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Jonas Lampart

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# Mathematical results on many-body quantum systems

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UNIVERSITÉ DE BOURGOGNE  
ÉCOLE DOCTORALE CARNOT-PASTEUR

**Résultats mathématiques sur des systèmes quantiques à  
plusieurs corps**

THÈSE D'HABILITATION À DIRIGER DES RECHERCHES

présentée par

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au

JURY

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# Preface

## Foreword

This habilitation thesis contains an overview and summary of the research I have published after obtaining my PhD. This research touches upon a variety of topics, grouped into six separate chapters. The unifying theme of all this work is a connection to the theory of many-body quantum systems. In some cases, the mathematical results are of direct relevance to such systems, like  $N$ -body systems or particle-field systems. In others, the connection lies in the fact that the studied equations are used as effective descriptions of many-body systems, for example in the mean-field approximation.

The goal is to give an account of my own work in a unified presentation. I have tried to be reasonably consistent with the notation across chapters, and conventions for repeatedly used notation are spelled out in an index. The chapters are not meant to be complete reviews on each topic, so only references to results of particular relevance for the discussion are given. The bibliography of each chapter is thus an incomplete selection from the literature. More detailed accounts on specific points can generally be found in the original articles. The style of the presentation varies from one chapter to another. In some cases, I have decided to give a rather brief synthesis of the main results and ideas. In others, I have chosen to present the original research from a slightly different point of view. Generally, the statements of the results have been optimised for readability and coherence with the explanations, rather than detail or generality. They thus often differ from the theorems stated in the original articles in this regard.

I want to express my gratitude towards all of my collaborators who have contributed to the research presented here, and to the joy of doing this work. I am also grateful to all colleagues who have provided inspiration by their own work, and their questions.

What follows is a brief summary of the chapters summarising the content of articles with a common theme, in roughly chronological order. Not covered are the articles [2, 6] contained in my PhD thesis, as well as the articles [1, 9, 10] on a closely related topic. The recent preprint [24], which would have constituted a chapter of its own, is also omitted.



## Chapter 1: A many-body RAGE theorem

In this chapter I review the article [3] in collaboration with Mathieu Lewin on an  $N$ -body version of the RAGE Theorem. The original RAGE theorem may be loosely paraphrased as stating that, in the long-time average of a unitary evolution, only the bound states of the generating Hamiltonian survive. Other components of the initial datum vanish in the corresponding limit. Our result provides an account of this vanishing in a general setting of  $N$ -body systems. In the long-time average, the system decomposes into bound states, including of smaller subsystems where some particles have been ejected. More precisely, using the notion of geometric convergence, we find that any limit point of the time-averaged state of an  $N$ -body system can be decomposed into  $n$ -particle components,  $0 \leq n \leq N$ , which are linear combinations of projections to bound states of the corresponding  $n$ -body system. Our result applies to  $N$ -body Schrödinger operators with slowly decaying potentials, which I will also discuss.

## Chapter 2: Inverse problems and time-dependent density functional theory

This chapter summarises the articles [4, 16] that are concerned with the inverse problem of mapping a time-dependent potential to the (one-particle) density of the corresponding solution to the Schrödinger equation, for a given initial condition. The possibility of reconstructing the potential from the density of the solution is a foundational issue in time-dependent density functional theory. It would imply that the time-dependent density contains, in principle, a complete characterisation of the system. It turns out that this inverse problem is related to the control problem of whether the initial state can be brought to a given final state by applying an external potential.

The first section is dedicated to results obtained in collaboration with Søren Fournais, Mathieu Lewin and Thomas Østergaard Sørensen [4]. The first part discusses a proof that the potential-to-density map  $V \mapsto \rho_V$  is one-to-one (up to addition of constants) in the case of highly regular potentials. This statement is known as the Runge-Gross Theorem and the proof relies on Taylor expansion in time, similarly to the original argument. This approach faces serious problems in the presence of singularities, which are examined in the second part.

The second section is about results from [16] on the range of the map  $V \mapsto \rho_V$ . The main result is that, as a set of time-dependent densities, this set is meagre in the sense of Baire for potentials that are bounded in space and satisfy a local integrability condition in time. As a consequence, the inverse problem is ill posed. The statement is proved first for the wave-function  $V \mapsto \psi_V$ , and obtained for the density as a corollary. A second corollary is that the control problem cannot be solved for generic

target states.

### Chapter 3: The Dirac equation with scalar fields

This chapter summarises the works [5, 22] on the Dirac equation in contact with scalar (or vector) fields.

The subject of the article [5] with Mathieu Lewin is the vacuum polarisation for the Dirac equation in an external scalar field. It was postulated by Dirac that the states of negative energy should be completely filled in the vacuum, thus forcing a fermionic particle to have positive energy and predicting the existence of an anti-particle, the positron. The negative energy subspace of the Dirac operator in an external field depends of this field, and thus there should be an associated difference in the energies of the corresponding vacuum states. Any naive formula for this energy will yield an infinite value, but one can provide regularised formulas. In [5] we use such a formula to derive an expansion of the polarisation energy for slowly varying external fields in terms of local functionals, i.e., integrals over point-wise functions of the field and its derivatives. We also give a non-rigorous discussion of the physical implications of the leading order term, including some numerics.

The topic of [22] in collaboration with Loïc Le Treust, Simona Rota Nodari and Julien Sabin is the Dirac-Klein-Gordon system in the strong coupling limit. This system is a model for a particle, described by the Dirac equation, interacting with relativistic, massive scalar or vector fields. The limit in question is that of simultaneous strong coupling and large masses of the fields. In this regime, the fields can have large derivatives, allowing them to adjust quickly to the evolution of the Dirac equation. One thus expects that the interaction becomes an instantaneous self-interaction in the limit, which yields the non-linear Dirac equation with self-consistent mass and current terms. Our result is the convergence of the solution to the Dirac equation as part of the system to that of the non-linear equation, and an estimate on the difference. We also generalise this to the Dirac-Fock equation for a Hilbert-Schmidt operator, which describes many particles in a mean-field approximation.

### Chapter 4: Interior boundary conditions

Here, I summarise the articles [7, 12, 11, 15, 13, 14, 17, 21, 23] on the use of interior boundary conditions in non-relativistic quantum field theory. This approach to the ultraviolet problem in quantum field theory seeks to identify a suitable domain for the Hamiltonian operator by imposing (generalised) boundary conditions on the singular set of the interactions. Usually, this set consists of configurations where several particles collide. The boundary conditions relate sectors with different numbers of particles, thereby encoding processes of particle creation. The strategy has similarities

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with singular perturbations for Schrödinger operators with a fixed number of particles, and, as in that case, the results coincide with those obtained by regularisation and renormalisation, whenever both are known.

In the first section, I start by explaining the general idea in a minimal example. I will then discuss the article [7] in collaboration with Julian Schmidt, Stefan Teufel, and Roderich Tumulka, which gives a characterisation of the domain of self-adjointness for a singular van Hove Hamiltonian. In light of these examples, I will present joint work with Tim Binz [14] on an abstract theory of interior boundary conditions which elucidates the relation to the concept of boundary triples and allows for a classification.

The second section is devoted to the discussion of Hamiltonians for systems of particles interacting with a quantum field by linear coupling, often called polaron Hamiltonians. I will explain the construction of their self-adjoint realisations by the method of interior boundary conditions and its relation to renormalisation. These results are contained in the article [12] with Julian Schmidt, and the later publications [11, 15, 13, 21]. I will proceed in the order of increasing strength of the singularities. I start with Hamiltonians that may be realised as quadratic forms, then discuss the Nelson Hamiltonian, which can be renormalised using a dressing transformation, and finally consider stronger singularities for which no dressing transformation is known. The latter class contains the important example of the Bogoliubov-Fröhlich Hamiltonian, modelling the interaction of an impurity with the excitation field in a Bose-Einstein condensate. This Hamiltonian and its renormalisation also feature in Chapter 6 on the Bose polaron.

In the final section I will explain how the knowledge of the Hamiltonian, without need for ultraviolet regularisation, can be used in the study of its spectrum. I focus on the property of the operator to improve positivity, which implies simplicity of any ground state. This property was proved in the article [17] for the Nelson model, and similar arguments were applied to the Fröhlich model in the article [23] with David Mitrouskas and Krzysztof Myśliwy to study the energy-momentum relation. The recent preprint [20] with Benjamin Hinrichs proves the existence of ground states of the Bogoliubov-Fröhlich Hamiltonian at fixed, small enough momentum.

## **Chapter 5: A model for plasmons in a finite medium**

In this chapter I present the work [8] in collaboration with Vincent Dorier, Hans Jauslin and Stéphane Guérin on a model for plasmons in the presence of a finite-size dielectric. Plasmons are a term for joint excitations of the electro-magnetic field and charge carriers in a medium. In our case, the latter are modelled by an oscillating polarisation field. In the first part of the chapter, I will discuss the model on the levels of both classical and quantum fields and the main results of [8] concerning the relations of physical quantities with those in the un-coupled model.

In the second part I give an outline of the proof of the mathematical statement underlying that discussion, using methods of stationary scattering theory.

## Chapter 6: Effective equations for many-boson systems

This chapter concerns the works [18, 25], and [19] about the derivation of effective equations for systems involving many bosons in the limit of large boson number.

The articles [18, 25] are about the Bose polaron problem. The system of interest consists of a large number of bosons and one, or few, impurities of a different type, at temperatures low enough for the bosons to form a Bose-Einstein condensate. Such systems are of interest in physics since the impurities can probe the properties of the Bose gas. Their model parameters can be controlled quite precisely in experiments, whence they are envisaged as platforms for studying impurity physics of less accessible systems, like solids, by analogy. This, however, requires a thorough theoretical understanding of the system and the relevant models. An important paradigm in the field is Bogoliubov theory, which describes the excitations out of a perfect condensate, created by the interactions, by a quantum field.

Together with Peter Pickl we prove in [18] that the dynamics of a boson-impurity system can be approximated by the Bogoliubov-Fröhlich Hamiltonian. The latter couples the impurity to Bogoliubov's excitation field with a linear coupling, similarly to the well-known Fröhlich Hamiltonian. We consider the system with periodic boundary conditions and a mean-field interaction, i.e., a weakly interacting system at high density.

With Arnaud Triay we study in [25] the ground state and low-lying eigenvalues of a dilute system in the Gross-Pitaevski regime. Contrary to the mean-field case, the interactions are strong but of short range compared to the very small density. Through rescaling, the problem can be brought into a form resembling the mean-field problem, but with rescaled potentials that become singular in the limit. These singularities make the renormalisation of the Bogoliubov-Fröhlich Hamiltonian necessary, which is achieved using the methods of [13]. This leads to a universal contribution to the ground state energy, with the excitation spectrum described by the renormalised Hamiltonian.

The subject of the article [19] with Marco Falconi, Nikolai Leopold, and David Mitrouskas is a system of bosons interacting via a relativistic scalar field, described by the Nelson Hamiltonian. In the mean-field limit of a dense, weakly interacting system we prove validity of Bogoliubov theory for the system of field and particles and show how the renormalisation of the Nelson model induces a renormalisation of the corresponding Bogoliubov approximation.

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# 1 A many-body RAGE theorem

This chapter is based on the article [7] on the many-body RAGE theorem. I will take the opportunity to revisit this result and present a slightly modified version of the abstract statement, and its proof. This variant was not presented in our original work, as we did not believe it would apply to the relevant case of  $N$ -body Schrödinger operators (compare [7, Remark 1]), and understood only later that this would indeed apply, as explained in Corollary 1.3 below.

The RAGE (Ruelle, Amrein-Georgescu, and Enss) Theorem is a fundamental result relating the long-time behaviour of a unitary group  $e^{-itH}$  to the spectrum of its self-adjoint generator  $H$ . In its basic form, it can be stated as follows. Let  $H, D(H) \subset \mathcal{H}$  be self-adjoint and  $0 \leq \gamma \in \mathfrak{S}^1(\mathcal{H})$  be a trace-class operator. Consider the ergodic mean,

$$M_T = \frac{1}{T} \int_0^T e^{-itH} \gamma e^{itH} dt. \quad (1.1)$$

This defines a bounded family  $(M_T)_{T \geq 0}$  in  $\mathfrak{S}^1(\mathcal{H})$ , so there exist convergent subsequences for the weak\*-topology. That is, there exists  $M_\infty \in \mathfrak{S}^1(\mathcal{H})$  (in fact, it is unique) so that for every compact  $K \in \mathfrak{K}(\mathcal{H})$

$$\mathrm{Tr}(KM_T) \xrightarrow{T \rightarrow \infty} \mathrm{Tr}(KM_\infty). \quad (1.2)$$

The RAGE Theorem states that  $M_\infty$  is an operator on the pure-point space of  $\mathcal{H}_{\mathrm{pp}}(H)$ . Moreover, it commutes with  $e^{-itH}$  and can thus be decomposed into a linear combination of projections onto eigenvectors of  $H$ . This means that only the bound states of  $H$  are discernible in the long-time average when testing with a compact operator.

In the context of many-body operators this theorem obviously applies, but it fails to capture the presence of bound states of subsystems. Consider for instance the Hamiltonians for  $n$  electrons in the field of a Hydrogen nucleus,

$$H_n = \sum_{j=1}^n \left( -\Delta_{x_j} - \frac{1}{|x_j|} \right) + \sum_{1 \leq j < \ell \leq n} \frac{1}{|x_j - x_\ell|}. \quad (1.3)$$

It is known that  $H_3$  has no bound states [6, 9],  $H_2$  has finitely many [6, 5], and of course  $H_1$  has an infinity of bound states. Therefore, the RAGE Theorem applied to  $H_3$  only yields that  $M_T$  converges weakly\* to zero. However, from  $n$ -body scattering

theory [3, 10], we know that the system will decompose into a number of free electrons and bound states of  $H_0 = 0$ ,  $H_1$ ,  $H_2$ .

The idea behind the many-body RAGE Theorem is to capture the effect of decomposition into subsystems, without describing the scattering process in detail. This has the benefit of requiring much weaker hypothesis. The refinement is achieved by changing the topology for  $M_T$  to one which allows for convergence to states with fewer particles, the geometric topology [8].

**The geometric topology.** We now introduce the geometric topology from a C\* algebraic point of view. Let  $\mathfrak{H}$  be the one-particle Hilbert space and  $N \in \mathbb{N}$  the initial number of particles. For  $0 \leq n \leq N$  let  $K \in \mathbb{K}(\mathfrak{H}^{\otimes n})$  be a compact operator that commutes with permutations of the tensor factors, and define for  $m \geq n$  the operator

$$K \otimes_s 1_{\mathfrak{H}^{\otimes(m-n)}} := \sum_{\substack{I \subset \{1, \dots, m\} \\ |I|=n}} K_I \otimes 1_{I^c} \in \mathbb{B}(\mathfrak{H}^{\otimes m}), \quad (1.4)$$

where in each summand  $I$  denotes the  $n$  indices of the tensor factors on which  $K$  acts, and the identity acts on the remaining  $|I^c| = m - n$  factors. Let

$$\mathfrak{G} \subset \bigoplus_{n=0}^N \mathbb{B}(\mathfrak{H}^{\otimes n}) \quad (1.5)$$

be the C\*-algebra generated by operators of the form

$$\mathbb{K} = \sum_{m=n}^N K \otimes_s 1_{\mathfrak{H}^{\otimes(m-n)}}, \quad (1.6)$$

for  $K \in \mathbb{K}(\mathfrak{H}^{\otimes n})$  and some  $0 \leq n \leq N$  (with the convention that  $\mathfrak{H}^{\otimes 0} = \mathbb{C}$ ). This is a unital algebra with identity  $\mathbb{1} = \bigoplus_{n=0}^N 1_{\mathfrak{H}^{\otimes n}}$ . The operators of this form correspond to looking for bound subsystems of size  $n$ . The algebra  $\mathfrak{G}$  is closely related to the  $N$ -body algebra discussed in [1], with the main difference that in the non-compact factors we simply have an identity. This corresponds to the fact that we do not want to describe specifically how the particles that escape behave.

Since elements of  $\mathfrak{G}$  commute with permutations of the tensor factors, they can be restricted to both the symmetric and anti-symmetric tensor products, so our results will cover both fermions and bosons.

**Definition 1.1.** The geometric topology is the weak\* topology on  $\mathfrak{G}'$ . We denote the associated convergence by  $\xrightarrow{\mathfrak{g}}$ .

Any element  $\gamma \in \mathfrak{G}'$  defines a continuous linear functional on  $\mathbb{K}(\mathfrak{H}^{\otimes n})$  by its restriction to operators of the form (1.6) with the given  $n \leq N$ . This functional is given by



1 A many-body RAGE theorem

$K \mapsto \text{Tr}(K\gamma^{(n)})$  with a trace-class operator  $\gamma^{(n)}$ , called the  $n$ -particle reduced density matrix. Geometric convergence is thus equivalent to weak\* convergence of  $\gamma^{(n)}$  for every  $0 \leq n \leq N$ .

Moreover,  $\gamma$  can be represented by a trace-class operator on  $\bigoplus_{n=0}^N \mathfrak{H}^{\otimes n}$  in the following way. The  $N$ -particle reduced density matrix can be extended to a functional  $G_N$  on  $\mathfrak{G}$  by, using the notation of (1.6),

$$G_N(\mathbb{K}) = \text{Tr}(\gamma^{(N)}(K \otimes_s 1_{\mathfrak{H}^{\otimes(N-n)}})). \quad (1.7)$$

Subtracting this from  $\gamma$  gives a functional  $\eta_N = \gamma - G_N$  with vanishing  $N$ -particle density,  $\eta_N^{(N)} = 0$ . In this way, we recursively define

$$G_n = \eta_{n+1}^{(n)}, \quad \eta_n = \eta_{n+1} - G_n, \quad (1.8)$$

where the extension to  $\mathfrak{G}$  is implicit. We clearly have  $\eta_0 = 0$ , since all of its reduced densities vanish. Undoing the recursive definition of  $\eta_0$ , this implies

$$0 = \eta_1 - G_0 = \gamma - \sum_{n=0}^N G_n, \quad (1.9)$$

so

$$\gamma = \sum_{n=0}^N G_n \in \mathfrak{G}^1\left(\bigoplus_{n=0}^N \mathfrak{H}^{\otimes n}\right). \quad (1.10)$$

The operator  $G_n$  really corresponds to the  $n$ -particle component of  $\gamma$ , whereas  $\gamma^{(n)}$  contains also the partial traces of  $G_m$ ,  $m > n$ .

**The Hamiltonian.** We consider general  $n$ -particle Hamiltonians built from a one-particle operator  $h$  and a two-body interaction  $w$  by

$$\begin{aligned} H_0 &= 0 \\ H_1 &= h \\ H_n &= \sum_{j=1}^n h_j + \sum_{0 \leq j < \ell \leq n} w_{j\ell}, \quad n \geq 2, \end{aligned} \quad (1.11)$$

where  $h_j$  acts on the  $j$ -th factor and  $w_{j\ell}$  on the  $j$ -th and  $\ell$ -th factors. We also introduce the notation for the induced Hamiltonian on  $\bigoplus_{n=0}^N \mathfrak{H}^{\otimes n}$ ,

$$\mathbb{H} = \bigoplus_{n=0}^N H_n. \quad (1.12)$$

In order to ensure that  $H_n$  has a self-adjoint realisation for any  $n$  we assume that  $h$  is self-adjoint, bounded from below, and that  $w_{12} = w_{21}$  is form-bounded by  $h_1 + h_2$  with relative bound zero.

The non-trivial assumption, which will ensure the decomposition into bound sub-systems, is that for all  $t > 0$  and  $K \in \mathbb{K}(\mathfrak{H})$ , the operator

$$(K \otimes_s 1) \int_0^t e^{is(h_1+h_2)} w_{12} e^{-is(h_1+h_2)} ds \in \mathbb{K}(\mathfrak{H} \otimes \mathfrak{H}) \quad (1.13)$$

is compact. In [7], a similar condition using the resolvent of  $h_1 + h_2$  instead of the integrated unitary group is given. There, we actively use the energy norm and thus the lower bound on  $h$ . For the argument given here one may drop this assumption if the relative bound of  $w_{12}$  is in the sense of operators.

In order to state the result, let  $\gamma \in \mathfrak{S}^1(\mathfrak{H}^{\otimes N})$  be non-negative and  $\text{Tr } \gamma = 1$ . This defines an element of  $\mathfrak{G}'$  by the natural extension (1.7). Then, set

$$M_T = \frac{1}{T} \int_0^T e^{-itH_N} \gamma e^{itH_N} dt \in \mathfrak{G}'. \quad (1.14)$$

For any  $T > 0$ , this defines a positive element of  $\mathfrak{G}'$  which is normalised by  $M_T(\mathbb{1}) = 1$ , i.e., a state on  $\mathfrak{G}$ . Hence, the family  $(M_T)_{T \geq 0}$  is pre-compact in the geometric topology and, since  $\mathfrak{G}$  has an identity, every limit point is a state [2, Thm.2.3.15]. Moreover, by the decomposition (1.10) every limit point has well defined  $n$ -particle components and is given by a trace-class operator. Note that, since  $\mathfrak{G}$  is separable, there exist geometrically convergent subsequences of  $M_T$ .

Since every limit point is a state, the vanishing phenomenon we observed for the RAGE Theorem in the absence of bound states does not happen here. The limit is always normalised, and in the worst case it just concentrates on the sector with zero particles, i.e., it equals its zero particle component and  $G_0 = 1$ .

**Theorem 1.2.** *Let  $h, w$  satisfy the hypothesis above, in particular property (1.13). Let  $M_\infty$  be a limit point of  $M_T$  for the geometric topology and for  $0 \leq n \leq N$  denote by  $G_n$  its  $n$ -particle component from (1.7). Then  $G_n$  is a linear combination of projections onto eigenvectors of  $H_n$ .*

*Sketch of the proof.* Let  $(M_{T_k})_{k \in \mathbb{N}}$  be a geometrically convergent subsequence of  $M_T$  with limit  $M_\infty$ . By a shift in the  $dt$ -integral, it is clear that  $e^{-i\mathbb{H}s} M_{T_k} e^{i\mathbb{H}s}$  converges to the same limit  $M_\infty$  for any  $s > 0$ . We will prove that also

$$e^{-iH_N s} M_{T_k} e^{iH_N s} = e^{-i\mathbb{H}s} M_{T_k} e^{i\mathbb{H}s} \xrightarrow{g} e^{-i\mathbb{H}s} M_\infty e^{i\mathbb{H}s} = \sum_{n=0}^N e^{-iH_n} G_n e^{iH_n}, \quad (1.15)$$

which is non-trivial since the left hand side involves only  $H_N$ , while on the right the whole family  $(H_n)_{0 \leq n \leq N}$  may appear. This then implies that  $M_\infty$  is  $\mathbb{H}$ -invariant

## 1 A many-body RAGE theorem

and  $G_n$  is  $H_n$ -invariant. Hence, each of its finite dimensional eigenspaces are  $H_n$  invariant and thus contained in  $\mathcal{H}_{\text{pp}}(H_n)$ . Consequently, it can be written as a linear combination of projections onto eigenvectors of  $H_n$ .

In order to prove that  $e^{-i\mathbb{H}s} M_{T_k} e^{i\mathbb{H}s}$  converges geometrically to  $e^{-i\mathbb{H}s} M_\infty e^{i\mathbb{H}s}$ , we will show that

$$\tau_t(\mathbb{K}) = e^{it\mathbb{H}} \mathbb{K} e^{-it\mathbb{H}} \quad (1.16)$$

defines a group of isometries of  $\mathfrak{G}$ . Then, geometric convergence implies for all  $\mathbb{K} \in \mathfrak{G}$

$$M_{T_k}(\tau_t(\mathbb{K})) \xrightarrow{k \rightarrow \infty} M_\infty(\tau_t(\mathbb{K})). \quad (1.17)$$

The non-trivial point is to show that  $\tau_t(\mathbb{K}) \in \mathfrak{G}$  for  $\mathbb{K} \in \mathfrak{G}$ . For this, it is sufficient to consider  $\mathbb{K}$  of the form (1.6). For simplicity of notation, we ignore the symmetrisation and the sum over  $m$  and consider  $K \otimes 1_{\mathfrak{F}^{\otimes(m-n)}}$ . Moreover, assume that  $w$  is bounded (otherwise one needs to perform an approximation argument). We need to write  $\tau_t(K \otimes 1_{\mathfrak{F}^{\otimes(m-n)}})$  as a sum of compact operators tensored with the identity. For  $n = m$  this is trivial, since the conjugation of a compact operator with a unitary is compact, so assume  $m > n$ . We can write  $\tau_t$  using the Dyson series (whose convergence is immediate for bounded  $w$ ). With  $H_m^0 = \sum_{j=1}^m h_j$ , the term of order zero in the series is simply

$$e^{iH_m^0}(K \otimes 1)e^{-iH_m^0} = \left( e^{iH_n^0} K e^{-iH_n^0} \right) \otimes 1, \quad (1.18)$$

which is of the claimed form. The first non-trivial term is

$$\begin{aligned} & i \int_0^t e^{i(t-s)H_m^0} \left[ \sum_{0 \leq j < \ell \leq m} w_{j\ell}, e^{isH_m^0}(K \otimes 1)e^{-isH_m^0} \right] e^{-i(t-s)H_m^0} \\ &= \sum_{0 \leq j < \ell \leq n} \left( i \int_0^t e^{i(t-s)H_n^0} [w_{j\ell}, e^{isH_n^0} K e^{-isH_n^0}] e^{-i(t-s)H_n^0} \right) \otimes 1 \\ & \quad + i \sum_{\substack{0 \leq j \leq n \\ n < \ell \leq m}} \int_0^t e^{i(t-s)H_m^0} [w_{j\ell}, e^{isH_n^0}(K \otimes 1)e^{-isH_n^0}] e^{-i(t-s)H_m^0}. \end{aligned} \quad (1.19)$$

After simplifying the commutators in this way, the first terms is clearly a product of a compact operator with the identity. The interesting term is the final one, where we add a new factor with index  $\ell > n$  in which we do not have compactness a-priori. In this term the commutator is now no longer of any use and we can simplify the first summand, for example, to

$$e^{iH_m^0 t} \left( \sum_{\substack{0 \leq j \leq n \\ n < \ell \leq m}} i \int_0^t \left( e^{-is(h_j+h_\ell)} w_{j\ell} e^{is(h_j+h_\ell)} K \otimes 1_\ell \right) \otimes 1_{\mathfrak{F}^{\otimes(m-n-1)}} \right) e^{-iH_m^0 t}. \quad (1.20)$$

It now follows from the hypothesis (1.13) that (1.20) is a sum of compact operators tensored with the identity. Since the Dyson series consists in iterating the integral operator from (1.19), the same argument applies to higher orders, where one can add compactness in one direction per iteration. This completes the proof by convergence of the series and closedness of  $\mathfrak{G}$ .  $\square$

A particularly important application of this theorem concerns Schrödinger operators. Let  $d \in \mathbb{N}$ ,  $\mathfrak{H} = L^2(\mathbb{R}^d)$  and choose the one-particle operator of the form  $h = -\Delta + V(x)$  and interaction potential  $w_{12} = W(x_1 - x_2)$  with  $W$  an even function. We have the following corollary, where the important point is that the decay of  $V, W$  at infinity may be arbitrarily slow (the regularity hypothesis can be improved).

**Corollary 1.3.** *Let  $V \in L^{1+d/2}(\mathbb{R}^d) + L_0^\infty(\mathbb{R}^d)$ ,  $W \in L^{1+d/2}(\mathbb{R}^d) + L_0^\infty(\mathbb{R}^d)$ , where  $L_0^\infty(\mathbb{R}^d)$  denotes the closure of functions with compact support in  $L^\infty(\mathbb{R}^d)$ . Then Theorem 1.2 holds for*

$$H_n = \sum_{j=1}^n (-\Delta_{x_j} + V(x_j)) + \sum_{1 \leq j < \ell \leq n} W(x_j - x_\ell).$$

*Sketch of the proof.* We need to show that the compactness property (1.13) holds. For simplicity consider the case  $V = 0$  (with the arguments below, one can show that  $e^{is\Delta} - e^{-ish}$  is compact). The key is to note that

$$\int_0^t e^{-is\Delta} W(x) e^{is\Delta} ds = L \tag{1.21}$$

is a compact operator due to the dispersive properties of  $e^{i\Delta}$  (by [4, Thm.2] the part in  $L^{1+d/2}$  gives an element of the Schatten space  $\mathfrak{S}^{2+d}$ , while for the part in  $L_0^\infty$  compactness follows from this and approximation by functions of compact support). Writing the Laplacian in relative and centre of mass coordinates, we thus have

$$\int_0^t e^{is(h_1+h_2)} w_{12} e^{-is(h_1+h_2)} ds = \int_0^t e^{is\Delta_{x_1-x_2}} W(x_1-x_2) e^{-is\Delta_{x_1-x_2}} ds, \tag{1.22}$$

which is of the form  $L \otimes_R 1$ , where the tensor product comes from the decomposition  $L^2(\mathbb{R}^{2d}) = L^2(\mathbb{R}_{x_1-x_2}^d) \otimes_R L^2(\mathbb{R}_{x_1+x_2}^d)$ , with respect to the relative and centre of mass coordinates. Since vectors of the form  $x_1$  and  $x_1 - x_2$  generate  $\mathbb{R}^{2d}$ , this implies that  $(K \otimes 1)L \otimes_R 1$  is compact, by the theory of semi-compact operators [1, Prop.1] (the argument is elementary: For Hilbert-Schmidt operators the product is also Hilbert Schmidt by inspection of its integral kernel, and the general case follows by approximation). The same applies to  $1 \otimes K$ , and this completes the proof.  $\square$

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## 2 Inverse problems and time-dependent density functional theory

In this chapter I review the articles [3, 6] that are concerned with the properties of the map  $V \mapsto \rho_V$ , mapping a time-dependent potential to the (one-particle) density of the corresponding solution to the Schrödinger equation. More precisely, let  $\psi_0 \in L^2(\mathbb{R}^{dN})$  be a fixed initial condition and  $\Psi_V(t)$  be the solution to the Cauchy problem

$$\begin{cases} i\partial_t \psi_V(t) = H_V(t)\psi_V(t) \\ \psi_V(0) = \psi_0, \end{cases} \quad (2.1)$$

where  $H_V$  is an  $N$ -particle Schrödinger operator with external time-dependent potential  $V$ . Then for any class of potentials  $\mathcal{V}$  for which the equation is well posed, the map  $V \mapsto \psi_V(t)$  is well defined, as is its one-particle density defined by

$$\rho_V(t, x) = N \int |\psi_V(t, x, y_1, \dots, y_{N-1})|^2 dy_1 \cdots dy_{N-1}. \quad (2.2)$$

We are interested in properties of this map that are relevant to the inverse problem of reconstructing the potential from the density, as well as the control problem of reaching a prescribed final state by choice of a potential.

### 2.1 The Runge-Gross theorem

In this section I summarise the main results of the article [3] on the Runge-Gross theorem in time-dependent density functional theory.

Density functional theory proposes methods to calculate, or approximate, the one-particle density of an  $N$ -particle quantum system directly – without first calculating the full  $N$ -body wave-function. Such methods are popular computational tools, due to their moderate cost. This leads to the question how much information about the full system is contained in the one-body density. More specifically, one may ask which quantities in the full system may be reconstructed from the density, given some a priori information, such as what kind of particles constitute the system.

We assume that the quantum system in question consists of  $N$  fermions or bosons, and that its time-dependent Hamiltonian, defined on the anti-symmetric  $L^2_a(\mathbb{R}^{dN})$  or symmetric  $L^2_s(\mathbb{R}^{dN})$   $L^2$ -space, is of the form

$$H_V(t) := H_0 + \sum_{i=1}^N V(t, x_i), \quad (2.3)$$

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with

$$H_0 = \sum_{i=1}^N -\Delta_{x_i} + V_0(x_i) + \sum_{1 \leq i < j \leq N} W(x_i - x_j). \quad (2.4)$$

The conditions on the potentials  $V$ ,  $V_0$ ,  $W$  on  $\mathbb{R}^d$  will be discussed in detail later. We consider  $V_0$  and  $W$  as quantities which are a priori known. If, for example, the particles in our system are electrons they will interact via Coulomb forces  $W(x) = 1/|x|$ .

In the time-independent case of ground-states, it is known that for  $V, V_0, W \in L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$  (for  $d \geq 3$ ) the potential  $V$  is uniquely determined by the ground state density. That is, if  $V_1, V_2 \in L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$  differ by more than a constant then the one-particle densities  $\rho_1$  and  $\rho_2$  corresponding to their ground states  $\psi_1, \psi_2$  are different. Equivalently, if  $\rho_1 = \rho_2$ , then  $V_1 = V_2 + \text{const.}$ . This statement is known as the Hohenberg-Kohn Theorem [4] (see Lieb [7] for a proof).

Runge and Gross [8] argued that a similar property should hold for time dependent systems. That is, the time-dependent density  $\rho(t, x)$  should determine the external potential  $V(t, x)$  up to a constant  $C(t)$  if the system starts with a given initial wavefunction  $\psi_0$ . The argument is based on an order-by-order analysis of the Taylor series in time of the density  $\rho(t, x)$  obtained from the solution  $\psi(t)$  of the Schrödinger equation with initial condition  $\psi_0$  and time-dependent Hamiltonian  $H_V$ . Such an expansion clearly relies on smoothness of  $\rho$  and  $V$  in the time variable, which is intimately related to the regularity in space. This led to a discussion in the physical chemistry literature regarding the validity of the argument, see e.g. [10].

The first mathematical work concerning this question is our article [3], where we discuss the possibility of choosing a set  $\mathcal{I}$  of admissible initial conditions and  $\mathcal{V}$  of external potentials for which the statement above can be proven rigorously, using an argument similar to that of Runge and Gross. In order to avoid pathologies, these sets should satisfy the following conditions:

- The set  $\mathcal{I}$  is invariant under the dynamics generated by  $H_V$  for any  $V \in \mathcal{V}$ .
- $0 \in \mathcal{V}$  and if  $V(t, x)$ ,  $t \in [0, T)$  is an admissible potential, then so is the time-independent potential  $V(x, t_0)$  for any  $t_0 \in [0, T)$ .
- If the time-independent potential  $V(x) \in \mathcal{V}$ , then any eigenvectors of  $H_V$  are admissible initial conditions.

In order to have smooth solutions, we also need to restrict the set of initial conditions

$$\mathcal{I} \subset \bigcap_{V(x) \in \mathcal{V}} C^\infty(H_V), \quad (2.5)$$

## 2.1 The Runge-Gross theorem

where the intersection is over all time-independent potentials, and we denote the set of  $H_V$ -smooth vectors by  $C^\infty(H_V) := \bigcap_{k \in \mathbb{N}} D(H_V^k)$ . Now, depending on the set  $\mathcal{V}$ , the intersection above may be very small – and will in general not be invariant under the dynamics of the operators  $H_V$ . In order to avoid this we have to restrict  $\mathcal{V}$  so that

$$C^\infty(H_V) = C^\infty(H_0) \quad (2.6)$$

for every  $V \in \mathcal{V}$ . This condition clearly shows that the possible choice of  $\mathcal{V}$  depends strongly on  $H_0$  – and thus on  $V_0$  and  $W$ .

**Smooth potentials.** If the potentials  $V_0$  and  $W$  are smooth, we have natural choices for  $\mathcal{I}$  and  $\mathcal{V}$  and the Runge-Gross argument becomes a rigorous theorem. To be more precise, let  $V_0, W \in C_b^\infty(\mathbb{R}^d, \mathbb{R})$ ,  $W$  even, and set

$$\begin{aligned} \mathcal{I} &= \bigcap_{k \in \mathbb{N}} H^{2k}(\mathbb{R}^{dN}) \cap L_{a/s}^2(\mathbb{R}^{dN}) \\ \mathcal{V} &= C_b^\infty([0, T] \times \mathbb{R}^d, \mathbb{R}) \end{aligned} \quad (2.7)$$

for some  $T > 0$ . We then have:

**Theorem 2.1.** *Let  $V_1, V_2 \in \mathcal{V}$  and  $\psi_0 \in \mathcal{I}$  with one-particle density  $\rho_0$ . Denote by  $\psi_k(t)$ ,  $k \in 1, 2$  the solution at time  $t \in [0, T)$  of the Schrödinger equation with Hamiltonian  $H_{V_k}$  and initial condition  $\psi_k(0) = \psi_0$ . Denote by  $\rho_k$  the corresponding one-particle density. If  $\rho_1 = \rho_2$ , then for all  $\ell \in \mathbb{N}$*

$$\int_{\mathbb{R}^d} \rho_0(x) |\nabla \partial_t^\ell (V_1 - V_2)|^2(0, x) dx = 0. \quad (2.8)$$

*If additionally the set  $\rho_0^{-1}(0)$  has zero Lebesgue measure, then  $\partial_t^\ell V_1(x) = \partial_t^\ell V_2(x) + c_\ell$  for some constant  $c_\ell$ . If furthermore  $(V_1 - V_2)(t, x)$  is real-analytic in  $t$  for every  $x$  we also have  $V_1(t, x) = V_2(t, x) + C(t)$ , with  $C(t) = \sum_{\ell \in \mathbb{N}} \frac{c_\ell}{\ell!} t^\ell$ .*

For the proof of this theorem, one first applies a result of Kato [5] to show that  $\psi_k(t) \in \mathcal{I}$  depends smoothly on time. Then Equation (2.8) is obtained recursively by calculating weak time-derivatives of  $\rho_1 - \rho_2$  at  $t = 0$ , which must equal zero since  $\rho_1 = \rho_2$ . For instance, the weak second derivative yields

$$0 = \left. \frac{d^2}{dt^2} \right|_{t=0} \int_{\mathbb{R}^d} \varphi(x) (\rho_1 - \rho_2)(t, x) dx = 2N \int (\nabla \varphi)(x) \nabla (V_2 - V_1)(0, x) dx. \quad (2.9)$$

Choosing the test-function  $\varphi = V_2 - V_1$  gives (2.8) for  $\ell = 0$ . The additional statements follow easily from (2.8).



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**Singular potentials.** If  $V_0$  or  $W$  are not smooth, the condition (2.6) will lead to strong restrictions on the set  $\mathcal{V}$ . For example, it is relatively easy to see that if  $H_0$  is the one-dimensional Schrödinger operator with a delta-potential at  $x = 0$ , any potential satisfying (2.6) must be smooth on  $\mathbb{R}$  and vanish to infinite order at  $x = 0$  (compare [3, Theorem 3]). For the Coulomb potential, we have a similar result.

**Proposition 2.2.** *Let  $d = 3$ ,  $N = 1$  and  $V_0 = -\frac{1}{|x|}$  be the Coulomb potential. If  $V \in C^\infty(\mathbb{R}^3, \mathbb{R})$  is radial and  $C^\infty(H_V) = C^\infty(H_0)$ , then*

$$\frac{d^k V}{dr^k}(0) = 0$$

for all  $k \geq 1$ .

The proof proceeds by examining the boundary conditions at  $x = 0$  that elements of  $D(H_0^k)$  must satisfy. If we restrict to radial functions and absorb the factor  $r^2$  from the integration measure into the wave-function, the operator  $H_0$  is mapped to the operator

$$h_0 = -\frac{d^2}{dr^2} - \frac{1}{r} \tag{2.10}$$

on  $L^2(\mathbb{R}_+)$  with Dirichlet boundary condition at  $r = 0$ . If  $D(H_V^k) = D(H_0^k)$  for  $k = 1, 2, 3$  then  $V$  must map  $D(H_0^3)$  to  $D(H_0^2)$ . Consequently, the Dirichlet condition in the form  $h_0 V \psi(0) = 0$  must be satisfied for  $\psi \in D(h_0^3)$ . Since  $(h_0 \psi)(0) = 0$  for  $\psi \in D(h_0^2)$ , this gives

$$h_0 V \psi(0) = [h_0, V] \psi(0) = -2V'(0) \psi'(0) = 0. \tag{2.11}$$

Since  $h_0$  has eigenfunctions with non-vanishing derivative at  $r = 0$ , this shows that  $V'(0) = 0$ . The derivatives of higher order are treated by iterating this type of argument.

We expect similar statements to hold generically for general non-smooth potentials  $V_0$ . The restrictions on  $\mathcal{V}$  are even more severe for singular interactions  $W$ .

**Proposition 2.3.** *Let  $d = 3$ ,  $N = 2$ ,  $V_0 = 0$ ,  $W(x) = \frac{1}{|x|}$  be the Coulomb interaction and  $H_0$  the operator acting on symmetric functions given by these choices. If  $V \in C_b^6(\mathbb{R}^3)$  satisfies  $D(H_V^4) = D(H_0^4)$  then  $V$  is constant.*

To prove this, one separates the relative and centre-of-mass coordinates and then applies similar arguments as in the case of a singular one-body potential  $V_0$ . This yields  $\Delta V = 0$ . As  $V$  is bounded, it must thus be constant.

We see that for the Coulomb interaction the relation (2.6) already implies that  $V$  is constant, and there is nothing of interest to prove afterwards. Equation (2.8) can still be shown to hold for  $\ell \leq 3$  ( $\ell \leq 4$  for fermions), under reasonable assumptions. In order to obtain more information, an approach that avoids Taylor expansions of high order is clearly necessary.

## 2.2 Time-dependent densities and control theory

In this section I present the results of [6] on range of the map  $V \mapsto \psi_V$ . As the difference between the density  $|\psi_V|^2$  and its marginal  $\rho_V$  plays no role here, we use the notation corresponding to the case with  $N = 1$  particles, and denote

$$H_V(t) = -\Delta + V(t, x). \quad (2.12)$$

The time-dependent potential  $V(t, x)$  will be assumed bounded in space and locally  $p$ -integrable in time,  $p > 1$ .

An important idea in this area goes back to Ball, Marsden and Slemrod [1]. These authors considered a general evolution equation of the form

$$\begin{cases} \partial_t \psi_u(t) = A\psi_u(t) + u(t)B\psi_u(t) \\ \psi_u(0) = \psi_0, \end{cases} \quad (2.13)$$

where  $(A, D(A))$  is a generator of a strongly continuous semi-group on some Banach space  $X$ ,  $B$  is a bounded operator, and  $u(t) \in L^p_{\text{loc}}([0, \infty))$ ,  $p > 1$  is a function of time, the control parameter. They proved that for any given  $B$  and  $\psi_0$ , the attainable set

$$\mathcal{A} = \bigcup_{p>1} \left\{ \psi_u(t) \mid t \geq 0, \psi_u \text{ solves (2.13) with } u \in L^p_{\text{loc}}([0, \infty)) \right\} \quad (2.14)$$

is a countable union of compact subsets of  $X$ . If  $X$  has infinite dimension, this means that it has empty interior, by Baire's theorem. Consequently, a generic target state  $\psi_1$  is not attainable (the complement of  $\mathcal{A}$  is the intersection of open and dense sets, a dense  $G_\delta$ -set). For the Schrödinger equation, this entails (cf. Turinici [9]) that for  $V(t, x) = u(t)V_0(x)$  with fixed  $V_0 \in L^\infty(\mathbb{R}^d, \mathbb{R})$  the attainable set

$$\mathcal{A} = \bigcup_{p>1} \left\{ \psi_V(t) \mid t \geq 0, V(t, x) = u(t)V_0(x) \text{ with } u \in L^p_{\text{loc}}([0, \infty)) \right\} \quad (2.15)$$

is meagre in the sphere

$$S(\|\psi_0\|) = \left\{ \psi \in L^2(\mathbb{R}^d) : \|\psi\| = \|\psi_0\| \right\}. \quad (2.16)$$

This leaves the question whether the result depends on fixing  $V_0$  before choosing the target state. In terms of physical modelling of the control problem, this corresponds to a device that generates a given potential, whose strength can be tuned in time. But once the target state is decided on, we may well ask if any potential can be used to attain it, and then try to engineer a device to do so. To resolve this question, we consider the class

$$\mathcal{V} = \bigcup_{p>1} L^p_{\text{loc}}([0, \infty), L^\infty(\mathbb{R}^d, \mathbb{R})). \quad (2.17)$$

of time-varying potentials. The main result of [6] can be stated as follows.

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**Theorem 2.4.** *For every  $\psi_0 \in L^2(\mathbb{R}^d)$  and  $T > 0$  the set of trajectories up to time  $T$*

$$\mathcal{T} = \left\{ t \mapsto \psi_V(t) : V \in \mathcal{V} \right\}$$

*is a countable union of compact subsets in  $C([0, T], S(\|\psi_0\|))$ .*

Since  $\psi \mapsto |\psi|^2$  is continuous from  $L^2(\mathbb{R}^d)$  to  $L^1(\mathbb{R}^d)$  and continuous images of compact sets are compact, we immediately have as a corollary that the set of time-dependent densities

$$\mathcal{R} = \left\{ t \mapsto |\psi_V(t)|^2 : V \in \mathcal{V} \right\} \quad (2.18)$$

is a countable union of compact subsets in the space of continuous functions of time to the sphere in  $L^1(\mathbb{R}^d)$ . The same applies to any marginals.

Moreover, as the evaluation  $\psi_V \mapsto \psi_V(t)$  is continuous, the result of Turinici for the attainable set extends to the class  $\mathcal{V}$ .

The proof of the theorem, which we sketch below, relies crucially on the local smoothing property of the group  $e^{it\Delta}$ . It is thus essential that the problem is set on  $\mathbb{R}^d$ , or some non-compact space where the wave-function can disperse. By contrast, the result of [1], and its generalisations with fixed  $V_0(x)$  [9, 2], apply without restrictions to the underlying configuration space.

*Sketch of the proof.* It is sufficient to show that the operator  $V \mapsto \psi_V$  is compact, since the restriction of  $\mathcal{V}$  to  $[0, T]$  is a countable union of closed, bounded sets. To do this, it is convenient to work with larger spaces that are duals of Banach spaces, so we actually prove the result for this larger class. For  $p > 1$  denote by  $p' = (1 - p^{-1})^{-1}$  the dual Hölder exponent, and set

$$\bar{\mathcal{V}}_T = \bigcup_{p>1} \left( L^{p'}([0, T], L^1(\mathbb{R}^d, \mathbb{R})) \right)'. \quad (2.19)$$

The elements of the dual to  $L^{p'}([0, T], L^1)$  are absolutely continuous  $L^\infty$ -valued measures, but not necessarily functions in  $L^p([0, T], L^\infty)$  since  $L^\infty$  does not have the Radon-Nikodym property. It is straightforward to define the solution to the Schrödinger equation with such a potential by the integral equation.

Using Grönwall's Lemma, we can reduce the problem to the linearised solution operator

$$V \mapsto \int_0^t e^{i\Delta(t-s)} \psi(s) V(ds) = L_\psi V, \quad (2.20)$$

where  $V \in L^{p'}([0, T], L^1)'$  is an  $L^\infty$ -valued measure. By the Banach-Alaoglu Theorem, which applies since we are now working in the dual of a Banach space, it is then

sufficient to prove that  $L_\psi V_n$  tends to zero in  $C([0, T], L^2)$  for any sequence  $V_n$  that converges weakly\* to zero. Considering  $L_\varphi^* L_\psi$  leads us to the expression

$$KV(s) = \overline{\varphi}(s) \int e^{i(s-s')\Delta} \psi(s') V(ds'). \quad (2.21)$$

The key technical point is now to show that  $K : L^{p'}([0, T], L^1)' \rightarrow C([0, T], L^1)$  is compact. This proceeds in the following steps.

- By continuity in  $\varphi, \psi$ , one may assume that these are smooth functions, rapidly decaying in  $x$ .
- It follows that for fixed  $s$ ,  $x \mapsto KV(s, x)$  is rapidly decreasing.
- $KV(s)$  is also somewhat regular in  $x$ , as  $\varphi(s)$  is smooth and the operator  $\int e^{-is'\Delta}$  is locally smoothing, with localisation coming from  $\varphi, \psi$ .
- It follows from the above points that  $V \mapsto KV(s) \in L^1(\mathbb{R}^d)$  is compact by the Rellich–Kondrachov Theorem. Compactness as a map to  $C([0, T], L^1(\mathbb{R}^d))$  follows from the Arzelà–Ascoli Theorem, since the spatial regularity can be translated into regularity of the evolution under  $e^{i\Delta s}$ .

Theorem 2.4 can likely be generalised to potentials in  $L^p_{\text{loc}}(\mathbb{R}, L^q(\mathbb{R}^d))$  with appropriate restrictions on  $p, q$  and more regular situations where the wave-function is treated as an element of some Sobolev space.  $\square$

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## 2 Inverse problems and time-dependent density functional theory

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### 3 The Dirac equation with scalar fields

In this chapter we consider two problems involving the Dirac operator and scalar (or vector) fields [7, 6]. Both of these problems are motivated by the relativistic mean-field theory of nuclear physics. The first concerns the polarisation of the vacuum in approximately homogeneous nuclear matter. The second is on the reduction of a dynamical interaction with the fields to an instantaneous self-interaction of the particles, described by the Dirac equation.

#### 3.1 Vacuum polarisation in a scalar field

This section summarises the article [7] on the vacuum polarisation of the Dirac operator in a scalar field, in the semi-classical regime.

The three-dimensional Dirac operator with an external scalar field  $\varphi$  is

$$D_\varphi = -i\alpha \cdot \nabla + \beta(1 + \varphi), \tag{3.1}$$

where the Dirac matrices  $(\alpha_i)_{i=1}^3, \beta \in \mathbb{C}^{4 \times 4}$  are self-adjoint, square to one, and anti-commute pairwise. The mass of the particle, Planck's constant, and the speed of light have been set to one.

In the picture of the Dirac sea, the vacuum state corresponds to a fully occupied subspace of negative energy, i.e., the spectral projection  $1_{(-\infty, 0)}(D_\varphi)$ . The corresponding energy would be the trace of the negative part of  $D_\varphi$ , which equals minus infinity. Of course, the quantity of interest is the energy difference relative to the free case  $\varphi = 0$ , which would be the trace of  $(D_0)_- - (D_\varphi)_-$ . Moreover, since the spectrum of  $D_\varphi$  is symmetric with respect to zero, this trace is formally equal to that of

$$-\frac{1}{2}(|D_\varphi| - |D_0|). \tag{3.2}$$

However, though better behaved, this still does not have a finite trace under any reasonable assumptions on  $\varphi$  in three space dimensions. One solution to this problem is to subtract further terms of the expansion of  $|D_\varphi|$  at  $\varphi = 0$ , until the trace is finite. If one defines a regularised vacuum polarisation in this way, one can make an ansatz for the full vacuum polarisation by adding a polynomial expression in  $\varphi$ , whose coefficients are interpreted as renormalised parameters, to be determined experimentally. Here, we will discuss the regularised expression defined by subtracting terms up to order four in  $\varphi$ .

### 3 The Dirac equation with scalar fields

**Definition 3.1.** For  $\varphi \in H^1(\mathbb{R}^3, \mathbb{R})$  the regularised vacuum polarisation energy is defined by

$$\mathcal{E}_{\text{vac}}(\varphi) = \frac{1}{2} \text{Tr} \left[ -|D_\varphi| + \sum_{j=0}^4 \frac{1}{j!} \frac{d^j}{ds^j} \Big|_{s=0} |D_{s\varphi}| \right].$$

It is shown in [7, Proposition 2.1] that this quantity is finite and defines a continuous function of  $\varphi$  that is smooth on the open set where  $0 \notin \sigma(D_\varphi)$ .

This regularised vacuum energy has been studied in the nuclear physics literature. For a constant field  $\varphi > -1$ , the energy per unit volume was calculated in [8, 1, 12], with the result

$$\mathcal{V}(\varphi) = -\frac{1}{4\pi^2} (1 + \varphi)^4 \log(1 + \varphi) - P(\varphi), \quad (3.3)$$

where

$$P(\varphi) = -\frac{1}{4\pi^2} \left( \varphi + \frac{7}{2}\varphi^2 + \frac{13}{3}\varphi^3 + \frac{25}{12}\varphi^4 \right)$$

is the fourth-order Taylor polynomial of the first term. Assuming that  $\varphi$  is not constant but varies slowly, the leading term of  $\mathcal{E}_{\text{vac}}(\varphi)$  should be given by the integral over  $\mathcal{V}(\varphi(x))$ . This is precisely the result of [7, Theorem 1.1]. Corrections should involve derivatives of  $\varphi$  and were also discussed in the physics literature (see [7] for references), and [7, Theorem 3.1] shows existence of such an expansion to arbitrary order. The precise statement for the leading order is:

**Theorem 3.2.** *Let  $\varphi \in C^\infty(\mathbb{R}^3, \mathbb{R})$  be such that*

- $|\varphi| < 1$ ;
- $(1 + |x|^2)^{(1+|\alpha|)/2} \partial_x^\alpha \varphi \in L^\infty(\mathbb{R}^3)$  for every multiindex  $\alpha \in \mathbb{N}^3$ .

*Then we have*

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^3 \mathcal{E}_{\text{vac}}(\varphi(\varepsilon \cdot)) = \int_{\mathbb{R}^3} \mathcal{V}(\varphi(x)) dx,$$

*where  $\mathcal{V}$  is given by (3.3).*

The formula from Theorem 3.2 has an analogue in the case of an electro-magnetic field, the well-known Euler-Heisenberg energy [5, 4, 3].

We will now sketch how to arrive at this formula, referring to the original article [7] for more precise statements and error estimates. A first step is to write

$$|D_\varphi| = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{D_\varphi^2}{D_\varphi^2 + \omega^2} d\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left( 2 - \frac{i\omega}{D_\varphi + i\omega} + \frac{i\omega}{D_\varphi - i\omega} \right) d\omega \quad (3.4)$$

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which holds by the functional calculus. One can then use the resolvent formula to evaluate the difference of this expression and its expansion in  $\varphi$ . This yields

$$\mathcal{E}_{\text{vac}}(\varphi) = \frac{1}{2} \text{Tr} \left( \int I(\omega, \varphi) + I(-\omega, \varphi) d\omega \right) \quad (3.5)$$

with

$$I(\omega, \varphi) = i\omega(D_\varphi + i\omega)^{-1}(\beta\varphi(D_0 + i\omega)^{-1})^5. \quad (3.6)$$

One can exchange the trace and the integral in (3.5), and then expand  $(D_\varphi \pm i\omega)^{-1}$  in a Neumann series, using that  $|\varphi| < 1$ . Calculating term-by-term, using integration by parts to eliminate the factor  $\omega$  and cyclicity of the trace, one arrives at an integral of the trace of a power series in  $\beta\varphi(D_0 + i\omega)^{-1}$  (respectively its adjoint for  $I(-\omega, \varphi)$ ). Summing this series yields

$$\mathcal{E}_{\text{vac}}(\varphi) = -\frac{1}{4\pi} \int \text{Tr} (F(\beta\varphi(D_0 + i\omega)^{-1}) + F((D_0 - i\omega)^{-1}\beta\varphi)) d\omega \quad (3.7)$$

with the explicit function  $F(z) = \log(1+z) - r(z)$ ,  $r$  a polynomial of degree four.

Now for a semi-classical pseudo-differential operator, like  $A = \beta\varphi(\varepsilon \cdot)(D_0 + i\omega)^{-1}$ , an analytic function  $F(A)$  is given to leading order by the quantisation of  $F(a_0(x, p))$ , with the principal symbol

$$a_0(x, p) = \beta\varphi(x)(\alpha \cdot p + \beta - i\omega)^{-1}. \quad (3.8)$$

The reason is that  $F(A)$  is given by Cauchy's formula, and the principal symbol of  $(z - A)^{-1}$  is  $(z - a_0)^{-1}$ . Moreover, if  $F(a_0(x, p)) \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ , the trace of the quantisation is

$$\text{Tr} (\text{Op}_\varepsilon F(a_0)) = \frac{1}{(2\pi\varepsilon)^3} \int F(a_0(x, p)) dx dp. \quad (3.9)$$

Evaluating the integrals over  $p$  and  $\omega$  yields the claimed formula.

A detailed proof of these statements using pseudo-differential calculus automatically yields an asymptotic expansion

$$\varepsilon^3 \mathcal{E}_{\text{vac}}(\varphi(\varepsilon \cdot)) = \sum_{j=0}^k \int \mathcal{V}_k(\varphi)(x) dx + \mathcal{O}(\varepsilon^{k+1}), \quad (3.10)$$

where  $\mathcal{V}_k(\varphi)(x)$  is a function of  $\partial^\alpha \varphi(x)$  with  $|\alpha| \leq k$ . Moreover, one can check that  $\mathcal{V}_1 = 0$ , cf. [7, Theorem 3.1].

In [7, Section 4.2] we also provide a brief numerical study of the linear response function of a homogeneous system and observe that the vacuum polarisation has a stabilising effect.



## 3.2 The strong-coupling limit of the Dirac-Klein-Gordon system

In this section we present the results of [6] on the Dirac-Klein-Gordon system in the regime of strong coupling and large field masses. This system couples the Dirac equation to an equation for a scalar field described by the Klein-Gordon equation. We also allow for a massive vector field described by the Proca equation. Such equations arise, for example, in the relativistic mean-field theory of nuclear physics [11]. There, they model the interaction of nucleons via meson fields, like the scalar  $\sigma$ -meson and the vectorial  $\omega$ -meson. The latter are simplified representations of the strong nuclear force, and as such they are both strong and of short range, which corresponds to the regime we consider below.

### 3.2.1 The one-body problem

We now discuss the case of a single particle described by the Dirac equation interacting with the fields. Its wavefunction  $\psi$  should satisfy the equation

$$i\partial_t\psi = \alpha \cdot (-i\nabla + A)\psi + \beta(m + \varphi)\psi + V\psi, \quad (3.11)$$

with  $\alpha, \beta$  as in (3.1). The field  $\varphi$  is the scalar field and coupled to  $\psi$  by the Klein-Gordon equation

$$(\partial_t^2 - \Delta + m_\sigma^2)\varphi = -g_\sigma^2\rho_s(\psi), \quad (3.12)$$

with the scalar density

$$\rho_s(\psi) = \langle \psi, \beta\psi \rangle_{\mathbb{C}^4}. \quad (3.13)$$

The four-dimensional vector field  $\omega = (V, A)$  satisfies the analogous equation

$$(\partial_t^2 - \Delta + m_\omega^2)\omega = g_\omega^2 J(\psi), \quad (3.14)$$

with the four-current

$$J(\psi) = (|\psi|^2, \langle \psi, \alpha\psi \rangle). \quad (3.15)$$

Since this current is divergence-free (i.e., the charge  $|\psi|^2$  satisfies the continuity equation), the equation preserves the Lorentz gauge condition under which the differential operator equals the vectorial d'Alembert operator. However, due to the mass term it is not gauge invariant.

We are interested in the regime where both masses  $m_\sigma^2, m_\omega^2$  and couplings  $g_\sigma^2, g_\omega^2$  are large, with

$$\lambda_\sigma = \frac{g_\sigma^2}{m_\sigma^2}, \quad \lambda_\omega = \frac{g_\omega^2}{m_\omega^2} \quad (3.16)$$

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fixed. After dividing the field equations by the respective masses, one is tempted to set

$$\varphi = -\lambda_\sigma \varphi_s(\psi), \quad \omega = \lambda_\omega J(\psi), \quad (3.17)$$

as is usually done in the physics literature. This replaces the dynamical self-interaction of  $\psi$  by an instantaneous one, and the equation becomes the non-linear Dirac equation

$$i\partial_t \psi = \alpha \cdot (-i\nabla + \langle \alpha \psi, \psi \rangle) \psi + \beta(m + \langle \beta \psi, \psi \rangle) \psi + |\psi|^2 \psi. \quad (3.18)$$

Of course, dropping the differential operators from the field equations is problematic. They may have small pre-factors, but these can, and will, be compensated by rapid oscillations of the solution. The result of [6] is that these oscillations average out as far as the evolution of  $\psi$  is concerned, and the non-linear Dirac equation indeed provides a good approximation for  $m_\sigma, m_\omega \rightarrow \infty$ . From this point on, one can also consider the non-relativistic limit of (3.11), i.e., let  $m \rightarrow \infty$  as well, which leads to a system of non-linear Schrödinger equations [10]. The combination of these limits was studied for ground states in [2, 9].

**Theorem 3.3.** *Let  $s > \frac{5}{2}$  and*

$$\psi_{\text{nl}} \in C((-T_{\text{min}}^{\text{nl}}, T_{\text{max}}^{\text{nl}}), H^s(\mathbb{R}^3, \mathbb{C}^4))$$

*be the maximal solution to (3.18) with initial condition  $\psi_{\text{in}} \in H^s(\mathbb{R}^3, \mathbb{C}^4)$ . Let  $\lambda_\sigma, \lambda_\omega \geq 0$ ,  $m_\sigma, m_\omega > 0$  and let*

$$(\psi, \varphi, \omega) \in C((-T_{\text{min}}, T_{\text{max}}), H^s(\mathbb{R}^3, \mathbb{C}^4) \times H^s(\mathbb{R}^3, \mathbb{R}) \times H^s(\mathbb{R}^3, \mathbb{R}^4)),$$

*be the maximal solution to the Dirac-Klein-Gordon system with initial conditions  $\psi|_{t=0} = \psi_{\text{in}}$  and*

$$\begin{aligned} (\varphi, \partial_t \varphi)|_{t=0} &\in H^s(\mathbb{R}^3, \mathbb{R}) \times H^{s-1}(\mathbb{R}^3, \mathbb{R}), \\ (\omega, \partial_t \omega)|_{t=0} &\in H^s(\mathbb{R}^3, \mathbb{R}^4) \times H^{s-1}(\mathbb{R}^3, \mathbb{R}^4). \end{aligned}$$

*Then, for all fixed  $\lambda_\sigma, \lambda_\omega \geq 0$ , we have*

$$\liminf_{m_\sigma, m_\omega \rightarrow \infty} T_{\text{min}/\text{max}} \geq T_{\text{min}/\text{max}}^{\text{nl}}.$$

*and, for any compact  $I \subset (-T_{\text{min}}^{\text{nl}}, T_{\text{max}}^{\text{nl}})$  and  $0 \leq s' < s$ ,*

$$\lim_{m_\sigma, m_\omega \rightarrow \infty} \|\psi - \psi_{\text{nl}}\|_{C(I, H^{s'}(\mathbb{R}^3, \mathbb{C}^4))} = 0.$$

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This means that the solution to the Dirac equation (3.11) subject to evolving fields converges to the solution to the non-linear Dirac equation (3.18) with the same initial condition, as long as the latter is defined. The proof gives a rate of convergence of  $\min\{m_\sigma, m_\omega\}^{-\min\{(s-s'), 1\}}$  which depends on the regularity expended in the final bound.

The main difficulty in proving this result is the loss of regularity incurred by dropping the terms

$$m_\sigma^{-2}(\partial_t^2 - \Delta), \quad m_\omega^{-2}(\partial_t^2 - \Delta) \quad (3.19)$$

from the field equations. This makes the equations more singular, while we might also want appropriate bounds on derivatives to prove convergence. However, the specific structure of the equations mitigates this problem somewhat. If one writes the equations for the differences

$$\tilde{\varphi} = \varphi + \lambda_\sigma \varphi_s(\psi), \quad \tilde{\omega} = \omega - \lambda_\omega J(\psi),$$

one obtains, e.g.,

$$(\partial_t^2 - \Delta + m_\sigma^2)\tilde{\varphi} = \lambda_\sigma(\partial_t^2 - \Delta)\rho_s(\psi), \quad (3.20)$$

where the right hand side of (3.12) has cancelled with  $m_\sigma^2 \lambda_\sigma \rho_s$ , eliminating the large coupling. Now in  $(\partial_t^2 - \Delta)\rho_s(\psi)$  all terms involving second derivatives cancel out, since  $(-i\alpha \cdot \nabla)^2 = -\Delta$  and  $\psi$  solves a wave equation up to lower-order terms. This leads to equations of the form

$$\begin{aligned} (\partial_t^2 - \Delta + m_\sigma^2)\tilde{\varphi} &= P_\sigma(\psi, \tilde{\varphi}, \tilde{\omega}, \nabla\psi, \nabla\tilde{\varphi}, \nabla\tilde{\omega}) + \partial_t Q_\sigma(\psi, \tilde{\varphi}, \tilde{\omega}) \\ (\partial_t^2 - \Delta + m_\omega^2)\tilde{\omega} &= P_\omega(\psi, \tilde{\varphi}, \tilde{\omega}, \nabla\psi, \nabla\tilde{\varphi}, \nabla\tilde{\omega}) + \partial_t Q_\omega(\psi, \tilde{\varphi}, \tilde{\omega}) \end{aligned} \quad (3.21)$$

for appropriate functions  $P_\sigma, P_\omega, Q_\sigma, Q_\omega$ . This effectively gains one derivative with respect to the generic case, if one works in sufficiently high regularity to estimate products like  $|\nabla\psi|^2$ . This is the reason for assuming the high initial regularity,  $H^s$ ,  $s > 5/2$ , which allows us to deal with such products using the Kato-Ponce inequality

$$\|fg\|_{H^s} \leq C(\|f\|_{H^s}\|g\|_{L^\infty} + \|f\|_{L^\infty}\|g\|_{H^s}). \quad (3.22)$$

With this, one can easily prove a well-posedness result for the equations (3.21) coupled to the Dirac equation. The fields  $\tilde{\varphi}, \tilde{\omega}$  have an oscillatory part, essentially due to the initial conditions, and a small part due to the non-linear terms. Inserting this into the Duhamel representation for  $\psi$  and integrating by parts to deal with the oscillatory terms gives the claimed convergence during the existence time of the solution.

To show that the solution exists at least as long as  $\psi_{\text{nl}}$  asymptotically, one proves bounds on  $\tilde{\varphi}, \tilde{\omega}$  in terms of  $\psi$ , and then uses the closeness of  $\psi$  to  $\psi_{\text{nl}}$  to prove that no blowup can occur for  $(\psi, \tilde{\varphi}, \tilde{\omega})$  inside the existence interval of  $\psi_{\text{nl}}$ .

### 3.2.2 The mean-field problem

For a mean-field description of a many-particle system, the wavefunction  $\psi$  is replaced by a one-particle density matrix  $\gamma$ , which we assume to be Hilbert-Schmidt. The equation for  $\gamma$  is

$$i\partial_t\gamma = [\alpha \cdot (-i\nabla + A) + \beta(m + \varphi) + V, \gamma], \quad (3.23)$$

and the coupling to the field equations is given by

$$\begin{aligned} \rho_s(\gamma) &= \text{Tr}_{\mathbb{C}^4}(\beta\gamma(x, x)) \\ J(\gamma) &= (\text{Tr}_{\mathbb{C}^4}(\gamma(x, x)), \text{Tr}_{\mathbb{C}^4}(\alpha\gamma(x, x))), \end{aligned} \quad (3.24)$$

where  $\gamma(x, y) \in \mathbb{C}^{4 \times 4}$  is the integral kernel of  $\gamma$ .

The corresponding equation with instantaneous interaction is thus

$$i\partial_t\gamma = [\alpha \cdot (-i\nabla + \lambda \text{Tr}(\alpha\gamma(x, x))) + \beta(m + \text{Tr}(\beta\gamma(x, x))) + \text{Tr} \gamma(x, x), \gamma]. \quad (3.25)$$

The natural functional setting for  $\gamma$  is that of the spaces

$$\mathfrak{S}^{2,s} = \left\{ \gamma \in \mathfrak{S}^2(L^2(\mathbb{R}^3, \mathbb{C}^4)) \mid \|(1 - \Delta)^{s/2} \gamma (1 - \Delta)^{s/2}\|_{\mathfrak{S}^2} < \infty \right\} \quad (3.26)$$

whose norm we denote by  $\|\gamma\|_s$ . For  $\gamma = |\psi\rangle\langle\psi|$  a rank-one projection this is just the square of the  $H^s$ -norm of  $\psi$ .

In this setting, much of the analysis can be done in analogy with the one-particle case. An interesting technical point is the generalisation of the Kato-Ponce inequality (3.22), which is an important ingredient in our proof, and the study of non-linear partial differential equations in high regularity in general. One should think of the function  $f(x)g(x)$  as  $\gamma(x, x)$ , whose  $H^s$ -norm one would like to estimate by a combination of  $\|\gamma\|_s$ ,  $s > 3/2$ , and a weaker norm. We have such a bound from [6, Lemma 3.1].

**Lemma 3.4.** *For  $3/2 < s' \leq s$  there exists  $C$  so that for all  $\gamma \in \mathfrak{S}^{2,s}$  with  $\gamma \geq 0$*

$$\|\gamma(x, x)\|_{H^s(\mathbb{R}^3, \mathbb{C}^{4 \times 4})} \leq C \|\gamma\|_s^{1/2} \|\gamma\|_{s'}^{1/2}.$$

Note the additional positivity condition  $\gamma \geq 0$ . This is necessary for  $s' < s$ , as can be seen from examples of the type  $\gamma = |f\rangle\langle g| + |g\rangle\langle f|$  where  $f$  and  $g$  concentrate at different points in momentum space (see [6, Remark 3.2]). It is not clear in this setting what norm could take the place of the  $L^\infty$ -norm from (3.22), being weaker than all the  $s'$ -norms but stronger than the  $3/2$ -norm.

Apart from its role in our analysis, this inequality can be used to prove blowup criteria for Hartree-type equations for density matrices. By reducing the regularity in

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one of the factors, one obtains from Grönwall's Lemma that at the maximal existence time of the solution in  $\mathfrak{S}^{2,s}$ , the  $s'$ -norm must blow up, for any  $3/2 < s' < s$ . The existence time is thus independent of  $s$ . We are not aware of such results in the literature on this type of equation.

The convergence result in the many-body setting is [6, Theorem 2].

**Theorem 3.5.** *Let  $s > \frac{5}{2}$*

$$\gamma_{\text{nl}} \in C((-T_{\text{min}}^{\text{nl}}, T_{\text{max}}^{\text{nl}}), \mathfrak{S}^{2,s})$$

*be the maximal solution to (3.25) with initial condition  $\gamma_{\text{in}} \in \mathfrak{S}^{2,s}$ . Let  $\lambda_\sigma, \lambda_\omega \geq 0$ ,  $m_\sigma, m_\omega > 0$  and let*

$$(\gamma, \varphi, \omega) \in C((-T_{\text{min}}, T_{\text{max}}), \mathfrak{S}^{2,s} \times H^s(\mathbb{R}^3, \mathbb{R}) \times H^s(\mathbb{R}^3, \mathbb{R}^4)),$$

*be the maximal solution to (3.23) together with the field equations (3.12), (3.14), with initial conditions  $\gamma_{\text{in}}$ , and  $\varphi, \omega$  as in Theorem 3.3. Then, for all fixed  $\lambda_\sigma, \lambda_\omega \geq 0$ , we have*

$$\liminf_{m_\sigma, m_\omega \rightarrow \infty} T_{\text{min}/\text{max}} \geq T_{\text{min}/\text{max}}^{\text{nl}},$$

*and, for any compact  $I \subset (-T_{\text{min}}^{\text{nl}}, T_{\text{max}}^{\text{nl}})$  and  $0 \leq s' < s$ ,*

$$\lim_{m_\sigma, m_\omega \rightarrow \infty} \|\gamma - \gamma_{\text{nl}}\|_{C(I, \mathfrak{S}^{2,s'})} = 0.$$

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## 4 Interior boundary conditions

The language of quantum field theory (QFT) is at the core of modern physics. It is the basis of the physics of fundamental particles, but also ubiquitous in the description of atoms, molecules and condensed matter. From the very beginning, the mathematical formulation of QFT has been complicated by the appearance of ill-defined expressions and divergent integrals. Many tools have been developed to address this problem, and renormalisation techniques have made perturbative QFT a great success, with stunningly accurate predictions. However, success has been more limited on the mathematical formulation of the underlying theory, to which the renormalised perturbation series should provide an asymptotic approximation.

One of the main problems in QFT is the ultraviolet problem. It stems from the fact that particles are modelled as point-like, and consequently their interactions usually involve distributions whose local singularities lead to divergences in the ultraviolet, i.e. for large values of the Fourier variable. If one wants to see the interacting Hamiltonian as a modification (perturbation) of the non-interacting one, this means that it is certainly a singular perturbation.

A common approach to this problem is via renormalisation: one considers the Hamiltonian with a regularised interaction and tries to prove existence of a limiting object as the regularisation is removed, possibly up to subtraction of a divergent energy or modification (renormalisation) of other parameters in the model.

A different idea is to implement the singularities of the interaction by special boundary conditions. To understand this, consider a model in which a particle in  $\mathbb{R}^d$  interacts with a field, represented by an arbitrary number of bosons. The configuration space of the model is

$$\mathcal{K} = \bigcup_{n=0}^{\infty} \mathbb{R}^d \times \mathbb{R}^{dn} / S_n, \quad (4.1)$$

where points obtained by permuting the coordinates of the  $n$  bosons are identified. Assume we know the Hamiltonian  $H_0$ ,  $D(H_0)$  of the non-interacting theory, which is a self-adjoint operator on the natural Hilbert space  $L^2(\mathbb{R}^d) \otimes \Gamma(L^2(\mathbb{R}^d)) \cong L^2(\mathcal{K})$ . We would like to define a Hamiltonian with interaction, of the form

$$H = H_0 + H_{\text{int}}. \quad (4.2)$$

The basic building blocks of the relevant interactions are the creation and annihilation operators  $a^*$ ,  $a$ . In a simple case, which we consider in detail in Section 4.2,

$$H_{\text{int}} = a(v_x) + a^*(v_x), \quad (4.3)$$

#### 4.1 Singular perturbations and self-adjoint extensions

where  $a^*(v_x)$  acts (with a form-factor  $v \in L^2(\mathbb{R}^d)$ ) by taking the tensor product with  $v$  and projecting to symmetric tensors

$$a^*(v_x)\psi^{(n)} = \sqrt{n}P_{\text{sym}}v(x - \cdot) \otimes \psi^{(n)}. \quad (4.4)$$

However, in practice,  $v$  is often a singular function or distribution. The formula above does not yield a densely defined operator in this case, since the multiplication by  $v$  creates a singularity. These typically lie on the set of collision configurations of the particle and the bosons

$$\mathcal{C} = \left\{ (x, y_1, \dots, y_n) \in \mathcal{K} : \prod_{j=1}^n |x - y_j| = 0 \right\}. \quad (4.5)$$

The idea is now to view  $\mathcal{C}$  as the boundary of configuration space  $\mathcal{K}$  and impose conditions on the asymptotic behaviour of functions in  $D(H)$  there, so that singularities created by application of  $H_0$  (extended in a distributional sense) and  $H_{\text{int}}$  cancel. In this case the sum  $H_0 + H_{\text{int}}$  may be (densely) defined, even though  $H_{\text{int}}$  alone is not. These boundary conditions will relate the behaviour of the wave-function at some points on  $\mathcal{C}$ , the boundary, with its values at the point where the variables  $y_j$  with  $y_j = x$  are eliminated, an interior point. For this reason, these boundary conditions were called *interior boundary conditions* (IBCs) in [40, 41].

Landau and Peierls proposed a (simplified) formulation of quantum electrodynamics in the particle-position representation [26], which includes constraints that integrate to IBCs [44]. Similar ideas have since reappeared sporadically, and often independently, in the literature [30, 29, 31, 42, 32, 45, 15, 37, 38, 43, 27].

In the following sections I will summarise the results of the articles [25, 24, 18, 20, 4, 21, 22, 23] that systematically investigate this idea in the context of non-relativistic quantum field theory.

#### 4.1 Singular perturbations and self-adjoint extensions

From the point of view of functional analysis, the approach by IBCs means that we are looking for a suitable domain  $D(H)$  for the Hamiltonian including the interaction. This is necessarily different from the domain  $D(H_0)$  of free Hamiltonian. In the case of ordinary boundary conditions, say for the Laplacian on some domain  $\Omega \subset \mathbb{R}^d$ , one may proceed as follows. First, one considers a restriction  $\mathring{H}_0$  of  $H_0$  to functions that avoid the singularities (the boundary). Then, one obtains an extension of  $H_0$  by taking the adjoint,  $H_0 \subset \mathring{H}_0^*$ . Different boundary conditions can now be imposed on  $\mathring{H}_0^*$  to obtain a self-adjoint operator. Indeed, boundary conditions classify the self-adjoint extensions of  $\mathring{H}_0$ . The abstract structure is similar in the case of interior boundary conditions, though the difference between  $H$  and  $H_0$  consists not only of boundary conditions, but also has an additive, regular part.



#### 4 Interior boundary conditions

It has been known for a long time that extension theory can be used to define singular perturbations, for example the perturbation of the Laplacian by a  $\delta$ -“potential” in  $\mathbb{R}^3$ . In this case, the result coincides with that obtained by a renormalisation procedure [16, 1]. One may thus view IBCs as a generalisation of this approach to models from quantum field theory.

##### 4.1.1 The minimal example

The general ideas we have discussed are best illustrated in a concrete and simple model, studied independently by Yafaev and Moshinsky [45, 30, 29, 31]. In this model, a particle, whose position is fixed at  $x = 0 \in \mathbb{R}^3$  can create and annihilate a single boson at the origin. The relevant Hilbert space is thus  $\mathcal{H} = \mathbb{C} \oplus L^2(\mathbb{R}^3)$ , where the second summand corresponds to having one boson, and the first to no bosons (i.e.,  $\mathbb{C} = L^2(\{0\})$ ). We take the free evolution of the boson to be generated by minus the Laplacian. Since creation and annihilation is supposed to take place only at  $x = 0$ , the formal expression for the Hamiltonian should naturally be

$$\begin{pmatrix} 0 & \delta_0 \\ \delta_0^* & -\Delta \end{pmatrix}. \quad (4.6)$$

Here,  $\delta_0$  is the Dirac distribution in  $x = 0$ , i.e.,  $\delta_0(f) = f(0)$ . The expression is not densely defined as  $\delta_0$  is not closable and thus  $\delta_0^*$  is not densely defined.

The non-interacting Hamiltonian is given by

$$H_0(z, \psi) = (0, -\Delta\psi), \quad D(H_0) = \mathbb{C} \oplus H^2(\mathbb{R}^3). \quad (4.7)$$

We restrict  $H_0$  to functions that avoid the singularity at  $x = 0$ , setting (this is exactly the kernel of  $\delta_0 : \mathbb{C} \oplus H^2 \rightarrow \mathcal{H}$ )

$$D(\mathring{H}_0) = \mathbb{C} \oplus H_0^2(\mathbb{R}^3), \quad \mathring{H}_0 = H_0|_{D(\mathring{H}_0)}. \quad (4.8)$$

The domain of the extension  $\mathring{H}_0^*$  is easy to determine in this case. It is given by

$$D(\mathring{H}_0^*) = D(H_0) \oplus \ker(\mathring{H}_0^* + 1) = D(H_0) \oplus \text{span}(0, g), \quad (4.9)$$

where

$$g(x) = -\frac{e^{-|x|}}{4\pi|x|}. \quad (4.10)$$

Note that, in the sense of distributions,

$$-\Delta g = -g - \delta_0. \quad (4.11)$$

#### 4.1 Singular perturbations and self-adjoint extensions

The singular set, i.e., the boundary, is the position of the particle  $x = 0$ . To determine the relevant boundary values, it is instructive to perform an integration by parts. For rapidly decreasing  $\varphi, \psi$  differentiable in  $\mathbb{R}^3 \setminus \{0\}$  we have

$$\begin{aligned} \int \bar{\varphi}(x)(-\Delta\psi)(x)dx &= \int_0^\infty \int_{S^2} r\bar{\varphi}(r\omega) \underbrace{r(-\partial_r^2 + \frac{2}{r}\partial_r)\psi(r\omega)}_{=-\partial_r^2 r\psi} d\omega dr \\ &= \int (-\Delta\bar{\varphi}(x))\psi(x)dx + \lim_{r \rightarrow 0} \int_{S^2} (r\bar{\varphi}(r\omega))\partial_r r\psi(r\omega)d\omega \\ &\quad - \lim_{r \rightarrow 0} \int_{S^2} (\partial_r r\bar{\varphi}(r\omega))r\psi(r\omega)d\omega. \end{aligned} \quad (4.12)$$

For functions of the form  $\psi = \varphi + cg$ ,  $\varphi \in H^2(\mathbb{R}^3)$ , we have

$$\lim_{r \rightarrow 0} r(\varphi(r\omega) + cg(r)) = -\frac{c}{4\pi}, \quad (4.13)$$

and

$$\lim_{r \rightarrow 0} \int_{S^2} \partial_r(r(\varphi(r\omega) + cg(r)))d\omega = 4\pi\varphi(0) + c. \quad (4.14)$$

The relevant boundary values of  $(z, \psi) = (z, \varphi + cg) \in D(\mathring{H}_0^*)$  are thus

- the value of the regular part  $\varphi \in H^2(\mathbb{R}^3)$  at  $x = 0$ ,
- the coefficient  $c$  of  $g$ ,
- the value of  $z$  (this corresponds to the value of the wave function of the particle with no boson at the origin, the boundary).

Relating  $\varphi(0)$  and  $c$  in such a way as to make  $\mathring{H}_0^*$  symmetric gives rise to the self-adjoint operators that describe a boson interacting with the particle at the origin with a point interaction [16, 1]. The boson is never created or annihilated, and these do not correspond to the expression (4.6). If we apply (4.6) to a vector of the form  $(z, \varphi + cg)$ , we obtain

$$(\varphi(0) + c\delta_0(g), -\Delta\varphi - cg - c\delta_0 + z\delta_0). \quad (4.15)$$

An obvious choice to make the second part an element of  $L^2(\mathbb{R}^3)$  is to take  $c = z$ , which corresponds to the boundary condition on  $(z, \psi)$

$$B\psi := -4\pi \lim_{r \rightarrow 0} r\psi(r\omega) = z. \quad (4.16)$$

With this choice we obtain

$$(\varphi(0) + z\delta_0(g), \underbrace{-\Delta\varphi - zg}_{=\mathring{H}_0^*\psi}). \quad (4.17)$$

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Now  $g$  diverges at  $x = 0$  so  $\delta_0(g)$  is not defined, and it might seem that we have not gained much. However, the formula (4.14) provides a natural extension of  $\delta_0$  to the relevant functions, i.e,

$$A\psi := \frac{1}{4\pi} \lim_{r \rightarrow 0} \int_{S^2} \partial_r r \psi(r\omega) d\omega. \quad (4.18)$$

Then we may define

$$\begin{aligned} D(H) &:= \left\{ (z, \psi) \in D(\mathring{H}_0^*) \mid B\psi = z \right\}, \\ H(z, \psi) &:= \mathring{H}_0^* \psi + A\psi. \end{aligned} \quad (4.19)$$

This is clearly well defined and, by our earlier calculations, corresponds to the formal expression (4.6) up to the choice of extension  $A$ .

The formula for  $H$  can be re-expressed in a more manifestly symmetric way. Define a bounded operator by

$$G : \mathbb{C} \rightarrow \mathcal{H}, \quad z \mapsto zg. \quad (4.20)$$

Then  $\psi - Gz = \varphi$  is the regular part of the wave-function, and

$$D(H) = \left\{ (z, \psi) \in \mathcal{H} \mid \psi - Gz \in H^2(\mathbb{R}^3) \right\}. \quad (4.21)$$

Moreover, since  $(\mathring{H}_0^* + 1)G = 0$ , we have for  $(z, \psi) \in D(H)$

$$(\mathring{H}_0^* + 1)\psi = (\mathring{H}_0^* + 1)(\psi - Gz) = (-\Delta + 1)(\psi - Gz). \quad (4.22)$$

For  $\varphi \in H^2(\mathbb{R}^3)$  it holds

$$\bar{z}G^*(-\Delta + 1)\varphi = \langle Gz, (-\Delta + 1)\varphi \rangle = \bar{z} \underbrace{\langle (-\Delta + 1)G, \varphi \rangle}_{=-\delta_0} = -\bar{z}\varphi(0), \quad (4.23)$$

so for  $(z, \psi) \in D(H)$

$$-G^*(-\Delta + 1)(\psi - Gz) = A\psi - \frac{z}{4\pi} \quad (4.24)$$

If we interpret  $G$  as the operator on  $\mathcal{H}$  given by  $G(z, \psi) = (0, zg)$  and use the additive notation  $(z, \psi) = z + \psi \in \mathbb{C} \oplus L^2(\mathbb{R}^3)$ , we can thus write

$$\begin{aligned} H(z + \psi) &= (H_0^* + 1)(z + \psi) + A\psi - z - \psi \\ &= (1 - G^*)(H_0 + 1)(1 - G)(z + \psi) + \frac{z}{4\pi} - z - \psi. \end{aligned} \quad (4.25)$$

With this representation we can easily prove self-adjointness of  $H$ .

#### 4.1 Singular perturbations and self-adjoint extensions

**Proposition 4.1.** *The operator  $H$ ,  $D(H)$  defined by (4.19) is self-adjoint.*

*Proof.* Since  $G^2 = 0$ ,  $1 - G$  is invertible with bounded inverse  $(1 - G)^{-1} = 1 + G$ . Hence  $(1 - G)^*(H_0 + 1)(1 - G)$  with domain  $D(H)$  is a symmetric, invertible operator, whence self-adjoint. By (4.25),  $H$  is the perturbation of this self-adjoint operator by a bounded operator, and thus self-adjoint.  $\square$

The self-adjoint operator constructed in this way can also be obtained by a renormalisation procedure. If one replaces the distribution  $\delta_0$  by the regularisation with Fourier transform  $\hat{v}_\Lambda(k) = (2\pi)^{-3/2}1_{|k| \leq \Lambda}$ , the operators

$$H_\Lambda = \begin{pmatrix} 0 & \langle v_\Lambda \rangle \\ v_\Lambda & -\Delta \end{pmatrix} \quad (4.26)$$

are self-adjoint with domain  $D(H_\Lambda) = \mathbb{C} \oplus H^2(\mathbb{R}^3)$ . With  $G_\Lambda(z, \psi) = (0, z(\Delta - 1)^{-1}v_\Lambda)$  they can be written as

$$H_\Lambda + 1 = (1 - G_\Lambda^*)(H_0 + 1)(1 - G_\Lambda) - G_\Lambda^*(H_0 + 1)G_\Lambda. \quad (4.27)$$

One can check that the first part converges to  $(1 - G^*)(H_0 + 1)(1 - G)$  in norm-resolvent sense. The operator  $G_\Lambda^*(H_0 + 1)G_\Lambda$  acts only on the sector with no particle. It evaluates to the multiplication by

$$-G_\Lambda^*(H_0 + 1)G_\Lambda = -\langle v_\Lambda, (1 - \Delta)v_\Lambda \rangle = -\frac{1}{(2\pi)^3} \int_{|k| \leq \Lambda} \frac{1}{k^2 + 1} dk \sim -\frac{\Lambda}{2\pi^2}. \quad (4.28)$$

Hence, after adjusting the Hamiltonian on the sector with no particles, i.e., the energy of the vacuum, by a divergent family  $E_\Lambda$ , the Hamiltonians  $H_\Lambda - E_\Lambda P_1$  converges in norm-resolvent sense to  $H$  from Proposition 4.1, where  $P_1$  is the projection to the first summand in  $\mathbb{C} \oplus L^2(\mathbb{R}^3)$ . The divergence of  $E_\Lambda$  is given by (4.28), while the precise asymptotics are fixed by the choice of extension  $A$  of  $\delta_0$  used in the definition of  $H$ .

#### 4.1.2 Van Hove Hamiltonians

If we consider the above model without the restriction that there be at most one boson, the formal expression for the Hamiltonian is

$$d\Gamma(-\Delta + E_0) + a(\delta_0) + a^*(\delta_0), \quad (4.29)$$

where we introduced the rest-energy of the bosons  $E_0 \geq 0$ . Such Hamiltonians are known as (singular) van Hove Hamiltonians [6]. In the article [25] we investigated the domain of a well-defined version of this formal expression and showed that it is given in terms of IBCs. This is a natural generalisation of the considerations above to an arbitrary number of bosons.

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Let  $\mathcal{H} := \Gamma(L^2(\mathbb{R}^3))$  be the Fock space and  $H_0 = d\Gamma(-\Delta + E_0)$ . Define  $\mathring{H}_0$  as the restriction of this to the kernel of  $a(\delta_0)$  (which is well-defined on  $D(H_0)$ ). To better understand this, fix  $n \in \mathbb{N}$  and let  $\mathcal{C}^{(n)}$  be the collision configurations of  $n$  bosons with the particle at the origin, i.e.,

$$\mathcal{C}^{(n)} = \left\{ x \in \mathbb{R}^{3n} \mid \prod_{j=1}^n |x_j| = 0 \right\}. \quad (4.30)$$

On  $\mathcal{H}^{(n)}$ ,  $\mathring{H}_0$  acts (up to the constant  $nE_0$ ) as the restriction of minus the Laplacian on  $\mathbb{R}^{3n}$  to functions vanishing on  $\mathcal{C}^{(n)}$ . Denote this operator by  $\Delta_n$ , i.e.,

$$D(\Delta_n) = \left\{ \psi \in L^2(\mathbb{R}^3)^{\otimes n} \mid \psi \in H^2(\mathbb{R}^{3n}), \psi|_{\mathcal{C}^{(n)}} = 0 \right\}, \quad \Delta_n \psi = \Delta \psi. \quad (4.31)$$

The boundary values have to be imposed on the extension of the Laplacian given by  $\Delta_n^*$  and link the function with  $n$  bosons to the one with  $n-1$  bosons. The expressions for the boundary values analogous to (4.16), (4.18) are

$$A\psi^{(n)}(x_1, \dots, x_{n-1}) = \frac{\sqrt{n}}{4\pi} \lim_{r \rightarrow 0} \partial_r \int_{S^2} r\psi^{(n)}(r\omega, x_1, \dots, x_{n-1}) d\omega \quad (4.32)$$

$$B\psi^{(n)}(x_1, \dots, x_{n-1}) = -4\pi\sqrt{n} \lim_{r \rightarrow 0} r\psi^{(n)}(r\omega, x_1, \dots, x_{n-1}). \quad (4.33)$$

One now encounters a difficulty that is familiar from the theory of boundary conditions for the Laplacian on  $\Omega \subset \mathbb{R}^d$ . While in one dimension the boundary consists of points and both Neumann- and Dirichlet boundary values are merely numbers, in higher dimensions the boundary values can be functions, and even distributions, on the boundary. In general the Dirichlet values are elements of  $H^{-1/2}(\partial\Omega)$  while the Neumann values are merely in  $H^{-3/2}(\partial\Omega)$  (these spaces are natural, since they are dual to the ranges of the trace maps on  $H^2(\Omega)$ , so they are the maximal spaces on which Green's identity can hold). Similarly, our boundary values are now distributions on the boundary, the space with one fewer boson.

One can indeed show that the limits in (4.32), (4.33) exist for  $\psi^{(n)} \in D(\Delta_n^*)$  in an appropriate distributional sense (see [25, Lemma 5.2]). The IBC  $B\psi^{(n)} = \psi^{(n-1)}$  is then well-defined.

We define

$$D(H) = \left\{ \Psi \in D(\mathring{H}_0^*) \mid B\Psi = \Psi, A\Psi \in \mathcal{H} \right\} \quad (4.34)$$

$$H\Psi = \mathring{H}_0^*\Psi + A\Psi.$$

The main result on this operator is:

**Theorem 4.2.** *The operator defined by (4.34) is self-adjoint if  $E_0 > 0$  and essentially self-adjoint if  $E_0 = 0$ . It holds that  $D(H) \cap D(d\Gamma((-\Delta)^{1/2})) = \{0\}$ .*

#### 4.1 Singular perturbations and self-adjoint extensions

The fact that one only has essential self-adjointness for  $E_0 = 0$  is related to a lack of control for large  $n$ . The property  $D(H) \cap D(d\Gamma((-\Delta)^{1/2})) = \{0\}$  shows that  $H$  is a singular perturbation of  $H_0$ . In particular, it is not a perturbation in the sense of quadratic forms.

Van Hove type Hamiltonians with regular interactions, i.e.,

$$H_v = d\Gamma(-\Delta + E_0) + a(v) + a^*(v) \quad (4.35)$$

with  $v \in L^2(\mathbb{R}^3)$ , are unitarily equivalent (for  $E_0 > 0$ ) to  $H_0 + E$  with

$$E = - \int_{\mathbb{R}^3} \frac{|\hat{v}(k)|^2}{k^2 + E_0} dk \quad (4.36)$$

via a Weyl transformation. This can be used to define a renormalised version of the singular Hamiltonian (4.29) by taking a sequence  $v_n \in L^2$  that converges to  $\delta_0$  in the sense of distributions, e.g., setting  $\hat{v}_n(k) = (2\pi)^{-3/2} 1_{|k| \leq n}$ . The sequence of numbers  $E_n$  then diverges, but one can show that  $H_{v_n} - E_n$  converges to a self-adjoint operator  $H_{\text{ren}}$  in strong resolvent sense [6]. This renormalised operator coincides with the one constructed in Theorem 4.2 up to a constant:

**Theorem 4.3.** *Let  $E_0 > 0$  and  $H$  be the self-adjoint operator given by (4.34). Then*

$$H = H_{\text{ren}} + \frac{\sqrt{E_0}}{4\pi}. \quad (4.37)$$

#### 4.1.3 An abstract setting and a classification result

One can take a more abstract view of the discussion in the previous sections, which is explored in [4]. In these sections, we worked with the following data:

- A Hilbert space  $\mathcal{H}$ ;
- A self-adjoint reference operator  $H_0$ ,  $D(H_0) \subset \mathcal{H}$ ;
- A restriction and an extension  $\mathring{H}_0 \subset H_0 \subset \mathring{H}_0^*$ ;
- Two boundary operators  $A, B$  defined on  $D(\mathring{H}_0^*)$ ;

These objects were related by the properties that  $H_0 = \mathring{H}_0^*|_{\ker(B)}$  and  $\mathring{H}_0 = H_0|_{\ker(A)}$ , so  $\mathring{H}_0$  is the “minimal” operator, for which all boundary values vanish. From these objects, we constructed a self-adjoint operator  $H$ ,  $D(H)$  that contains  $A$  as an additive perturbation. But this really maps to the space of boundary values, so to formalise this properly we need additionally

- A Hilbert space  $\partial\mathcal{H}$  ( $\partial\mathcal{H} = \mathbb{C}$  for Section 4.1.1 and  $\partial\mathcal{H} = \mathcal{H}$  for Section 4.1.2);

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- A bounded operator  $I : \partial\mathcal{H} \rightarrow \mathcal{H}$  (the inclusion  $\mathbb{C} \rightarrow \mathbb{C} \oplus L^2(\mathbb{R}^3)$  for Section 4.1.1 and  $I = 1_{\Gamma(L^2(\mathbb{R}^3))}$  for Section 4.1.2).

With the appropriate choices for these objects, we can write the operator  $H$  for both cases as

$$\begin{aligned} D(H) &= \left\{ \Psi \in D(\mathring{H}_0^*) \mid B\Psi = I^*\Psi, A\Psi \in \partial\mathcal{H} \right\} \\ H\Psi &= \mathring{H}_0^*\Psi + IA\Psi. \end{aligned} \quad (4.38)$$

In this setting, one can consider Robin-type boundary conditions of the form

$$\alpha A\Psi + \beta B\Psi = I^*\Psi, \quad (4.39)$$

say for  $\alpha, \beta \in \mathbb{R}$  (more generally these could also be operators). It is then natural to also include both boundary operators in the Hamiltonian as

$$H = \mathring{H}_0^* + \gamma IA + \delta IB. \quad (4.40)$$

It is, in general, necessary to include these terms to obtain a symmetric operator, i.e.  $H$  is symmetric subject to the Robin condition (4.39) if  $\beta\gamma - \alpha\delta = 1$ . Note that for  $I = 0$ , which we did not exclude, we are in the familiar situation of (generalised) Robin conditions that has been studied extensively [2]. The specificity of interior boundary conditions is that  $I \neq 0$ . Indeed, in both cases studied so far  $I$  is injective so the condition  $B\Psi = I^*\Psi$  relates boundary values to the part  $II^*\Psi$  of the data in  $\mathcal{H}$  and  $IA$  is a non-trivial term in the operator.

These general operators are studied in [4]. An important role therein is played by two families of operators indexed by  $z \in \rho(H_0)$ . The abstract Dirichlet operator

$$G_z := (A(z - H_0)^{-1})^*, \quad (4.41)$$

describes the extension  $H_0 \subset \mathring{H}_0^*$  using solutions to the inhomogeneous equation

$$(\mathring{H}_0^* - z)\Psi = 0, \quad B\Psi = \Phi, \quad (4.42)$$

and was already introduced in Section 4.1.1. The ‘‘Dirichlet to Neumann’’ operator

$$T_z := AG_z. \quad (4.43)$$

fixes the extension of  $A = a(\delta_0)$  from  $D(H_0)$  to  $D(A) \subset D(\mathring{H}_0^*)$ .

Note that the operator  $H$  is not a self-adjoint extension of  $\mathring{H}_0$  if  $I \neq 0$ , since the conditions  $B\Psi = A\Psi = 0$  and  $B\Psi = I^*\Psi$  defining the operators are not compatible (on a dense set). In order to use the theory of self-adjoint extensions to classify boundary conditions such as (4.39), it is natural to consider the stronger condition

$$A\Psi = B\Psi = (\alpha + \beta)^{-1}I^*\Psi. \quad (4.44)$$

#### 4.1 Singular perturbations and self-adjoint extensions

With this condition on  $\Psi$ , the action of the operator (4.40) can be written as

$$H\Psi = \mathring{H}_0^* + (\gamma + \delta)(\alpha + \beta)^{-1}II^*. \quad (4.45)$$

Hence all the operators with  $\alpha + \beta = \text{const.}$  and  $\gamma + \delta = \text{const.}$  are extensions of one symmetric operator. Let thus  $\alpha + \beta = 1 = \gamma + \delta$  and define

$$\begin{aligned} D(\mathring{H}) &= \left\{ \Psi \in D(\mathring{H}_0^*) : A\Psi = B\Psi = I^*\Psi \right\} \\ \mathring{H} &= \mathring{H}_0^* + (\gamma + \delta)(\alpha + \beta)^{-1}II^*. \end{aligned} \quad (4.46)$$

Informally, the results of [4] state that the ‘‘maximal operator’’  $\mathring{H}^*$  and the corresponding boundary operators  $B - I^*$ ,  $A - I^*$  enjoy very similar properties to the case  $I = 0$ . More precisely,  $(\partial\mathcal{H}, B - I^*, A - I^*)$  form a quasi-boundary triple for  $\mathring{H}^*$  and one can apply general results for such structures [3, 2].

To be precise, let us assume that the families  $G_z$  and  $T_z$  satisfy the following hypothesis (that can be slightly weakened):

- i) The unbounded operator  $IT_zI^*$  on  $\mathcal{H}$  is relatively bounded with respect to  $(1 - G_zI^*)^*(H_0 - z)(1 - G_zI^*)$  with bound  $a < 1$ .
- ii) The bounded operator  $1 - I^*G_z$  is invertible on  $\partial\mathcal{H}$  and leaves  $D(T_z)$  invariant.

By an argument similar to the one of Section 4.1.1, these hypothesis guarantee that  $H^{0,1}$  (the extension of  $\mathring{H}$  with boundary condition  $B\Psi = I^*\Psi$  and  $\gamma = 1$ ,  $\delta = 0$ ) is self-adjoint (see [4, Thm.3.12] and also Section 4.2.1).

**Theorem 4.4.** *Assume the hypothesis i) and ii) and let  $\mathfrak{R}$  be a symmetric relation on  $\partial\mathcal{H}$ . Then*

$$\begin{aligned} D(H_{\mathfrak{R}}) &= \left\{ \Psi \in D(\mathring{H}^*) : ((B - I^*)\Psi, (A - I^*)\Psi) \in \mathfrak{R} \right\} \\ H_{\mathfrak{R}} &= \mathring{H}^*|_{D(H_{\mathfrak{R}})} \end{aligned} \quad (4.47)$$

*is symmetric.*

The action of  $H_{\mathfrak{R}}$  will explicitly contain boundary terms. Indeed, using the generalisation of Green’s identity (see [4, Lem.3.3])

$$\langle \mathring{H}_0^*\Phi, \Psi \rangle_{\mathcal{H}} - \langle \Phi, \mathring{H}_0^*\Psi \rangle_{\mathcal{H}} = \langle B\Phi, A\Psi \rangle_{\partial\mathcal{H}} - \langle A\Phi, B\Psi \rangle_{\partial\mathcal{H}}, \quad (4.48)$$

together with the conditions  $B\Psi = I^*\Psi = A\Psi$  on  $D(\mathring{H})$ , we find the expression

$$\mathring{H}^* = \mathring{H}_0^* - IB + IA + II^*. \quad (4.49)$$

This can then be simplified using the relation  $\mathfrak{R}$ , e.g., for  $\mathfrak{R} = 0 \oplus \partial\mathcal{H}$  we recover  $H^{0,1}$ .



#### 4 Interior boundary conditions

The pre-fix “quasi” to the boundary triple relates to the fact that  $\partial\mathcal{H}$  may not be the “full” space of boundary values. In order to classify self-adjoint extensions, we need to take into account the maximal space of boundary values  $\partial\mathcal{H} \subset \mathcal{G}'$ . This comes a space of regular boundary values  $\mathcal{G} \subset \partial\mathcal{H}$  and an isometry  $\iota : \partial\mathcal{H} \rightarrow \mathcal{G}'$  (for the Laplacian on a domain with  $\partial\mathcal{H} = L^2(\partial\Omega)$ , these are  $H^{1/2}(\partial\Omega) \subset L^2(\partial\Omega) \subset H^{-1/2}(\partial\Omega)$ , the space of Neumann values on the domain of the Dirichlet operator and its dual). Let  $S_z$  be the family of Dirichlet-to-Neumann operators, associated with  $(\partial\mathcal{H}, B - I^*, A - I^*)$ .

**Theorem 4.5.** *Assume the hypothesis  $i)$ ,  $ii)$  and additionally that  $D(\mathring{H})$  is dense. Let  $H_{\mathfrak{R}}$  be as above and  $\lambda \in \mathbb{R}$  be in the resolvent set of  $H^{0,1}$ . Then  $H_{\mathfrak{R}}$  is self-adjoint if and only if  $\iota(\mathfrak{R} - S_\lambda)\iota$  defines a self-adjoint relation and  $\iota D(\mathfrak{R}) \subset D(S_\lambda)$ .*

Here, the adjoint of a relation is defined exactly like the adjoint of the relation  $(\Psi, O\Psi)$  for an operator  $O$ ,  $D(O)$ , and the domain of a relation is simply the projection to the first component. The adjoint relation is always well defined, and in this sense the hypothesis that  $D(\mathring{H})$  is dense is not needed for the symmetry statement of Theorem 4.4.

Every self-adjoint extension of  $\mathring{H}$  gives rise to some boundary relation. If we consider only extensions with with regular boundary values, i.e., for which  $(B - I^*)\Psi \in \partial\mathcal{H}$ ,  $(A - I^*)\Psi \in \partial\mathcal{H}$ , the statement gives a complete classification if  $\mathbb{R} \cap \rho(H^{0,1}) \neq \emptyset$ . The latter holds under the additional hypothesis that  $H_0$  is bounded from below. In the case where  $\iota(\mathfrak{R} - S_\lambda)\iota$  is given by the graph of an invertible operator, we have  $\lambda \in \rho(H_{\mathfrak{R}})$  and obtain a formula relating the resolvents of  $H^{0,1}$  and  $H_{\mathfrak{R}}$  in  $\lambda$ .

**Example 4.6.** For the minimal example of Section 4.1.1, the elements of  $D(\mathring{H}_0^*)$  are of the form  $\Psi = (z, \varphi + cg)$  with  $z \in \mathbb{C}$ ,  $\varphi \in H^2(\mathbb{R}^3)$  and  $g(x) = -e^{-|x|}/(4\pi|x|)$ . The conditions  $B\Psi = I^*\Psi = A\Psi$  mean that

$$c = z, \quad \varphi(0) + \frac{c}{4\pi} = z, \quad (4.50)$$

where the second condition simplifies to  $\varphi(0) = z(1 - (4\pi)^{-1})$  using the first. These two conditions define the (dense) domain of

$$\mathring{H} = \mathring{H}_0^* + II^*, \quad (4.51)$$

where  $II^*$  is the projection to the first summand in  $\mathbb{C} \oplus L^2(\mathbb{R}^3)$ . As  $\dim(\partial\mathcal{H}) = 1$ , the self-adjoint extensions of this symmetric operator are parameterised by the symmetric relations on  $\mathbb{C}$ , i.e. they are given by boundary conditions of the form

$$a(A - I^*)\Psi + b(B - I^*)\Psi = 0 \Leftrightarrow \frac{a}{a+b}A\Psi + \frac{b}{a+b}B\Psi = I\Psi, \quad (4.52)$$

with  $[a : b] \in \mathbb{R}\mathbb{P}^1 \cong S^1$ . Changing the sum of the parameters in the second equation amounts to changing  $I$  or the coupling constant of the model and leads to a different family of self-adjoint operators that do not extend  $\mathring{H}$ .

In this example, all technical hypothesis are trivially satisfied since  $\dim(\partial\mathcal{H}) = 1$ . They are non-trivially satisfied for some of the models we introduce in the next section, but not for the model from Section 4.1.2 with the canonical choice of  $H_0$  (we will explain this in more detail in Section 4.2.3).

## 4.2 Polaron models in non-relativistic quantum field theory

Polaron models arise frequently in the physics of condensed matter. The general idea is that small local perturbations of a system in equilibrium can be described by a bosonic field of elementary excitations. An impurity in the system will be influenced by the bulk properties of the system, which are not affected by its presence. It will also interact with the excitation field, and vice versa. The nature of this interaction will be reflected, for example, in the transport properties of the medium.

For example, local distortions of an ionic crystal can be modelled by a polarisation field. An electron moving through the medium will deform the lattice in its vicinity, and also experience a force due to any existing polarisation. Assuming that the wave-function varies slowly on the scale of the lattice, one is led to consider a continuum model with Hamiltonian

$$\underbrace{\Omega(i\nabla_x) + d\Gamma(\omega(i\nabla))}_{=H_0} + a(v_x) + a^*(v_x), \quad (4.53)$$

where  $\Omega$  is the effective dispersion of the electron,  $\omega$  that of the polarisation waves, and  $v$  is the interaction potential between the two. These quantities are determined by the bulk properties of the crystal. In this specific example, the model is known as Fröhlich's large polaron model [7]. Similar models are now considered in a multitude of situations. Whenever the excitation field is a scalar, the expression (4.53) is the most simple and natural form of a Hamiltonian. An example of particular interest to us will be the Bogoliubov-Fröhlich model of an atom interacting with excitations out of a bulk Bose-Einstein condensate.

In the upcoming sections we will discuss the construction of self-adjoint operators corresponding to the formal expression (4.53) in the presence of ultraviolet singularities following [24, 18, 20, 22]. We will mostly focus on the main examples that are the Fröhlich polaron, the Nelson model, and the Bogoliubov-Fröhlich model. We will restrict to the case of a single particle for simplicity, though the articles [24, 18] allow for an arbitrary number.

To obtain a heuristic understanding of the problem, it is instructive to consider the (essentially) homogeneous case

$$\hat{v}(k) = |k|^{-\alpha}, \quad \omega(k) = (m^{2/\beta} + k^2)^{\beta/2}, \quad \Omega(p) = |p|^\gamma, \quad (4.54)$$

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with  $0 \leq \alpha < d/2$ ,  $\beta, \gamma, m > 0$  (it is really sufficient to have upper/lower bounds by these functions). The ultraviolet problem concerns the behaviour of the model at short distances. This corresponds to the behaviour for large  $\lambda$  after a unitary rescaling induced by  $f(x) \mapsto \lambda^{-d/2} f(x/\lambda)$ . The rescaled Hamiltonian has the form

$$H_\lambda = \lambda^\gamma \Omega(i\nabla_x) + \lambda^\beta d\Gamma(\omega_\lambda(i\nabla)) + \lambda^{d/2-\alpha} H_{\text{int}}, \quad (4.55)$$

with  $\omega_\lambda(k) = (m^{2/\beta} \lambda^{-2} + k^2)^{\beta/2}$ . For  $d/2 - \alpha < 0$  the Hamiltonian does not have an ultraviolet singularity, but an infrared (long distance) singularity. We may observe that for sub-critical scaling,

$$d/2 - \alpha < \max\{\gamma, \beta\}, \quad (4.56)$$

the growth of the interaction is small relative to that of the free part as  $\lambda \rightarrow \infty$ . We may thus expect that the problem can be treated perturbatively, in some sense. In the language of theoretical physics one would call such models super-renormalisable.

Taking  $\beta = \gamma$  for simplicity, we have the following picture:

- 1) We have  $\hat{v}(\Omega + \omega)^{-1/2} \in L^2(\mathbb{R}^d)$  if

$$d - 2\alpha < \gamma, \quad (4.57)$$

and the interaction defines a quadratic form on  $D(H_0^{1/2})$ . We explain how to construct the self-adjoint operator associated with the sum of the forms following [24] in Section 4.2.1.

- 2) We have  $\hat{v}(\Omega + \omega)^{-1} \in L^2(\mathbb{R}^d)$  if

$$d - 2\alpha < 2\gamma. \quad (4.58)$$

The map  $a(v_x) : D(H_0) \rightarrow \mathcal{H}$  is continuous, so  $\mathring{H}_0 = H_0|_{\ker(a(v_x))}$  is a closed, symmetric operator. We can thus hope to construct  $H$  by IBCs on  $D(\mathring{H}_0^*)$ . For  $d - 2\alpha < 3\gamma/2$  the operator obtained in this way coincides with known renormalised versions of  $H$ , as we will explain in Section 4.2.2. In Section 4.2.3 we generalise this construction to models with  $3\gamma/2 < d - 2\alpha < 2\gamma$ , for which no renormalisation procedure was previously known.

- 3) The interaction is (super-) critical,  $v\Omega^{-1} \notin L^2(\mathbb{R}^d)$ , for

$$2\alpha + \gamma \leq d, \quad (4.59)$$

and it is not clear if  $H$  can be constructed. One may expect that  $\mathring{H}_0$  is essentially self-adjoint and thus the extension  $H_0 \subset \mathring{H}_0^*$  is trivial (as for  $-\Delta|_{H_0^2(\mathbb{R}^d \setminus \{0\})}$  in  $d \geq 4$ ).

### 4.2.1 Quadratic forms and the Fröhlich polaron

The Fröhlich Polaron models the interaction of one (or several) electrons with phonons in a solid. The Hamiltonian is of the general form (4.53) with  $\Omega(i\nabla) = -\Delta$ ,  $\omega \equiv 1$  and  $\hat{v}(k) = (4\pi|k|)^{-1}$ , i.e., we have

$$H_0 = -\Delta_x + \mathcal{N}, \quad H_{\text{int}} = a^*(|x - \cdot|^{-2}) + a(|x - \cdot|^{-2}). \quad (4.60)$$

In this section we characterise the domain of  $H$  in terms of IBCs and give a short proof of self-adjointness. This can easily be generalised to the general Hamiltonian (4.53) with  $2\alpha + \gamma > d$ ,  $\beta \geq 0$ ,  $m > 0$  (see [24] for a proof in the case  $\gamma = 2$ ).

The only necessary technical ingredient is the inequality

$$\|a(v_x)H_0^{-1/2}\Psi\|_{\mathcal{H}} \leq C\|(\mathcal{N} + 1)^{1/4}\Psi\|_{\mathcal{H}}, \quad (4.61)$$

which easily follows from the Cauchy-Schwartz inequality in Fourier representation.

With this, we know that the quadratic form corresponding to  $H$

$$Q(\Psi, \Psi) = \langle \Psi, H_0 \Psi \rangle + 2\text{Re}\langle \Psi, a(v_x) \Psi \rangle \quad (4.62)$$

is well defined on  $D(Q) = D(H_0^{1/2})$ . The form of the interaction is bounded relative to the free one. However, the relative bound is not necessarily less than one, so this does not immediately yield existence of a self-adjoint realisation  $H$ . This problem can be solved in a variety of ways (cf. [11]). We present here a solution based on IBCs that is rather simple and also illustrates well the structure of the arguments we use for more singular models in the upcoming sections.

In order to construct the self-adjoint operator  $H$  with quadratic form  $Q$ , we do not need to go through the full programme of restricting  $H_0$  to the kernel of  $a(v_x)$  and taking the adjoint  $\hat{H}_0^*$ . It is sufficient to parametrise directly a smaller extension that allows us to impose the boundary conditions.

Let  $G_z$ ,  $z \in \rho(H_0)$ , be the family of abstract Dirichlet operators (cf. 4.1.3), i.e.,

$$G_z = (a(v_x)(z - H_0)^{-1})^* \quad (4.63)$$

and denote  $G := G_{-1}$ . As an extended domain we consider

$$D = D(H_0) \oplus G\mathcal{H}. \quad (4.64)$$

We define the boundary operator  $B$  by  $BD(H_0) = 0$  and  $BG = 1$ , so the condition  $B\Psi = \Psi$  is equivalent to  $(1 - G)\Psi \in D(H_0)$ .

**Theorem 4.7.** *Define  $H$  by*

$$\begin{aligned} D(H) &= \left\{ \Psi \in D(H_0) \oplus G\mathcal{H} \mid (1 - G)\Psi \in D(H_0) \right\} \\ H &= (1 - G)^*(H_0 + 1)(1 - G) - a(v_x)(1 + H_0)^{-1}a^*(v_x) - 1. \end{aligned} \quad (4.65)$$

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Then  $H$  is self-adjoint,  $D(H^{1/2}) \subset D(H_0^{1/2})$ , and for all  $\Psi \in D(H)$

$$\langle \Psi, H\Psi \rangle = Q(\Psi, \Psi). \quad (4.66)$$

*Sketch of the proof.* From (4.61) one obtains that  $G$  is bounded and that  $\sum_{k=0}^{\infty} G^k$  converges in the strong operator topology. Hence  $(1 - G)$  is invertible with bounded inverse. This implies that  $D(H)$  is dense and

$$K = (1 - G)^*(H_0 + 1)(1 - G) \quad (4.67)$$

is invertible, in particular self-adjoint. Also from (4.61), we see that the ‘‘Dirichlet to Neumann’’ operator

$$T = a(v_x)G = -a(v_x)(H_0 + 1)^{-1}a^*(v_x) \quad (4.68)$$

is  $\mathcal{N}^{1/2}$ -bounded. Since  $(1 - G)^{-1}$  is also bounded on  $D(\mathcal{N})$  (by the same argument) and  $H_0 \geq \mathcal{N}$ , this implies that  $T$  is infinitesimally  $K$ -bounded, so  $H$  is self-adjoint and  $D(\mathcal{N}) \subset D(H)$ .

We have  $D(H^{1/2}) \subset D(H_0^{1/2})$  since by (4.61)  $G$  maps  $D(\mathcal{N}^{1/2}) \subset D(H^{1/2})$  to  $D(H_0^{1/2})$ . The equality of the forms then follows by expanding  $K$ , which yields

$$H = H_0 - \underbrace{G^*(H_0 + 1)}_{=-a(v_x)} - \underbrace{(H_0 + 1)G}_{=-a^*(v_x)} + \underbrace{G^*(H_0 + 1)G}_{=-T} + T = H_0 + a(v_x) + a^*(v_x). \quad (4.69)$$

□

**Remark 4.8.** Note that in the proof of Theorem 4.7 we have essentially just verified that  $T$  and  $G$  satisfy the technical hypothesis *i*), *ii*) from Section 4.1.3. In particular this shows that these hypothesis indeed imply self-adjointness, and after proving self-adjointness of  $H$  in this way we immediately obtain the large family of symmetric operators given in Theorem 4.4. For certain sub-classes of this family one can prove self-adjointness using that  $T \leq 0$  (compare [4, Sect.5], where local Robin conditions for a model in the same regularity class as the Fröhlich model are treated).

#### 4.2.2 The Nelson model

In this section we discuss the construction of the Nelson model using IBCs and the appropriate class to which this construction generalises. The Nelson model is of the form (4.53) with  $\Omega(p) = p^2$ ,  $\omega(k) = \sqrt{k^2 + m^2}$  and  $\hat{v} = \omega^{-1/2}$ . We thus have  $2\alpha + \gamma = 3$ , which equals  $d$  for the most interesting case.

In [33] Nelson showed that this model can be renormalised in the following sense: Let

$$H_\Lambda := -\Delta_x + d\Gamma(\omega) + a^*(v_{\Lambda,x}) + a(v_{\Lambda,x}) \quad (4.70)$$

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with the regularised interaction  $\hat{v}_\Lambda(k) = \omega(k)^{-1/2} 1_{|k| \leq \Lambda}$ . Let also

$$E_\Lambda = - \int_{|k| \leq \Lambda} \frac{dk}{\omega(k)(k^2 + \omega(k))} \quad (4.71)$$

and note that  $E_\Lambda \sim e \log \Lambda$  as  $\Lambda \rightarrow \infty$ . Then  $H_\Lambda - E_\Lambda$  converges in strong resolvent sense to a self-adjoint operator which we call  $H_{\text{ren}}$  (in fact, convergence holds in norm, see [12]). This shows that the model is truly singular and provides a construction for an operator that corresponds to the formal expression (4.53).

However, the operator  $H_{\text{ren}}$  is not very explicit, and Nelson put forward the problem of finding a direct description of  $H_{\text{ren}}$  and its domain, as well as determining whether  $D(H_{\text{ren}}) \cap D(H_0^{1/2}) = \{0\}$ . Such a description is provided by IBCs, and it is then straightforward to prove that indeed  $D(H_{\text{ren}}) \cap D(H_0^{1/2}) = \{0\}$  (see also [12] for a proof based on Nelson's construction). Moreover, the method lends itself to the generalisation for differential operators with non-constant coefficients, such as the Laplacian of a Riemannian manifold. This generalisation was carried out for the Nelson model in the master's thesis [17] (see [9] for a construction inspired by Nelson's method).

We start the construction as in the previous section by setting

$$G = -(a(v_x)(H_0 + 1)^{-1})^*, \quad (4.72)$$

where  $H_0 = -\Delta_x + d\Gamma(\omega)$ . One can check that  $G$  is bounded. The boundary operator  $B$  is again defined as the left inverse of  $G$ , and the natural domain for  $H$  is

$$D_{\text{IBC}} = \left\{ \Psi \in D(H_0) \oplus G\mathcal{H} \mid (1 - G)\Psi \in D(H_0) \right\}. \quad (4.73)$$

However, we are now faced with the problem that  $A = a(v_x)$  does not extend in a straightforward way to the range of  $G$ . We already encountered this problem in the minimal example of Section 4.1.1. There, we found a natural formula providing such an extension from an integration by parts. Here, the extension will be fixed in a way that ensures compatibility with Nelson's renormalisation procedure. This is naturally formulated in Fourier space, but after a Fourier transform still corresponds to expanding functions in the range of  $G$  near the singular set of collision configurations between the bosons and the particle (the singularities are of the form  $\mathcal{F}(k^2 + \omega)^{-1} \omega^{-1/2} \sim |x|^{-1/2}$ , in this case).

An extension of  $A$  to the range of  $G$  is determined by specifying the, possibly unbounded, operator  $T = AG$ . A priori, we can just choose for  $T$  any symmetric operator, but this might not correspond to the model we wish to construct. To single out a choice of  $T$ , consider the regularised model, where

$$T_\Lambda = -a(v_{\Lambda,x})(H_0 + 1)^{-1} a(v_{\Lambda,x})^* \in \mathcal{B}(\mathcal{H}). \quad (4.74)$$

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In Fourier representation we can write

$$T_\Lambda = - \int_{|k| \leq \Lambda} \int_{|\ell| \leq \Lambda} e^{k \nabla_p} a_k \frac{\hat{v}(k) \hat{v}(\ell)}{p^2 + d\Gamma(\omega) + 1} a_\ell^* e^{-\ell \nabla_p} dk d\ell, \quad (4.75)$$

where  $e^{k \nabla_p}$  is the translation group in  $p$ , the dual variable to  $x$ . Rearranging terms and putting  $a_k, a_\ell^*$  into normal order, we obtain

$$\begin{aligned} T_\Lambda &= - \int_{|k| \leq \Lambda} \int_{|\ell| \leq \Lambda} \frac{\hat{v}(k) \hat{v}(\ell)}{(p-k)^2 + \omega(k) + d\Gamma(\omega) + 1} a_k a_\ell^* e^{(k-\ell) \nabla_p} dk d\ell \\ &= - \int_{|k| \leq \Lambda} \frac{\hat{v}(k)^2}{(p-k)^2 + \omega(k) + d\Gamma(\omega) + 1} dk \end{aligned} \quad (4.76)$$

$$- \int_{|k| \leq \Lambda} \int_{|\ell| \leq \Lambda} a_\ell^* \frac{\hat{v}(k) \hat{v}(\ell)}{(p-k)^2 + \omega(k) + \omega(\ell) + d\Gamma(\omega) + 1} a_k e^{(k-\ell) \nabla_p} dk d\ell. \quad (4.77)$$

Note that the integral in (4.76) diverges for  $\Lambda \rightarrow \infty$  in the same way as  $E_\Lambda$  above, which is essentially the value of the integral at  $p = 0$  and restricted to the zero-boson space. After subtracting this number, the integral becomes convergent also for  $\Lambda = \infty$ . We thus set for  $\Lambda \in \mathbb{R}_+ \cup \{\infty\}$

$$\Theta_{\Lambda,0} = - \int_{|k| \leq \Lambda} \left( \frac{\hat{v}(k)^2}{(p-k)^2 + \omega(k) + d\Gamma(\omega) + 1} - \frac{\hat{v}(k)^2}{k^2 + \omega(k)} \right) dk. \quad (4.78)$$

One can also show that the expression (4.77) makes sense as an unbounded operator when  $\Lambda = \infty$ , since the integral can be made convergent by using decay of  $a_k \Psi$  in  $k$ . Denote this operator by  $\Theta_{\Lambda,1}$ ,  $\Lambda \in \mathbb{R}_+ \cup \{\infty\}$ .

Note that under scaling as in (4.55),  $\Theta_{\infty,0}$ ,  $\Theta_{\infty,1}$  behave as  $\lambda^{d-2\alpha-\gamma} = \lambda^0$  (formally, each  $a$ ,  $a^*$  contributes  $\lambda^{d/2-\alpha}$  and  $H_0^{-1}$  contributes  $\lambda^{-\gamma}$ ), which corresponds to the (logarithmic) growth of  $E_\Lambda$ . We thus expect these operators to be (almost) bounded, which is made precise by the following key Lemma (compare [24, Sect.3], [21, Sect.A]):

**Lemma 4.9.** *For  $0 < \varepsilon \leq 1/2$  there exists  $C > 0$  so that for all  $\Psi \in D(H_0^\varepsilon) \cap D(\mathcal{N})$  the inequalities*

$$\begin{aligned} \|\Theta_{\infty,0} \Psi\| &\leq C \|H_0^\varepsilon \Psi\| \\ \|\Theta_{\infty,1} \Psi\| &\leq C \|\mathcal{N}^{1-2\varepsilon} H_0^\varepsilon \Psi\| \end{aligned}$$

hold.

We thus define  $T = \Theta_{\infty,0} + \Theta_{\infty,1}$ ,  $D(T) = D(H_0^\varepsilon) \cap D(\mathcal{N})$  and this gives an extension of  $A$  to  $GD(T)$ .

**Theorem 4.10.** *The operator*

$$H = (1 - G^*)(H_0 + 1)(1 - G) + T - 1$$

*is self-adjoint on  $D(H) = D_{\text{IBC}}$ . Moreover, we have  $H = H_{\text{ren}}$ .*

This theorem also covers the massless case,  $\omega(k) = |k|$ , [36, 21] and can be generalised to the case where  $-\Delta$ ,  $\omega$  are replaced by (pseudo-) differential operators with non-constant coefficients [17].

The proof of self-adjointness follows the same steps as Theorem 4.7, using Lemma 4.9 to show that  $T$  is infinitesimally bounded relative to the first term in  $H$ , which essentially amounts to bounding  $TG$  relative to  $\mathcal{N}$ . This relative bound holds only for models that are not too singular. The proof in [24] covers all (massive) models with  $\gamma = 2 \geq \beta \geq 0$  and

$$\alpha > \frac{1}{2} - \frac{\beta^2}{8 + \beta^2} \tag{4.79}$$

in  $d = 3$  dimensions. Schmidt [35] gave a generalisation to models with  $\gamma \neq 2$ . These limits can be improved if one is content with a relative form-bound for  $T$ , in which case one obtains less explicit information on  $D(H)$ . However, a modified construction does give bounds in the sense of operators and an explicit domain, see Remark 4.12.

The equality of  $H$  and  $H_{\text{ren}}$  is a simple consequence of the fact that one can write, with the analogous definition of  $G_\Lambda$ ,

$$H_\Lambda = (1 - G_\Lambda^*)(H_0 + 1)(1 - G_\Lambda) + T_\Lambda - 1, \tag{4.80}$$

and  $T = \lim_{\Lambda \rightarrow \infty} (T_\Lambda - E_\Lambda)$  (in the norm of  $B(D(T), \mathcal{H})$ ).

### 4.2.3 Strongly singular Hamiltonians

There are cases in which the interaction is too singular for both Nelson's renormalisation procedure and the IBC construction of the previous section to work, while still being in the sub-critical class with  $v\Omega^{-1} \in L^2(\mathbb{R}^d)$ .

An important example of such a model is the Bogoliubov-Fröhlich model for an impurity particle interaction with the excitations of a Bose-Einstein condensate in three dimensions. The formal Hamiltonian for this model is composed of

$$H_0 = -\Delta_x + d\Gamma(\omega), \tag{4.81}$$

where  $\omega(k) = \sqrt{k^4 + c^2 k^2}$  is the Bogoliubov dispersion of the excitations, and

$$H_{\text{int}} = a(v_x) + a^*(v_x), \quad \hat{v}(k) = \sqrt{\frac{k^2}{\omega(k)}} \tag{4.82}$$



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is the interaction obtained from the  $\delta$ -interaction through a Bogoliubov transformation. In terms of the scaling parameters we have  $d = 3$ ,  $\gamma = \beta = 2$ ,  $\alpha = 0$ . Note that this is the same behaviour as for the van Hove model considered in Section 4.1.2, which would correspond to the case of an immobile impurity of “infinite mass”.

To see why the method of the previous section cannot be applied to this model as such, consider the quadratic form of  $H$  in the representation of Theorem 4.10

$$\begin{aligned} \langle \Psi, H\Psi \rangle &= \langle (1 - G)\Psi, (H_0 + 1)(1 - G)\Psi \rangle + \langle \Psi, T\Psi \rangle - \|\Psi\|^2 \\ &= \langle (1 - G)\Psi, (H_0 + T + 1)(1 - G)\Psi \rangle \\ &\quad + 2\operatorname{Re}\langle (1 - G)\Psi, TG\Psi \rangle + \langle G\Psi, TG\Psi \rangle - \|\Psi\|^2 \end{aligned} \quad (4.83)$$

and note that the first term allows us to control  $H_0^{1/2}(1 - G)\Psi$ .

The scaling behaviour of  $T$  (compare (4.55)) is  $\lambda^{d-2\alpha-\beta} = \lambda$ , which corresponds to that of  $H_0^{1/2}$  and one can indeed show that  $T$  is  $H_0^{1/2}$ -bounded by generalising Lemma 4.9. Thus,  $T(1 - G)\Psi$  is under control. However, the scaling of  $G^*TG$  is  $\lambda^{2d-4\alpha-3\beta} = \lambda^0$  (there are two of each  $a, a^*$  contributing  $\lambda^{d/2-\alpha}$ , and three resolvents contributing  $\lambda^{-\beta}$ ), which is a critical case. Indeed, for regular  $\Psi$ ,  $G\Psi$  behaves as  $|x - y|^{-1}$  for  $|x - y| \rightarrow 0$ , and applying  $H_0^{1/2}$  leads to  $|x - y|^{-2}$  which cannot be paired with another function behaving as  $|x - y|^{-1}$ , i.e.,  $\langle G\Psi, TG\Psi \rangle$  does not seem to make sense at all (see [20] for a detailed analysis in a simplified model).

This problem can be approached by trying to include  $T$  with  $H_0$  in some way, as it is  $H_0^{1/2}$ -bounded. Set  $\tilde{H}_0 = H_0 + T$ , which is self-adjoint on  $D(H_0)$ , and, for  $z \in \rho(\tilde{H}_0)$ ,  $\tilde{G}_z = (a(v_x)(z - \tilde{H}_0)^{-1})^*$ . Then on a formal level we have

$$H_0 + H_{\text{int}} = (1 - \tilde{G}_z^*)(\tilde{H}_0 - z)(1 - \tilde{G}_z) + a(v_x)(z - \tilde{H}_0)^{-1}a^*(v_x) - T + z. \quad (4.84)$$

Recall that  $T$  was constructed as a renormalised version of  $a(v_x)(-1 - H_0)^{-1}a^*(v_x)$ , so we can expect cancellations to occur with  $a(v_x)(z - \tilde{H}_0)^{-1}a^*(v_x)$ . Our guess for the domain  $D(H)$  would now be given by the condition  $(1 - \tilde{G}_z)\Psi \in D(H_0)$ . The functions in this domain have singularities of the form  $a|x - y|^{-1} + b \log|x - y|$  as  $|x - y| \rightarrow 0$  (see [20]), which shows that this gives a different domain than the condition  $(1 - G)\Psi \in D(H_0)$ , for which there is no logarithmic term.

To make this approach rigorous, one can set  $T =: T_1$  and construct an operator  $T_2$  that is a renormalised version of

$$a(v_x)(1 + H_0)^{-1}T_1(1 + H_0)^{-1}a^*(v_x) \quad (4.85)$$

by the same procedure as for  $T_1$ , i.e., putting creation/annihilation operators into normal order and subtracting the value of the term with no remaining creation/annihilation operators after replacing  $p \mapsto 0$ ,  $d\Gamma(\omega) \mapsto 0$ . There will also be a remainder  $R_z$ , given by the difference of  $T_2$  and the expression in (4.84)

With this, we obtain the following result [18, 19, 22].

## 4.2 Polaron models in non-relativistic quantum field theory

**Theorem 4.11.** *Let  $z \in \mathbb{R} \cap \rho(H_0 + T_1)$  and set*

$$\begin{aligned} H &= (1 - \tilde{G}_z^*)(H_0 + T - z)(1 - \tilde{G}_z) + T_2 + R_z + z \\ D(H) &= \left\{ \Psi \in \mathcal{H} \mid (1 - \tilde{G}_z)\Psi \in D(H_0) \right\}. \end{aligned}$$

*The following hold true:*

- 1)  *$H$  is self-adjoint and bounded from below.*
- 2) *There is a family  $(E_\Lambda)_{\Lambda \geq 0} \subset \mathbb{R}$  so that the operators  $H_\Lambda$  with ultraviolet cutoff  $\Lambda$  satisfy*

$$\lim_{\Lambda \rightarrow \infty} (H_\Lambda - E_\Lambda) = H \tag{4.86}$$

*in the norm resolvent sense.*

- 3) *For  $\Psi \in D(H)$  we have the identity*

$$H\Psi = H_0\Psi + a^*(v_x)\Psi + A\Psi, \tag{4.87}$$

*as elements of  $D(H_0)'$ , where  $A|_{D(H_0)} = a(v_x)$  and  $A\tilde{G}_z = (T_1 + T_2 + R_z)$ .*

Self-adjointness for the case  $\alpha = 0$ ,  $\beta = \gamma = 2$  of the Bogoliubov-Fröhlich model was proved in [18] by finding appropriate bounds on  $T_2$ ,  $R$ . The second statement on renormalisation was first proved in [19]. The asymptotics of  $E_\Lambda$  are given by

$$E_\Lambda = E_{\Lambda,1} + e_2 \log \Lambda + O(1), \tag{4.88}$$

where  $E_{\Lambda,1}$  has the same expression (4.71) as in the Nelson model (which is asymptotic to  $e_1\Lambda$  in this case). This is consistent with our expectation based on the scaling heuristics. The number  $e_2$  can be calculated explicitly (see [19]). It depends essentially on the mass  $M$  of the impurity and vanishes for  $M \rightarrow \infty$ , which explains why no logarithmic term is present in Section 4.1.2.

The third statement shows that  $H$  has the form we originally assumed, up to a choice of domain and definition of  $A$  on this domain. However, now  $A$  cannot be viewed as an extension of  $a(v_x)$  since  $T_1$  is not defined on  $D(H)$  and thus  $A\Psi$  is really an element of  $D(H_0)'$ . The modification of the domain arranges for the term  $T_1\Psi$  from  $A$  to cancel with a singularity created by application of  $H_0$ .

In [22], Theorem 4.11 is generalised to models with  $\beta = \gamma \in \{1, 2\}$  and

$$d - 2\alpha < 2\gamma, \tag{4.89}$$

which covers the whole sub-critical regime (with additional technical hypothesis of rotation invariance and differentiability). For this, one proceeds in  $n$  steps, with

$$n = \left\lfloor \gamma(2\alpha + 2\gamma - d)^{-1} \right\rfloor = \max \left\{ n \in \mathbb{N} : n(2\alpha + 2\gamma - d) \leq \gamma \right\}, \tag{4.90}$$

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i.e.,  $n = 1$  for the Nelson model,  $n = 2$  for Bogoliubov-Fröhlich. One constructs operators  $T_1, \dots, T_n$  and sets  $\tilde{H}_0 = H_0 + T_1 \cdots + T_n$ . The result is then analogous to Theorem 4.11 (inclusion of  $T_2$  into  $\tilde{H}_0$  in this case only changes the form of  $R$ ). In principle, one can apply the same construction for  $\beta \neq \gamma$ . The case  $\beta > \gamma$  poses no difficulties. If  $\beta < \gamma$  however, there will be an additional difficulty in controlling the operators  $T$  with respect to the number of bosons, since relying on  $\Omega(i\nabla)$  for regularity leads to bounds that grow with this number, as in Lemma 4.9. The condition under which the construction works will thus depend on  $d, \alpha, \beta, \gamma$  in a more complicated way, similarly to (4.79) for  $n = 1$ .

The scaling of  $T_j$  is  $\lambda^{j(d-2\alpha-2\gamma)+\gamma}$ , and  $n$  is exactly the largest number for which the exponent is non-negative. If we make explicit the coupling constant  $g$  to  $H_{\text{int}}$ , the numbers  $E_\Lambda$  to be subtracted for renormalisation have the form (with the understanding that  $\Lambda^0$  should be  $\log \Lambda$ )

$$E_\Lambda = \sum_{j=1}^n e_j g^{2j} \Lambda^{j(d-2\alpha-2\gamma)+\gamma} + \mathcal{O}(1). \quad (4.91)$$

This shows clearly the perturbative nature of the construction. Indeed, one can think of  $T = \sum_{j=1}^n T_j$  as an approximate solution to the equation

$$a(v_x)(z - H_0 - T)^{-1} a^*(v_x) = T + E, \quad (4.92)$$

suggested by (4.84). Using this equation it might be possible to generalise to specific models with critical scaling, at least for small coupling. An interesting example would be the pseudo-relativistic Nelson model studied in [13, 5], where  $\gamma = \beta = 1$ ,  $\alpha = 1/2$  and  $d = 3$ .

**Remark 4.12.** Note that when  $T_1$  is form-bounded by  $(1 - G^*)H_0(1 - G)$ , the expression (4.85) is well defined. In this case Theorem 4.11 yields the operator domain and  $E_\Lambda = E_{\Lambda,1} + O(1)$ . This is analogous to the construction of the Fröhlich polaron in Section 4.2 after  $n = 1$  steps.

### 4.3 Applications to spectral theory

In the previous section we discussed how to define rigorously polaron Hamiltonians and provided explicit expressions for the resulting operator and domain. These expressions can be used to analyse the spectrum of the operator. One advantage of this approach compared to the definition by renormalisation, i.e., as limit of regularised operators, is that it avoids the need to control a whole family of operators uniformly in the cutoff parameter.

**Positivity.** An example in which this has been put to use is the property of specific polaron models to improve positivity. This property is an important tool for further analysis of the spectrum, implying in particular that the ground state (if it exists) is simple. It was proved using the IBC representation for the Nelson model in [21] and the Fröhlich polaron in [23].

A bounded operator  $A$  on a Hilbert space  $\mathcal{H}$  is said to preserve positivity with respect to a Hilbert cone  $\mathcal{C}$  if  $A\mathcal{C} \subset \mathcal{C}$ . It improves positivity if for all non-zero  $\varphi, \psi \in \mathcal{C}$  one has  $\langle \varphi, A\psi \rangle > 0$ . For a semi-bounded operator  $H$  one can consider either the resolvent or the exponential and by equivalent definitions (see [34, Thm.XIII.44])  $H$  preserves/improves positivity if its resolvent or exponential do (for appropriate parameters).

We will first present an abstract form of the arguments used in [21, 23] and then explain briefly how these are applied in the specific context. We consider the Hilbert space

$$\mathcal{H} = \mathcal{H}_p \otimes \Gamma(L^2(\mathbb{R}^d)), \quad (4.93)$$

where  $\mathcal{H}_p$  is an auxiliary Hilbert space for the particle(s). Let  $\mathcal{C}_p \subset \mathcal{H}_p$  be a Hilbert cone, and define the cone of positive elements in  $\mathcal{H}$  as

$$\mathcal{C}_+ := \left\{ \Psi \in \mathcal{H} = \bigoplus_{n=0}^{\infty} \mathcal{H}^{(n)} \mid \forall n \in \mathbb{N}_0, \forall \varphi \in \mathcal{C}_p : \langle \varphi, \Psi^{(n)} \rangle_{\mathcal{H}_p} \geq 0 \text{ a.e. in } \mathbb{R}^{dn} \right\}. \quad (4.94)$$

The operators constructed in the previous section are of the form

$$H = \underbrace{(1 - G^*)H_0(1 - G)}_{=:K} + T, \quad (4.95)$$

with  $H_0 \geq 1$  and

$$G^* = a(-v_x)H_0^{-1}. \quad (4.96)$$

With this formula, if  $v < 0$  and  $H_0^{-1}$  preserves positivity, then  $G, G^*$  are positivity preserving. Moreover, if  $\Phi^{(n)} \geq 0$  is not identically zero, then  $a(-v_x)\Phi^{(n)}$  is also not zero, since it is given by the integral over a non-negative function that does not vanish everywhere.

In the abstract setting, we can formulate the following Lemma.

**Lemma 4.13.** *Assume  $G^*$  is a bounded operator with norm less than one that preserves positivity and maps  $\mathcal{H}^{(n)}$  to  $\mathcal{H}^{(n-1)}$  so that  $\Psi \in \mathcal{C}_+$  and  $G^*\Psi^{(n)} = 0$  for some  $n \in \mathbb{N}$  imply  $\Psi^{(n)} = 0$ . If  $H_0^{-1}$  is positivity preserving and its restriction to  $\mathcal{H}^{(0)}$  improves positivity, then  $K^{-1}$  improves positivity.*

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*Proof.* Clearly  $K^{-1} = (1 - G)^{-1}H_0^{-1}(1 - G^*)^{-1}$  preserves positivity. Take non-zero  $\Phi, \Psi \in \mathcal{H}$  and let  $n, m \in \mathbb{N}_0$  be so that  $\Phi^{(n)}, \Psi^{(m)} \neq 0$ . Then  $(G^*)^n \Phi^{(n)}, (G^*)^m \Psi^{(m)}$  are non-zero elements of  $\mathcal{H}^{(0)}$ . Since  $H_0^{-1}|_{\mathcal{H}^{(0)}}$  improves positivity, we may neglect some non-negative terms to obtain

$$\begin{aligned} \langle \Phi, K^{-1}\Psi \rangle_{\mathcal{H}} &= \sum_{j,k=0}^{\infty} \left\langle (G^*)^j \Phi, H_0^{-1}(G^*)^k \Psi \right\rangle \\ &\geq \left\langle (G^*)^n \Phi^{(n)}, H_0^{-1}(G^*)^m \Psi^{(m)} \right\rangle_{\mathcal{H}^{(0)}} > 0, \end{aligned} \quad (4.97)$$

which proves the claim.  $\square$

**Proposition 4.14.** *Let  $G^*, H_0$  satisfy the conditions of Lemma 4.13. If for  $\lambda$  sufficiently large,*

$$-T(K + \lambda)^{-1}$$

*is bounded of norm less than one and positivity preserving, then  $(H + \lambda)^{-1}$  improves positivity for all  $\lambda > -\inf \sigma(H)$ .*

*Proof.* By the assumed bound, we have for  $\lambda$  large enough

$$(K + T + \lambda)^{-1} = (K + \lambda)^{-1} \sum_{k=0}^{\infty} (-T(K + \lambda)^{-1})^k. \quad (4.98)$$

The resolvent of  $K$  near zero can be written as a power series whose terms are positivity improving. By analytic continuation,  $(K + \lambda)^{-1}$  improves positivity. Thus the summand with  $k = 0$  in (4.98) is positivity improving and by hypothesis all the others preserve positivity. This proves the claim for sufficiently large  $\lambda$ , and this extends to all  $\lambda > -\inf \sigma(H)$  by analyticity.  $\square$

In the article [23] we use these ideas to prove absence of a ground state and uniqueness of the minimum of the effective dispersion relation for the Fröhlich model discussed in Section 4.2.1. The proof is by contradiction following ideas of [10]. Assuming that there is a momentum  $P \neq 0$  so that the ground state energy of the Hamiltonian  $H(P)$  at fixed total momentum  $P$  is a minimum among all  $P$ , one concludes that an auxiliary operator, which is similar to the Fröhlich Hamiltonian but with the particle space  $\mathcal{H}_p = L^2(\mathbb{R}^3/(L\mathbb{Z})^3)$ ,  $LP \in 2\pi\mathbb{Z}^3$ , must have a degenerate ground-state. One arrives at the sought-after contradiction by proving that the auxiliary operator improves positivity (which implies that the ground state is simple) using the arguments above. The required conditions are easy to check. In particular,  $T$  is an operator with negative kernel (compare (4.68)).

The result of [21] is that the Nelson Hamiltonian at fixed total momentum improves positivity in Fourier representation. Fixing the momentum removes the center of mass,

so in this case  $\mathcal{H}_p = \mathbb{C}$ . This result was announced in [8], but the first complete proof appeared only much more recently [28]. The difficulty was that, defining  $H$  by renormalisation, it is clear that it preserves positivity if this holds for the cutoff Hamiltonians (since Hilbert cones are closed) but showing that the limit remains strictly positive is more subtle. In the proof of [21] using the representation of Theorem 4.10, this difficulty shows itself in the fact that  $-T$  no longer preserves positivity as the Fourier multiplier  $\Theta_{\infty,0}$  has a non-trivial positive part. The solution lies in including this positive part with  $H_0$  as done for the more singular models of Section 4.2.3. With the modified choices of  $H_0$ ,  $G$ , and  $T$  the proof then follows from Proposition 4.14.

**Eigenvectors.** Knowledge of the domain of self-adjointness is also useful for the construction of (approximate) eigenvectors. The recent preprint [14] proves that the Bogoliubov-Fröhlich Hamiltonian at fixed momentum  $P$  has a ground state if  $|P| \leq c/M$ , where  $M$  is the particle mass and  $c$  the speed of sound in the condensate (compare (4.81) and Section 6.1). This ground state corresponds to a stable polaron quasi-particle. This particle may move freely without exciting additional bosons, as long as its momentum does not exceed  $c/M$ , which is a manifestation of the superfluidity of the underlying condensate.

Our proof makes use of the information on the domain obtained from the construction of the Hamiltonian in [19] (see Section 4.2.3) in order to construct trial states. Thanks to this construction and a-priori estimates on the dependence of the energy on the momentum, the result does not require an ultra-violet cutoff, nor a small coupling assumption.

It would be interesting to prove the non-existence of a ground state eigenvector for  $|P| > p_c$  for a critical momentum  $p_c$ . There is numerical evidence for this [39], but the mathematical problem remains a challenge.

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## 5 A model for plasmons in a finite medium

Plasmons, or polaritons, are the joint excitations of the electro-magnetic field and internal degrees of freedom of a material, for example a metal. Their properties differ from those of free photons, even outside of the medium. This may give rise to measurable effects, such as the enhancement of spontaneous emission by atoms and molecules, similar to the Purcell effect in a cavity.

In this chapter I discuss a specific model for the electro-magnetic quantum field interacting with a finite-size dielectric medium. For this model, one can use methods from mathematical scattering theory to exhibit the structure of the joint excitations and provide explicit formulas (that can be treated numerically [9], and analytically [12]) for important quantities, such as the electric field operator. In addition to summarising the results of [4], I provide in the final section a sketch of the mathematical proofs that were omitted there.

### 5.1 Discussion of the model

In our microscopic model, the electro-magnetic field interacts with a medium occupying some region of space by coupling to the elementary vibrations of charges in the material. Such models are often employed in physics, thanks to their relative simplicity and the fact that they can be related to the macroscopic Maxwell equations with, in general, complex and frequency-dependent susceptibilities. Note that one cannot base the discussion directly on the macroscopic Maxwell equations since they are, in general, not Hamiltonian and it is thus unclear how they relate to a quantum-mechanical model.

We start by discussing the model on the level of classical fields, which also serves to fix the parameters in relation to known properties of the material. Matter will be included into the model in the form of a field of oscillating charges. For every  $\nu > 0$ , corresponding to the frequency of the oscillation, let  $X_\nu$  be a field, i.e.  $X_\nu : M \rightarrow \mathbb{R}^3$  is a function, where  $M \subset \mathbb{R}^3$  is the region of space occupied by the matter, which we assume to be compact. These fields are coupled to the electro-magnetic field by assigning to their configuration the polarisation density

$$\mathcal{P}(x) = \int_0^\infty \alpha(x, \nu) X_\nu(x) d\nu, \quad (5.1)$$

with a (real valued) function  $\alpha$  modeling the strength of the coupling to the medium. The form of  $\mathcal{P}$  corresponds to the assumption that the medium is isotropic, as oth-

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erwise  $\alpha$  would be a tensor. We also neglect a possible magnetic response, which could be included via an additional magnetisation field [10]. To the polarisation one associates charge and current densities by

$$\rho = -\operatorname{div} \mathcal{P}, \quad j = \frac{\partial \mathcal{P}}{\partial t}. \quad (5.2)$$

The coupled system of equations for the electric and magnetic fields  $E, B$ , and  $(X_\nu)_{\nu>0}$  reads

$$\frac{\partial E}{\partial t} = \operatorname{curl} B - \frac{\partial \mathcal{P}}{\partial t} \quad (5.3a)$$

$$\frac{\partial B}{\partial t} = -\operatorname{curl} E \quad (5.3b)$$

$$\operatorname{div} E = -\operatorname{div} \mathcal{P} \quad (5.3c)$$

$$\operatorname{div} B = 0 \quad (5.3d)$$

$$\frac{\partial^2 X_\nu}{\partial t^2} = -\nu^2 X_\nu + \alpha(\nu)E. \quad (5.3e)$$

This is a system of linear equations of Hamiltonian type, as made explicit in Equation (5.12) below.

**The macroscopic Maxwell equations.** One justification for using this model, and a way to determine the choice of coupling  $\alpha$  in a given situation, is its relation to the macroscopic Maxwell equations in the material. We can eliminate the fields  $X_\nu$  by substituting the solution of (5.3e) that vanishes as  $t \rightarrow -\infty$

$$X_\nu(t, x) = \int_{-\infty}^t \frac{\sin(\nu(t-s))}{\nu} \alpha(x, \nu) E(s, x) ds, \quad (5.4)$$

which gives

$$\mathcal{P}(t, x) = \int_0^\infty \int_{-\infty}^t \frac{\sin(\nu(t-s))}{\nu} \alpha^2(x, \nu) E(s, x) d\nu ds. \quad (5.5)$$

Taking the Fourier transform in the time variable yields

$$\hat{\mathcal{P}}(\omega, x) = \hat{E}(\omega, x) \left( \text{p.v.} \int_0^\infty \frac{\alpha(x, \nu)^2 d\nu}{\nu^2 - \omega^2} + \frac{i\pi}{2} \frac{\alpha^2(x, |\omega|)}{\omega} \right), \quad (5.6)$$

where p.v. is the Cauchy principal value. Equations (5.3a) and (5.3c) can be seen as Maxwell's equations for the displacement field  $D = E + \mathcal{P}$ . The Fourier transform of  $D$  is

$$\hat{D}(\omega, x) = \hat{E}(\omega, x) \left( 1 + \text{p.v.} \int_0^\infty \frac{\alpha(x, \nu)^2}{\nu^2 - \omega^2} d\nu + \frac{i\pi}{2} \frac{\alpha^2(x, |\omega|)}{\omega} \right) =: \epsilon(\omega, x) \hat{E}(\omega, x), \quad (5.7)$$

which defines the dielectric function  $\epsilon(x, \omega)$ . In practice, given some material whose effective dielectric function  $\epsilon$  is known, one can choose  $\alpha$  so as to reproduce this function (note that  $\alpha^2$  is completely determined by the imaginary part of  $\epsilon$ ). Two functional forms for  $\alpha$  that are often used in physics are the Lorentz model

$$\alpha(x, \omega) = \frac{\omega}{\sqrt{a^2(\omega^2 - \omega_0^2)^2 + b^2\omega^2}} 1_M(x) \quad (5.8)$$

and the Drude model

$$\alpha(x, \omega) = \frac{1}{\sqrt{a^2\omega^2 + b^2}} 1_M(x), \quad (5.9)$$

where  $a, b, \omega_0 > 0$  are free parameters, and  $1_M$  is the characteristic function of the compact set  $M \subset \mathbb{R}^3$ .

**The model in oscillator form.** Since the system of equations (5.3a)–(5.3e) is linear, we are essentially dealing with a free field theory. That is, the sum of two solutions is again a solution so localised wave-packets will pass through each other without interacting. In order to associate to these fields a quantum field, one should write the equations (or the Hamilton function) in ‘oscillator’ form [1], in complete analogy with the standard quantisation of the free electro-magnetic field. That is, we want to find a change of variables so that, expressed in terms of the new field  $\Psi$ , we have

$$\mathcal{H} = \langle \Psi, \Omega \Psi \rangle_{\mathfrak{H}} \quad (5.10)$$

for a Hilbert space  $\mathfrak{H}$  and a self-adjoint operator  $\Omega, D(\Omega)$  on  $\mathfrak{H}$ , and the symplectic form is

$$\sigma(\Psi, \Psi') = \text{Im} \langle \Psi, \Psi' \rangle_{\mathfrak{H}}. \quad (5.11)$$

The corresponding quantum theory is then defined on the Fock space  $\Gamma(\mathfrak{H})$  over  $\mathfrak{H}$  and its dynamics is generated by the Hamiltonian  $H = d\Gamma(\Omega)$ .

In terms of the vector potential  $A$  (in Coulomb gauge) and its conjugate momentum  $\Pi_A = -D$ , we can write a Hamiltonian for the system of equations as

$$\begin{aligned} \mathcal{H} = & \frac{1}{2} \int_{\mathbb{R}^3} \left( \Pi_A(x) + \int_0^\infty \alpha(x, \nu) X_\nu(x) d\nu \right)^2 - A(x) \Delta A(x) dx \\ & + \frac{1}{2} \int_{\mathbb{R}^3} \int_0^\infty (\Pi_{X_\nu}^2(x) + \nu^2 X_\nu^2(x)) d\nu dx, \end{aligned} \quad (5.12)$$

where  $\Delta$  is the vectorial Laplacian  $\Delta = \text{curl curl} - \text{grad div}$ , and thus  $\Delta A = \text{curl}^2 A$ . We now interpret the family  $X_\nu$  as one field  $X$  on  $M$ , taking values in  $L^2(\mathbb{R}_+, \mathbb{R}^3)$ ,

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and extend it to the whole of  $\mathbb{R}^3$  by zero. Setting  $\Phi = ((-\Delta)^{-1/2}\Pi_A, X) : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \times L^2(\mathbb{R}_+, \mathbb{R}^3)$  with conjugate momentum  $\Pi = (-(-\Delta)^{1/2}A, \Pi_X)$  brings  $\mathcal{H}$  into the form

$$\mathcal{H} = \frac{1}{2} \int_{\mathbb{R}^3} \Phi(x) \Omega^2 \Phi(x) dx + \frac{1}{2} \int_{\mathbb{R}^3} \Pi(x)^2 dx, \quad (5.13)$$

with the non-negative operator

$$\Omega^2 = \begin{pmatrix} \text{curl}^2 & (-\Delta)^{1/2} \langle \alpha(x, \cdot), \cdot \rangle_{L^2(\mathbb{R}_+)} \\ \alpha(x, \nu) (-\Delta)^{1/2} & \nu^2 + \alpha(x, \nu) \langle \alpha(x, \cdot), \cdot \rangle_{L^2(\mathbb{R}_+)} \end{pmatrix}, \quad (5.14)$$

Finally, we can move to the complex representation by setting

$$\Psi = \frac{1}{\sqrt{2}} \left( \Omega^{1/2} \Phi + i \Omega^{-1/2} \Pi \right), \quad (5.15)$$

and this gives the desired form (5.10). The natural Hilbert space  $\mathfrak{H}$  is the subspace of  $L^2(\mathbb{R}^3, \mathbb{C}^3 \times L^2(\mathbb{R}_+, \mathbb{C}^3))$  where the  $\mathbb{C}^3$ -component is divergence free, i.e., orthogonal to all gradient fields, and the second component has support in  $M$  (note that the appropriate spaces and the symplectic structure for the original fields can be defined by going backwards from here with the transformations given above). The domain of  $\Omega$  is discussed in Section 5.2.

**The quantum model of plasmons.** From the oscillator representation above, a model for quantum plasmons is defined on the Fock space over  $\mathfrak{H} = P_{\text{div}} L^2(\mathbb{R}^3, \mathbb{C}^3) \oplus L^2(M \times \mathbb{R}_+, \mathbb{C}^3)$ , where  $P_{\text{div}}$  is the projection to divergence-free fields, with Hamiltonian given by  $H = d\Gamma(\Omega)$ . This is the precise meaning of the often invoked quantisation rule by which one replaces the complex field  $\Psi$  by an annihilation operator and the complex conjugate field by a creation operator. The properties of the quantum plasmon Hamiltonian are completely encoded in the spectral theory of  $\Omega$ .

The Fock space can be identified with the tensor product of Fock spaces over  $\mathfrak{H}_1 = P_{\text{div}} L^2(\mathbb{R}^3, \mathbb{C}^3)$  and  $\mathfrak{H}_2 = L^2(M \times \mathbb{R}_+, \mathbb{C}^3)$ ,  $\Gamma(\mathfrak{H}_1 \oplus \mathfrak{H}_2) = \Gamma(\mathfrak{H}_1) \otimes \Gamma(\mathfrak{H}_2)$ , which intuitively corresponds to the degrees of freedom of the electro-magnetic field and the polarisation field, respectively. However, since  $\Omega$  is a two-by-two matrix operator with, in general, non-trivial off-diagonal entries,  $H = d\Gamma(\Omega)$  does not respect this decomposition. The simplest description of states would be in the spectral representation of  $\Omega$ , which does not have such a tensor structure.

The important question is of course how the interaction of the electro-magnetic field with matter affects the system, which is studied by comparing  $\Omega^2$  with its non-interacting counterpart

$$\Omega_0^2 = \begin{pmatrix} \text{curl}^2 & 0 \\ 0 & \nu^2 \end{pmatrix}. \quad (5.16)$$

The mathematical statement that forms the basis of the discussion in [4] is the following.

**Assertion 5.1.** *Let  $\rho$  be a smooth, rapidly decreasing function and denote by  $\Omega_\rho^2$  the operator  $\Omega^2$  with an ultra-violet cutoff function  $\rho$  on the interaction (see (5.26)). Let  $\alpha$  be of the Drude or Lorentz form (or satisfy the hypothesis of Theorem 5.3). Then*

- *the spectrum of  $\Omega_\rho$  equals  $[0, \infty)$  and is purely absolutely continuous;*
- *the wave operators  $W_\pm(\Omega_\rho^2, \Omega_0^2) := s\text{-}\lim_{t \rightarrow \mp\infty} e^{i\Omega_\rho^2 t} e^{-i\Omega_0^2 t}$  exist and are unitary.*

The precise statement is given in Theorem 5.3 below. The hypothesis are essentially assumptions on the coupling function  $\alpha$  that are compatible with both the Drude and the Lorentz form above. For technical reasons, one also needs to cut off the interaction at high energies of the electro-magnetic field with the cutoff  $\rho$ .

An immediate consequence is that the spectrum of  $\Omega$  is the same as that of  $\Omega_0$ , including multiplicity. This is important to keep in mind when writing down quantities by expanding into (generalised) eigenfunctions. In the physics literature, it has been suggested that the degeneracy should be lifted by the interaction. This intuition comes from the Friedrichs-Fano model, where an eigenvalue dissolves into a continuum, but is erroneous for the perturbation of continuous spectrum, which is described by scattering theory (see [13, 10, 3] for contributions to this debate in the physics literature).

A quantity of particular importance is the electric field operator outside of the medium  $M$ . For example, it describes the coupling of the electro-magnetic field to an atom outside the medium in the dipole approximation. At a point at  $x \notin M$ , the classical electric field  $E(x) = D(x)$  can be expressed in terms of the variables  $\Psi, \bar{\Psi}$  by

$$E(x) = D(x) = -\frac{1}{\sqrt{2}} \left( \Omega_0 \Omega^{-1/2} (\Psi + \bar{\Psi}) \right)_1, \quad (5.17)$$

where the index denotes projection to the first component. In general,  $\Omega^{-1/2}$  is not diagonal and a non-local operator. There is thus a contribution to the electric field outside of the medium that is induced by both components of the  $\Psi$ -field inside. The contribution of the second components of  $\Psi, \bar{\Psi}$  vanishes with the coupling  $\alpha$ . The expression for the field operator  $\mathbb{E}$  associated to  $E$  on the Fock space  $\Gamma(\mathfrak{H})$  is obtained by replacing the symbols  $\bar{\Psi}, \Psi$  with bosonic creation and annihilation operators. For the operator smeared with a regular function  $f \in L^2(\mathbb{R}^3, \mathbb{C}^3)$  this gives the expression

$$\mathbb{E}(f) = -\frac{1}{\sqrt{2}} \left( a(\Omega^{-1/2} \Omega_0(f, 0)) + a^*(\Omega^{-1/2} \Omega_0(f, 0)) \right) \quad (5.18)$$

Again, this operator is not of the form  $\Phi \otimes 1$  or  $1 \otimes \Phi$  in the tensor decomposition of the Fock space  $\Gamma(\mathfrak{H})$  and contains a term involving creation/annihilation operators of

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both factors. In the formulas suggested in [13, 10], based on the assumption of lifted degeneracy and an ansatz for the plasmon creation/annihilation operators, the terms with creation and annihilation operators for the first factor  $\Gamma(\mathfrak{H}_1)$  is absent. This leads to the issue that the formula does not reproduce the one of the electric field in vacuum when the coupling is set to zero. Pointing out and resolving this problem was the central point of our article [4]. Moreover, our construction of the wave operators is based on the solution of an integral equation that could be evaluated numerically in order to calculate generalised eigenfunctions of  $\Omega_\rho^2$  and gain information on the form the electric field and its coupling to matter.

**(In-)equivalence of the plasmon and photon representations.** The unitary equivalence of  $\Omega$  to  $\Omega_0$  shows that the quantum plasmon model with Hamiltonian  $H = d\Gamma(\Omega)$  and the model of decoupled photons and phonons with  $H_0 = d\Gamma(\Omega_0)$  behave the same from the spectral point of view. However, it would be misleading to identify both by using the unitary  $\Gamma(W_\pm)$ , as this does not correctly keep track of the physical meaning of quantities. For example, the electric field (5.18) is not the conjugation of the vacuum electric field  $\mathbb{E}_0$  by this unitary. The reason is, of course, that the relationship of these objects is determined by the relation of the classical fields. To correctly implement these in the quantum model, one has to consider the Hilbert spaces as representation spaces for the canonical commutation relations generated by these fields, on which the symplectic transformations act. Note that these transformations also depend on the interaction, e.g., by application of  $\Omega$ ,  $\Omega^{-1/2}$  in (5.15). Retracing the different changes of variables, one can spell out the relation between the fields  $\Psi$ ,  $\bar{\Psi}$  and their non-interacting analogues as

$$\Psi = \frac{1}{2} \left( (\Omega^{1/2} \Omega_0^{-1/2} + \Omega^{-1/2} \Omega_0^{1/2}) \Psi_0 + (\Omega^{1/2} \Omega_0^{-1/2} - \Omega^{-1/2} \Omega_0^{1/2}) \bar{\Psi}_0 \right), \quad (5.19)$$

with a similar formula for  $\bar{\Psi}$ . For the associated annihilation operators, this would correspond to a formula

$$a(f) = \frac{1}{2} a_0 \left( (\Omega_0^{-1/2} \Omega^{1/2} + \Omega_0^{1/2} \Omega^{-1/2}) f \right) + \frac{1}{2} a_0 \left( \overline{(\Omega_0^{-1/2} \Omega^{1/2} - \Omega_0^{1/2} \Omega^{-1/2}) f} \right) \quad (5.20)$$

The question of equivalence of these representations is thus whether there exists a unitary map  $U : \Gamma(\mathfrak{H}) \rightarrow \Gamma(\mathfrak{H})$ , called Bogoliubov transformation, so that  $U a_0^*(f) U^*$  satisfies the identity above. A unitary satisfying the relations

$$U a^*(f) U^* = a^*(Cf) + a(\bar{S}f), \quad U a(f) U^* = a(Cf) + a^*(\bar{S}f) \quad (5.21)$$

with bounded linear operators  $C, S$  exists if and only if

$$C^* C - S^* S = 1, \quad C^* \bar{S} - S^* \bar{U} = 0 \quad (5.22)$$

and  $S \in \mathfrak{S}^2(\mathfrak{H})$  is a Hilbert-Schmidt operator. The identities simply express the fact that  $Ua(f)U^*$  and  $Ua^*(f)U^*$  satisfy the canonical commutation relations. They are evidently satisfied in our case, and generally hold if the transformation arises from a symplectic transformation of the classical fields.

The condition that  $S$  be Hilbert-Schmidt is called the Shale condition. It relates to the transformation of the particle number operator under  $U$ . Indeed, the Hilbert-Schmidt norm is exactly the expectation value of the transformed number operator in the vacuum,

$$\langle \emptyset, UNU^* \emptyset \rangle = \sum_{j=1}^{\infty} \langle \emptyset, Ua^*(f_j)a(f_j)U^* \emptyset \rangle = \sum_{j=1}^{\infty} \langle \emptyset, a(\overline{Sf_j})a^*(\overline{Sf_j}) \emptyset \rangle = \text{Tr}(S^*S). \quad (5.23)$$

We should not expect the Shale condition to be satisfied for  $S = \Omega_0^{-1/2}\Omega^{1/2} - \Omega_0^{1/2}\Omega^{-1/2}$ , since  $\Omega^2$  is not a relatively compact perturbation of  $\Omega_0^2$ , due to the self-interaction of the polarisation field, which acts like a multiplication operator in  $x \in M$  (see the next section). If we compare  $\Omega_0^2$  to the operator where this self-interaction has been removed by application of a wave-operator (see (5.36)), the corresponding operator  $S$  should satisfy the Shale condition, at least with the cutoff  $\rho$  on the interaction with the electro-magnetic field.

## 5.2 Mathematical results

In this section we formulate the exact mathematical hypothesis for the main result, the existence and unitarity of the wave operators  $W_{\pm}(\Omega^2, \Omega_0^2)$  stated in Theorem 5.3 and sketch the proof.

**Self-adjointness.** First, it is necessary to properly define  $\Omega^2$ . To start with,  $\Omega_0^2$  is self-adjoint on the domain  $D(\Omega_0^2) = P_{\text{div}}H^2(\mathbb{R}^3, \mathbb{C}^3) \oplus L^2(M, L^2(\mathbb{R}_+, \nu^2 d\nu))$ . Its spectrum is purely absolutely continuous and covers  $[0, \infty)$ .

To control the interaction, it is convenient to assume that  $\nu \mapsto \alpha(x, \nu)$  is in  $L^2(\mathbb{R}_+)$ , uniformly in  $x$ , which is satisfied for both the Drude and the Lorentz model.

**Lemma 5.2.** *Assume  $\alpha \in L^\infty(\mathbb{R}^3, L^2(\mathbb{R}_+))$ , then  $\Omega^2 - \Omega_0^2$  is infinitesimally form bounded with respect to  $\Omega_0^2$ .*

*Proof.* We have

$$\Omega^2 - \Omega_0^2 = \begin{pmatrix} 0 & (-\Delta)^{1/2} \langle \alpha(x, \cdot), \cdot \rangle \\ \alpha(x, \cdot) (-\Delta)^{1/2} & \alpha(x, \cdot) \langle \alpha(x, \cdot), \cdot \rangle \end{pmatrix}. \quad (5.24)$$



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The lower diagonal is, up to normalisation, the projection to  $\alpha(x, \cdot)$  for any fixed  $x \in M$ , and thus bounded. The relative form-bound for the off-diagonal entries follows from the fact that the action of  $\Omega_0^2$  on the first component is  $\text{curl}^2 = -\Delta$ .  $\square$

We conclude from the KLMN theorem that  $\Omega^2$  defines a self-adjoint operator with

$$D((\Omega^2)^{1/2}) = D(\Omega) = D(\Omega_0). \quad (5.25)$$

Note that, in general,  $\Omega^2$  is not a perturbation of  $\Omega_0^2$  in the sense of operators since there is no reason for the second component of a vector in  $D(\Omega_0^2)$  to be differentiable in  $x$ , but the off-diagonal terms of  $\Omega^2$  contain derivatives.

**Construction of the wave operators.** Even though  $\Omega$  is well defined, we need to impose an ultra-violet cutoff on the interaction for the construction of the wave operators. Let

$$\Omega_\rho^2 = \begin{pmatrix} \text{curl}^2 & \rho(-\Delta)(-\Delta)^{1/2}\langle \alpha(x, \cdot), \cdot \rangle_{L^2(\mathbb{R}_+)} \\ \alpha(x, \nu)(-\Delta)^{1/2}\rho(-\Delta) & \nu^2 + \alpha(x, \nu)\langle \alpha(x, \cdot), \cdot \rangle_{L^2(\mathbb{R}_+)} \end{pmatrix}, \quad (5.26)$$

where  $\rho$  is a real, smooth, rapidly decreasing function.

**Theorem 5.3.** *Let  $\rho \in \mathcal{S}(\mathbb{R})$  take values in the interval  $[0, 1]$ . Let  $M \subset \mathbb{R}^3$  be compact, and  $\alpha \in L^2(\mathbb{R}_+, L^\infty(M, \mathbb{R}))$  be Hölder continuous of exponent  $r > 1/2$ . Assume moreover that  $\alpha(x, \nu) \neq 0$  for all  $\nu > 0$ ,  $x \in M$ , and that the modified coupling  $\tilde{\alpha}$  (defined in (5.39)) is of class  $C_0^{r,s}$  for some  $r, s > 1/2$  (with the definition of (5.49)). Then the wave operators  $W_\pm(\Omega_\rho^2, \Omega_0^2)$  exist and are complete. Moreover, the spectrum of  $\Omega_\rho^2$  is purely absolutely continuous and  $W_\pm(\Omega_\rho^2, \Omega_0^2)$  are unitary.*

The construction of the wave operators proceeds in two steps. First, we take care of the self-interaction of the medium, given by the diagonal entry of the interaction. This leads to a purely off-diagonal interaction with the modified coupling function  $\tilde{\alpha}$ . We then construct the wave operators for this case under an appropriate regularity assumption on  $\tilde{\alpha}$ . Finally, in order to show that the spectrum is absolutely continuous, we need to rule out the existence of eigenvalues. For this, we need to assume that the coupling  $\alpha(\nu)$  does not vanish at any  $\nu > 0$ .

In some of the arguments below we will focus on the case of  $W_+$ , with  $W_-$  being analogous.

**Rank one perturbations.** The lower block on the diagonal of  $\Omega^2$  reads

$$A_\alpha = \nu^2 + \alpha(x, \nu)\langle \alpha(x, \cdot), \cdot \rangle_{L^2(\mathbb{R}_+)}, \quad (5.27)$$

i.e., for fixed  $x \in M$  it is the perturbation of the multiplication by  $\nu^2$  by  $\|\alpha(x, \cdot)\|_{L^2(\mathbb{R}_+)}^2$  times the projection to  $\alpha(x, \cdot)$  in  $L^2(\mathbb{R}_+)$ . Note, however, that on the full Hilbert space

this is not a relatively compact perturbation, as it acts multiplicatively in the variable  $x \in M$ .

For a rank-one perturbation it is not difficult to show that the wave operators exist, a result that goes back to Kato and Kuroda. Since rank-one perturbations are solvable models, one even has an explicit formula for the wave operator [7]. We state the result below, fixing the value of  $x \in M$ .

**Proposition 5.4.** *Let  $\alpha \in L^2(\mathbb{R}_+, \mathbb{R})$  be locally Hölder continuous of exponent  $r > 1/2$  and define a self-adjoint operator on  $D(A_\alpha) = L^2(\mathbb{R}_+, \nu^2 d\nu)$  by*

$$(A_\alpha f)(\nu) = \nu^2 f(\nu) + \alpha(\nu) \langle \alpha, f \rangle. \quad (5.28)$$

Define for  $z \in \mathbb{C} \setminus \mathbb{R}_+$

$$F(z) = \langle \alpha, (A_0 - z)^{-1} \alpha \rangle = \int_0^\infty \frac{\alpha^2(\nu)}{\nu^2 - z} d\nu. \quad (5.29)$$

Then:

a) *The spectrum of  $A_\alpha$  equals  $[0, \infty)$  and the resolvent is given by*

$$\left( (A_\alpha - z)^{-1} f \right) (\lambda) = \frac{f(\lambda)}{\lambda^2 - z} - \frac{\alpha(\lambda)}{(1 + F(z))(\lambda^2 - z)} \int_0^\infty \frac{\alpha(\eta) f(\eta)}{\eta^2 - z} d\eta. \quad (5.30)$$

b) *If moreover  $\alpha(\nu) \neq 0$  for all  $\nu > 0$ , the spectrum of  $A_\alpha$  is purely absolutely continuous and the unitary wave operators  $W_\pm(A_\alpha, A_0)$  are given by*

$$(W_\pm(A_\alpha, A_0) f) (\lambda) = f(\lambda) - \alpha(\lambda) \lim_{\varepsilon \rightarrow 0} \int \frac{\alpha(\omega)}{1 + F(\omega^2 \pm i\varepsilon)} \frac{f(\omega)}{\lambda^2 - \omega^2 \mp i\varepsilon} d\omega. \quad (5.31)$$

Let us comment on how these statements are obtained, without going into the details of the proofs. Since  $\alpha \langle \alpha, \cdot \rangle$  is a positive, compact operator, it is clear that the spectrum of  $A_\alpha$  equals  $\mathbb{R}_+$ . The resolvent formula is easily checked.

In view of the resolvent formula, the singularities of  $(A_\alpha - z)^{-1}$  are located at exactly those  $z \in \mathbb{C}$  where  $1 + F(z)$  is not invertible, and it can be proved that these points form the singular spectrum of  $A_\alpha$  [2]. We already know that there is no spectrum in  $\mathbb{C} \setminus \mathbb{R}_+$ . For  $\omega^2 > 0$ , we denote

$$F_\pm(\omega^2) = \lim_{\varepsilon \rightarrow 0} F(\omega^2 \pm i\varepsilon) = \frac{i\pi\alpha(\omega)^2}{2\omega} + \text{p.v.} \int_0^\infty \frac{|\alpha(\lambda)|^2}{\lambda^2 - \omega^2} d\lambda, \quad (5.32)$$

where p.v. is the Cauchy principal value. The limit exists due to the regularity assumption on  $\alpha$ . If  $\alpha(\omega) \neq 0$ , the equation  $1 + F_\pm(\omega^2) = 0$  cannot hold for  $\omega > 0$  since

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$\text{Im } F_{\pm}(\omega^2) \neq 0$ , so  $\omega^2$  is not in the singular spectrum of  $A_{\alpha}$ . Concerning the remaining case  $\omega = 0$ , we may note that

$$\text{Re } F(i\varepsilon) = \int_0^{\infty} \frac{\alpha(\lambda)^2 \lambda^2}{\lambda^4 + \varepsilon^2} d\lambda > 0, \quad (5.33)$$

so  $\omega = 0$  is also not a singular point. We have thus established that the spectrum of  $A_{\alpha}$  is absolutely continuous.

Existence of the wave operators can be shown using Cook's method [8, Sect.10.4]. Since the argument also applies to the perturbation of  $A_{\alpha}$  by  $-\alpha\langle\alpha, \cdot\rangle$ , they are complete, and since the spectra are absolutely continuous they are unitary. The formula for the wave operators is obtained by writing

$$\begin{aligned} W_{\pm}(A_{\alpha}, T)f &= \lim_{t \rightarrow \mp\infty} e^{itA_{\alpha}} e^{-itA_0} f \\ &= f \mp i \lim_{\varepsilon \rightarrow 0} \int_0^{\infty} e^{\mp it(A_{\alpha} \mp i\varepsilon)} \alpha\langle\alpha, e^{\pm itA_0} f\rangle dt \\ &= f - \lim_{\varepsilon \rightarrow 0} \int_0^{\infty} \alpha(\nu) f(\nu) ((A_{\alpha} \mp i\varepsilon - \nu^2)^{-1} \alpha) d\nu, \end{aligned} \quad (5.34)$$

which gives the claimed formula by inserting the formula for the resolvent. This calculation is justified on a dense set of functions  $f$  by the construction of the wave operators, wherein one shows that the time integral exists for  $\varepsilon = 0$ .

We can now use the wave operators above to remove the self-interaction of the polarisation field. Let

$$W_{\alpha} = \begin{pmatrix} 1 & 0 \\ 0 & W_{+}(A_{\alpha}, A_0) \end{pmatrix}, \quad (5.35)$$

then

$$\begin{aligned} W_{\alpha}^* \Omega_{\rho}^2 W_{\alpha} & \quad (5.36) \\ &= \Omega_0^2 + \begin{pmatrix} 0 & i \text{curl } \rho(-\Delta) \langle \alpha(x, \cdot) W_{+}(A_{\alpha}, A_0), \cdot \rangle \\ W_{+}(A_{\alpha}, A_0)^* \alpha(x, \cdot) i \rho(-\Delta) \text{curl} & 0 \end{pmatrix}. \end{aligned}$$

The new interaction term can be computed explicitly. We have

$$\begin{aligned} & \langle \alpha(x, \cdot), W_{+}(A_{\alpha}, A_0) f(x, \cdot) \rangle \\ &= \int_0^{\infty} \alpha(x, \omega) f(x, \omega) d\omega - \lim_{\varepsilon \rightarrow 0} \int_0^{\infty} \int_0^{\infty} \frac{\alpha(x, \omega)^2}{\omega^2 - \eta^2 - i\varepsilon} \frac{\alpha(\eta) f(x, \eta)}{1 + F_{+}(x, \eta^2)} d\omega d\eta \\ &= \int_0^{\infty} \alpha(x, \omega) f(x, \omega) \left( 1 - \frac{F_{+}(x, \omega^2)}{1 + F_{+}(x, \omega^2)} \right) d\omega \\ &= \int_0^{\infty} \frac{\alpha(x, \omega)}{1 + F_{+}(x, \omega^2)} f(x, \omega) d\omega = \langle \tilde{\alpha}(x, \cdot), f(x, \cdot) \rangle \end{aligned} \quad (5.37)$$

where  $F(z)$  depends on  $x$  via  $\alpha$ . We thus have

$$i \operatorname{curl} \langle \alpha(x, \cdot) W_+(A_\alpha, A_0) = i \operatorname{curl} \langle \tilde{\alpha}(x, \cdot), \cdot \rangle, \quad (5.38)$$

which is of the same form as before, but with  $\alpha$  replaced by the modified coupling

$$\tilde{\alpha}(x, \nu) = \frac{\alpha(x, \omega)}{1 + F_+(x, \omega^2)} = W_+(A_\alpha, A_0)^* \alpha(x, \cdot). \quad (5.39)$$

Note that the new coupling is no longer real. For our main examples the modified coupling can be calculated explicitly using the residue calculus. For the Drude coupling (5.9), the result has a simple expression. For  $\omega > 0$  we have

$$F_+(\omega^2) = \frac{\pi}{2(a^2\omega^2 + b^2)} \left( \frac{i}{\omega} - \frac{a}{b} \right). \quad (5.40)$$

So, while  $\alpha(x, 0) = b^{-1}1_M(x)$  was positive,  $\tilde{\alpha}(x, 0) = 0$ . The Lorentz coupling (5.8) already vanishes at  $\omega = 0$  and this is not changed by passing to  $\tilde{\alpha}$ . Hence, now in both cases,  $\tilde{\alpha}(x, \cdot)$  is a differentiable function from  $\mathbb{R}_+$  to  $\mathbb{C}$  that vanishes at  $\omega = 0$ .

**Friedrichs-Fadeev theory.** We will use methods of stationary scattering theory to prove existence of the wave operators  $W_\pm(W_\alpha^* \Omega_\rho^2 W_\alpha, \Omega_0^2)$ . These go back to the pioneering work of Friedrichs [6] and were further developed by Fadeev [5]. These works concern perturbation of a multiplication operator with continuous spectrum by an integral operator, and prove existence of wave operators  $W_\pm$  via an integral equation for the kernel of  $1 - W_\pm$ . We refer to [14] for a detailed exposition of this material.

First, we will need to bring the operator  $W_\alpha^* \Omega_\rho^2 W_\alpha$  (cf. (5.36)) into the form of an operator of multiplication plus an integral operator.

For this, proceed by the following steps:

1. Apply the Fourier transform to the first component to pass to the spectral representation of  $-\Delta$ .
2. Parametrise the range of  $P_{\operatorname{div}}$  by choosing unit vectors  $e_j(k/|k|)$ ,  $j = 1, 2$  with  $k \cdot e_j(k) = 0$ .
3. Pass to spherical coordinates  $k \mapsto (\lambda, \theta) \in \mathbb{R}_+ \times S^2$ .
4. Perform a unitary change of measure  $L^2(\mathbb{R}_+, \lambda^2 d\lambda) \rightarrow L^2(\mathbb{R}_+, d\lambda)$ .

We thus obtain a transformed operator, which we denote as  $\tilde{\Omega}^2$ , acting on  $L^2(\mathbb{R}_+, \mathfrak{h})$  with

$$\mathfrak{h} = L^2(S^2, \mathbb{C}^2) \oplus L^2(M, \mathbb{C}^3). \quad (5.41)$$

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Its action is given by

$$(\tilde{\Omega}^2\Psi)(\lambda) = \lambda^2\Psi(\lambda) + (V\Psi)(\lambda), \quad V = \begin{pmatrix} 0 & \tilde{B} \\ \tilde{B}^* & 0 \end{pmatrix}, \quad (5.42)$$

with  $\tilde{B}: L^2(\mathbb{R}_+, L^2(M, \mathbb{C}^3)) \rightarrow L^2(\mathbb{R}_+, L^2(S^2, \mathbb{C}^2))$ ,

$$(\tilde{B}\psi)(\lambda, \theta)_j = \frac{\lambda^2\rho(\lambda)}{(2\pi)^{3/2}} \int_0^\infty \int_M \tilde{\alpha}(x, \mu) e^{-i\lambda\theta \cdot x} \langle e_j(\theta), \psi(\mu, x) \rangle_{\mathbb{C}^3} dx d\mu, \quad (5.43)$$

and its adjoint

$$(\tilde{B}^*\varphi)(\lambda, x) = \sum_{j=1,2} \frac{\tilde{\alpha}(x, \lambda)}{(2\pi)^{3/2}} \int_0^\infty \int_{S^2} e^{i\mu\theta \cdot x} \mu^2 \rho(\mu) e_j(\theta) \varphi_j(\mu, \theta) d\theta d\mu, \quad (5.44)$$

where  $d\theta$  denotes the volume measure on the unit sphere. Note that  $V$  is an integral operator whose kernel is a bounded operator on  $\mathfrak{h}$ . Since both  $S^2$  and  $M$  have finite volume and for fixed  $\lambda, \mu$  the kernel is a bounded function of  $\theta, x$ , it is obvious that  $V(\lambda, \mu)$  is Hilbert-Schmidt, and in particular compact.

We now discuss the construction of the wave operators for the model with cutoff, following the strategy of [14, Chap.4]. Note that we have written  $\tilde{\Omega}^2$  as a perturbation of multiplication by  $\lambda^2$ , and not  $\lambda$  as in [14], which will slightly alter the explicit formulas. Moreover, we have a different sign convention for  $W_\pm$ , in line with the usual time-dependent definition [11, Eq.10].

The strategy is to construct a family of operators  $T(z)$ , where  $z$  belongs to the upper or lower half plane in  $\mathbb{C}$ , satisfying

$$T(z) = V - V(\tilde{\Omega}^2 - z)^{-1}V. \quad (5.45)$$

Using the resolvent formula, we have

$$(\Omega_0^2 - z)^{-1}T(z) = (\Omega_0^2 - z)^{-1}V - (\Omega_0^2 - z)^{-1}V(\tilde{\Omega}^2 - z)^{-1}V = (\tilde{\Omega}^2 - z)^{-1}V. \quad (5.46)$$

Thus,  $T(z)$  satisfies the equation

$$T(z) = V - V(\Omega_0^2 - z)^{-1}T(z). \quad (5.47)$$

We will use this equation to show that  $T(z)$  has an (operator-valued) integral kernel  $t(\lambda, \mu, z)$ , which has a limit as  $z$  tends to a point  $\mu^2$  on the positive real line. The wave operators are then given by [14, Eq.4.2.1]

$$(W_\pm(\tilde{\Omega}_\rho^2, \Omega_0^2)\Psi)(\lambda) = \Psi(\lambda) - \lim_{\varepsilon \rightarrow 0} \int_0^\infty \frac{t(\lambda, \mu, \mu^2 \pm i\varepsilon)}{\lambda^2 - \mu^2 \mp i\varepsilon} \Psi(\mu) d\mu. \quad (5.48)$$

**Construction of the integral kernels.** To simplify the notation, we now restrict ourselves to the wave operator  $W_+$ , which is constructed from  $T(z)$  with  $z$  in the upper half plane  $\text{Im } z \geq 0$ . The construction will be done in an auxiliary space of Hölder continuous functions, which allows us to deal with the limits  $\text{Im } z \rightarrow 0$  on a point-wise basis. For a Banach space  $X$ , let  $C_0^{r,s}(X)$  be the subspace of the globally  $r$ -Hölder continuous functions  $f: [0, \infty) \rightarrow X$ , that vanish at  $\lambda = 0$  and for which the norm

$$\|f\|_{r,s} = \sup_{\lambda > 0} (1 + \lambda)^s \left( \|f(\lambda)\|_X + \sup_{|\eta| \leq 1} \frac{\|f(\lambda) - f(\lambda + \eta)\|_X}{|\eta|^r} \right). \quad (5.49)$$

is finite.

These spaces restrict the coupling functions, which should satisfy  $\tilde{\alpha} \in C_0^{r,s}(L^\infty(M))$  for some  $r, s > 1/2$ . In particular, this ensures that  $\tilde{\alpha} \in L^2(\mathbb{R}_+, L^2(M))$ . Both for the Lorentz and the Drude coupling we have  $\tilde{\alpha} \in C_0^{1,1}(L^\infty(M))$ .

Formulated for the integral kernel, Equation (5.47) for  $T(z)$  takes the form

$$t(\lambda, \mu, z) = V(\lambda, \mu) - \int_0^\infty \frac{V(\lambda, \eta)t(\eta, \mu, z)}{\eta^2 - z} d\eta. \quad (5.50)$$

For  $\text{Im } z > 0$ , and

$$t(\lambda, \mu, \omega^2) = V(\lambda, \mu) - \lim_{\varepsilon \rightarrow 0} \int_0^\infty \frac{V(\lambda, \eta)t(\eta, \mu, \omega^2)}{\eta^2 - \omega^2 - i\varepsilon} d\eta, \quad (5.51)$$

for  $z = \omega^2 = \lim_{\varepsilon \rightarrow 0} \omega^2 + i\varepsilon$ .

Observe that in these equations we may fix  $\mu, z$  and then view them as an equation for the function  $\lambda \mapsto t(\lambda, \mu, z) \in \mathfrak{B}(\mathfrak{h})$ . In order to obtain an equation for vector valued, rather than operator valued, functions, we apply the whole equation to an arbitrary but fixed vector  $\varphi \in \mathfrak{h}$ . Setting

$$\tau_z(\lambda, \mu) := t(\lambda, \mu, z)\varphi \quad (5.52)$$

we thus have an equation for the  $\mathfrak{h}$ -valued function  $\lambda \mapsto \tau_z(\lambda, \mu)$ , for every fixed  $\mu \in \mathbb{R}_+$ ,  $\text{Im } z \geq 0$ ,

$$\begin{aligned} \tau_z(\lambda, \mu) &= V(\lambda, \mu)\varphi - \int_0^\infty \frac{V(\lambda, \eta)\tau_z(\eta, \mu)}{\eta^2 - z} d\eta \\ &= V(\lambda, \mu)\varphi - \int_0^\infty k_z(\lambda, \eta)\tau_z(\eta, \mu) d\eta. \end{aligned} \quad (5.53)$$

For  $\text{Im } z = 0$  this equation is interpreted as in (5.51) and extends the integral operator  $K_z = V(\Omega_0^2 - z)^{-1}$  to this case. Our task is now to show that  $1 + K_z$  is invertible. We will achieve this by appealing to the Fredholm alternative and using the explicit form

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of the operators to show that the kernel is empty, which provides some simplifications compared to the general case [14]. We must thus first show that  $K_z$  is compact, on an appropriate space. For this, we use the following generalisation of the Arzelà-Ascoli Theorem.

**Lemma 5.5.** *Let  $r > r' \geq 0$  and  $s > s' \geq 0$ . Any bounded set  $F \subset C^{r,s}(\mathfrak{h})$ , such that, for every fixed  $\lambda$ ,  $F_\lambda = \{f(\lambda), f \in F\}$  is pre-compact in  $\mathfrak{h}$ , is pre-compact in  $C^{r',s'}(\mathfrak{h})$ .*

For the proof see [5].

**Lemma 5.6.** *Let  $\rho \in \mathcal{S}(\mathbb{R})$  and  $\tilde{\alpha} \in C_0^{r,s}(L^\infty(M))$  with  $r, s > 1/2$ . Then for  $z \in \mathbb{C}$ ,  $\text{Im } z \geq 0$ , and every  $r', s' \in [0, 1)$ , with  $r' < r$ ,  $s' < s$ , the operator  $K_z$  defines a compact operator on  $C_0^{r',s'}(\mathfrak{h})$ .*

*Sketch of the proof.* Let  $\Phi = \begin{pmatrix} f \\ g \end{pmatrix} \in C_0^{r',s'}(\mathfrak{h})$ . We discuss the case  $z = \omega^2 \in \mathbb{R}_+$  directly. The upper component of  $(K_{\omega^2}\Phi)(\lambda)$  equals (for  $j = 1, 2$ )

$$\lim_{\varepsilon \rightarrow 0} \frac{\lambda^2 \rho(\lambda)}{(2\pi)^{3/2}} \int_0^\infty \int_M \frac{\tilde{\alpha}(x, \eta) e^{-i\lambda\theta \cdot x} \langle e_j(\theta), g(\eta, x) \rangle_{\mathbb{C}^3}}{\eta^2 - \omega^2 \pm i\varepsilon} dx d\eta. \quad (5.54)$$

Using the regularity of  $\tilde{\alpha}$ ,  $g$  and the fact that both vanish at zero, one can show that the limit  $\varepsilon \rightarrow 0$  exists for all  $\omega$  (this is the reason for assuming  $r > 1/2$ ). The function vanishes as  $\lambda \rightarrow \infty$  because of the cutoff  $\rho$ , and also at  $\lambda = 0$  (here, the cutoff  $\rho$  is crucial, since there is no reason why  $g$  should be regular and thus the expression above might not decay for  $\lambda \rightarrow \infty$ ). Moreover, this defines a smooth function of  $\lambda$ , as it is the Fourier transform of a function with support in  $M$ . One concludes that it is an element of  $C_0^{r',s}(L^2(S^2, \mathbb{C}^2))$ . Moreover, for fixed  $\lambda$ , this is an element of the pre-compact set of smooth functions in  $L^2(S^2, \mathbb{C}^2)$  with derivatives bounded in terms of  $\|g(\mu, \cdot)\|_{L^2(M)}$ .

For the lower component, a similar property follows easily from the properties of  $\tilde{\alpha}$ ,  $\rho$  and the Fourier transform. Compactness of  $K_{\omega^2}$  is now a consequence of Lemma 5.5.  $\square$

From this Lemma and the Fredholm alternative we conclude that, for fixed  $z$ , either there is a unique  $\tau_z(\lambda, \mu)$ , solution to the equation

$$\tau_z = V\varphi - K_z\tau_z, \quad (5.55)$$

or otherwise the homogeneous equation

$$\Phi = -K_z\Phi \quad (5.56)$$

has at least one non-trivial solution. As we will now see, this does not happen for the model we are interested in.

**Lemma 5.7.** *Assume the hypothesis of Theorem 5.3 hold. Then for  $z \in \mathbb{C}$  with  $\text{Im } z \geq 0$  and for any  $r, s > 1/2$  the homogeneous equation (5.56) has no non-zero solution in  $C_0^{r,s}(\mathfrak{h})$ .*

*Proof.* For  $z$  in the resolvent set of  $\Omega_0^2$ , a solution  $\Phi$  to the homogeneous equation corresponds to an eigenfunction  $\Psi = (\Omega_0^2 - z)^{-1}\Phi$  of  $\tilde{\Omega}^2$ , since

$$(\tilde{\Omega}^2 - z)\Psi = \Phi + V(\Omega_0^2 - z)^{-1}\Phi = 0. \quad (5.57)$$

As  $\tilde{\Omega}^2$  is self-adjoint and non-negative, this implies  $\Phi = 0$ .

Now let  $z = \omega^2 \geq 0$  and let  $\Phi_\omega$  be a solution to (5.56). By [14, Lem.4.1.3], we must have  $\Phi_\omega(\omega^2) = 0$ . By Eq. (5.44), the second component of the solution  $\Phi_\omega(\omega^2)$  must equal  $\bar{\alpha}(x, \omega^2)\varphi_\omega(x)$ , for some  $\varphi_\omega \in L^2(M, \mathbb{C}^3)$ . Now for almost every  $x \in M$  we either have  $\bar{\alpha}(x, \omega^2) = 0$  or  $\varphi_\omega(x) = 0$ . The first case can only occur for  $\omega = 0$  by hypothesis. In the latter case,  $\bar{\alpha}(x, \lambda)\varphi_\omega(x)$  vanishes for all  $\lambda$ , and Eq. (5.54) then gives  $\Phi_\omega = 0$ .

This leaves only the possibility of a solution for  $\omega = 0$ . To exclude this, consider the equation satisfied by  $\varphi_0$  in this case. Using that the solution satisfies  $\Phi_0 = K_0^2\Phi_0$ , we obtain

$$\begin{aligned} \varphi_0(x) = \frac{1}{(2\pi)^3} \lim_{\varepsilon, \delta \rightarrow 0} \int_0^\infty \int_0^\infty \int_{S^2} \frac{\eta^4 \rho(\eta)^2 e^{i\eta\theta \cdot (x-y)} |\tilde{\alpha}|^2(x, \xi)}{\eta^2 + i\varepsilon} \frac{1}{\xi^2 - i\delta} \\ \times \sum_{j=1}^2 e_j(\theta) \langle e_j(\theta), \varphi_0(y) \rangle d\eta d\xi dy d\theta. \end{aligned} \quad (5.58)$$

Since  $\tilde{\alpha} = W_+(A_\alpha, A_0)^*\alpha$  (cf. Section 5.2), we have

$$\lim_{\delta \rightarrow 0} \int_0^\infty \frac{|\tilde{\alpha}|^2(x, \xi)}{\xi^2 - i\delta} d\xi = \lim_{\delta \rightarrow 0} \langle \alpha(x, \cdot), (A_\alpha - i\delta)^{-1}\alpha(x, \cdot) \rangle = \frac{F_+(x, 0)}{1 + F_+(x, 0)} =: \tilde{F}_+(x, 0). \quad (5.59)$$

By Equation (5.33), this quantity is of absolute value less or equal to one. Taking the limit  $\varepsilon \rightarrow 0$  and writing  $k = \eta\theta$ ,  $dk = \eta^2 d\eta d\theta$  we can rewrite the equation for  $\varphi_0$  as

$$\varphi_0(x) = \frac{1}{(2\pi)^3} \int \rho^2(|k|) e^{ik(x-y)} e_j(k) \langle e_j(k), \tilde{F}_+(y, 0)\varphi_0(y) \rangle dy dk, \quad (5.60)$$

i.e.,  $\varphi_0$  is an eigenfunction of this operator with eigenvalue one. But by  $\tilde{F}_+ \leq 1$ ,  $\rho \leq 1$  and isometry of the Fourier transform, this operator is a composition of maps of norm at most one. The bound must thus be saturated at every step, and thus  $\|\rho^2(k)\hat{\psi}(k)\| = \|\psi\|$ , where  $\psi(y) = \tilde{F}_+(y, 0)\varphi_0(y)$ , has to hold. Hence, the support of  $\hat{\psi}$  must lie in the set where  $\rho \equiv 1$ . Since  $\lim_{k \rightarrow \infty} \rho(k) = 0$ , this set is compact. But  $\hat{\psi}$  is the Fourier transform of a function with support in  $M$ , so an entire function. This leaves  $\hat{\psi} \equiv 0$  as the only possibility.

We have thus proved that the homogeneous equation has only the trivial solution.  $\square$



Note that we have used the cutoff  $\rho$  in this proof. In the case of the Lorentz coupling (5.8), we have  $\text{Im } F_+(0) = 0$  and thus  $\tilde{F}_+(0) < 1$ , so the argument would also work for  $\rho \equiv 1$ . For the Drude coupling (5.9) on the other hand, we have  $\tilde{F}_+(x, 0) = 1$  for  $x \in M$ , and the assumption that  $\rho(k) \rightarrow 0$  really is needed.

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## 6 Effective equations for many-boson systems

In this chapter I summarise the works [11, 13, 4] on the derivation of effective equations for many-boson systems. At very low temperatures, a system containing a large number of bosons is expected to exhibit Bose–Einstein condensation. This means that, in the ground state or low-temperature equilibrium states with  $N \gg 1$  bosons, an  $N$ -independent fraction of the bosons will participate in collective behaviour that can be described by a single one-particle state, the condensate. The remaining particles are considered to be excitations out of the perfect condensate, either due to temperature or interactions. Bogoliubov proposed an approximate description of these excitations by a free quantum field. Bose–Einstein condensation and Bogoliubov’s approximation have since been the subject of an extensive mathematical literature (see [19, 17, 18, 16, 15, 2, 6, 8] and references therein). In the following, I will discuss the justification of Bogoliubov’s theory and investigate its consequences in two specific situations. In the first, the bosons interact with an impurity particle, and in the second with an additional bosonic quantum field.

### 6.1 The Bose polaron

The Bose polaron system consists of a large number  $N \gg 1$  of bosons together with one, or few, particles of a different type. The latter are considered impurities in the Bose gas, and the interaction with these will slightly disturb the Bose gas. If there are only a few impurities, the interesting effects of this interaction should be visible at the level of excitations from the condensate, since disturbing the whole condensate would require an interaction energy of order  $N$ .

The system of  $N$  bosons and one impurity will be modelled by a Hamiltonian of the form

$$H_N = -\Delta_x - \sum_{j=1}^N \Delta_{y_j} + \sum_{1 \leq j < k \leq N} V_N(y_j - y_k) + \sum_{j=1}^N W_N(x - y_j) \quad (6.1)$$

with one-periodic boundary conditions, where  $x$  denotes the position of the impurity and  $y_j$  that of a boson. The choice of the  $N$ -dependent potentials will differ in the mean-field and dilute cases that we discuss separately below.

Due to the periodic boundary conditions, the condensate will simply correspond to the constant function on the torus. A single excitation is thus modelled by a function orthogonal to the condensate, i.e., with integral zero. The field of excitations

can be represented on the Fock space  $\Gamma(\mathfrak{H}_+)$  with  $\mathfrak{H}_+ = \{1\}^\perp \subset L^2(T^3)$ . Following Bogoliubov's ideas leads to an effective description of the system of impurity and excitations by a Hamiltonian of the form

$$-\Delta_x + d\Gamma(\omega) + a(v_x) + a^*(v_x) \quad (6.2)$$

on  $L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)$ . Here,  $\omega$  is the dispersion relation of the excitations, also called phonons since they are responsible for the propagation of sound waves in the system, and  $v$  is the effective phonon-impurity interaction. This is precisely the form of the Hamiltonians whose self-adjoint realisation is discussed in Section 4.2.

### 6.1.1 Mean-field dynamics

We now explain the results concerning the Bogoliubov-Fröhlich Hamiltonian in the mean-field setting of [11]. The mean-field limit corresponds to weak interactions at high density and the choice of potentials

$$V_N(y) = N^{-1}V(y), \quad W_N(x) = N^{-1/2}W(x), \quad (6.3)$$

for fixed  $V, W \in L^2(T^3)$ . In the case of  $V$ , this choice is motivated by asking that the interaction energy, which may be proportional to the number of boson pairs times  $V_N$ , to be of order  $N$ , like the kinetic energy. For  $W$ , the coupling strength  $N^{-1/2}$  is chosen so that the interaction of the particle with excitations out of the condensate is comparable to the energy of these excitations, as we now explain. If all the bosons condense in the state  $u_0 \equiv 1$ , then the energy of the system with (normalised) impurity wave-function  $\psi$  would be

$$\left\langle \psi \otimes u_0^{\otimes N}, \sum_{j=1}^N W_N(x - y_j) \psi \otimes u_0^{\otimes N} \right\rangle = \langle \psi, \psi \rangle N \int W_N = \sqrt{N} \int W. \quad (6.4)$$

This is large, but since the condensate is homogeneous it is a constant and will only modify the dynamics by a global phase. The first non-trivial contribution of the boson-impurity interaction will be seen in states with some excitations. Let  $\varphi \in \mathfrak{H}_+$ , then

$$\Phi = \frac{1}{\sqrt{N}} \sum_{j=1}^N u_0^{\otimes(N-j)} \otimes \varphi \otimes u_0^{\otimes(j-1)} \quad (6.5)$$

is a normalised element of  $L^2(T^3)^{\otimes_s N}$ . One easily calculates using the orthogonality of  $u_0, \varphi$ ,

$$\left\langle \psi \otimes \Phi, \sum_{j=1}^N W_N(x - y_j) \psi \otimes \Phi \right\rangle = \frac{N-1}{\sqrt{N}} \int W + N^{-1/2} \langle \psi \otimes \varphi, W \psi \otimes \varphi \rangle, \quad (6.6)$$

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and

$$\left\langle \psi \otimes \Phi, \sum_{j=1}^N W_N(x - y_j) \psi \otimes u_0^{\otimes N} \right\rangle = \langle \psi \otimes \varphi, W\psi \otimes u_0 \rangle. \quad (6.7)$$

We see in (6.6) a constant term, and a term that appears to be small, while the coupling between the states with one and zero excitations (6.7) is of order one.

The extraction of the different terms observed above from the interaction is conveniently implemented by the excitation map [16, 15],

$$U_X : L^2(T^3)^{\otimes_s N} \rightarrow \Gamma(\mathfrak{H}_+), \quad u_0^{\otimes j} \otimes_s \Phi \mapsto \Phi, \quad (6.8)$$

where  $\Phi \in \mathfrak{H}_+^{\otimes_s(N-j)}$ , and the normalisation of the symmetric tensor product is such that this is an isometry, i.e., as in (6.5). Identifying  $L^2(T^3)^{\otimes_s N}$  with a subspace of Fock space, the map can be expressed as

$$U_X = \bigoplus_{j=0}^N P_+^{\otimes j} \frac{a(u_0)^{N-j}}{\sqrt{(N-j)!}}, \quad (6.9)$$

with the orthogonal projection  $P_+ : L^2(T^3) \rightarrow \mathfrak{H}_+$ . With this formula, one easily checks that

$$\begin{aligned} U_X \sum_{j=1}^N W_N(x - y_j) U_X^* &= \frac{(N - \mathcal{N}_+)_+}{\sqrt{N}} \int W + N^{-1/2} d\Gamma(P_+ W_x P_+) \\ &+ a^*(P_+ W_x u_0) \frac{\sqrt{(N - \mathcal{N}_+)_+}}{\sqrt{N}} + \frac{\sqrt{(N - \mathcal{N}_+)_+}}{\sqrt{N}} a(P_+ W_x u_0) \end{aligned} \quad (6.10)$$

with  $\mathcal{N}_+$  the number operator on  $\Gamma(\mathfrak{H}_+)$  and  $W_x(y) = W(x - y)$ , as before. Observe that, assuming  $\mathcal{N}_+$  is of order one, the leading non-trivial interaction term is a linear coupling with form factor  $v = P_+ W u_0 = W - \int W$ .

Similarly, we can write (see [11, Lem.3.1], [13, Prop.4.2])

$$U_X \sum_{1 \leq j < k \leq N} V_N(y_j - y_k) U_X^* = \frac{1}{2}(N - 1) \int V + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4 \quad (6.11)$$

with (as quadratic forms on  $\Gamma(\mathfrak{H}_+)$ )

$$\begin{aligned} \mathcal{L}_2 &= (N - \mathcal{N}_+)_+ d\Gamma(V_N^*) \\ &+ \frac{1}{2} \sqrt{(1 - \mathcal{N}_+/N)_+} \sqrt{(1 - (\mathcal{N}_+ + 1)/N)_+} \int N V_N(y_1 - y_2) a_{y_1} a_{y_2} + \text{adj.}, \end{aligned} \quad (6.12)$$

$$\mathcal{L}_3 = \frac{1}{2} \sqrt{(1 - \mathcal{N}_+/N)_+} \int \sqrt{N} V_N(y_1 - y_2) a_{y_1}^* a_{y_2} a_{y_1} + \text{adj.}, \quad (6.13)$$

$$\mathcal{L}_4 = \frac{1}{2} \int V_N(y_1 - y_2) a_{y_1}^* a_{y_2}^* a_{y_1} a_{y_2}. \quad (6.14)$$

## 6.1 The Bose polaron

There is no term “ $\mathcal{L}_1$ ” linear in creation and annihilation operators, since  $u_0$  is constant, and thus  $V * |u_0|^2$  is orthogonal to  $\mathfrak{H}_+$ . Note that  $\mathcal{L}_3$  carries a pre-factor  $N^{-1/2}$  and  $\mathcal{L}_4$  a factor  $N^{-1}$  due to the definition of  $V_N$ . The Bogoliubov Hamiltonian is obtained by adding  $d\Gamma(-\Delta)$  to  $\mathcal{L}_2$  and setting  $\mathcal{N}_+/N$  to zero, i.e.,

$$H_{\text{Bog}} = d\Gamma(-\Delta) + d\Gamma(V*) + \frac{1}{2} \int V(y_1 - y_2) a_{y_1} a_{y_2} + \text{adj.} \quad (6.15)$$

Under appropriate conditions on  $V$ , this operator is essentially self-adjoint on the domain of  $d\Gamma(-\Delta) \subset \Gamma(\mathfrak{H}_+)$ . It is unitarily equivalent to  $d\Gamma(\omega(i\nabla)) + E_0$  for a constant  $E_0$  and  $\omega(k) = \sqrt{k^4 + 2\hat{V}(k)k^2}$  (see [22]), but we will not make use of this here.

The Bogoliubov-Fröhlich Hamiltonian for the mean-field model is then

$$H_{\text{BF}} = -\Delta_x + H_{\text{Bog}} + a(P_+ W_x) + a^*(P_+ W_x). \quad (6.16)$$

It is self-adjoint on  $H^2(\mathbb{R}^3) \otimes \Gamma(\mathfrak{H}_+) \cap D(H_{\text{Bog}})$ .

The main result of [11] concerns the difference of the dynamics generated by  $H_N$  to those of  $H_{\text{BF}}$  when intertwined by  $U_X$ . The hypothesis on the initial conditions  $\Psi_N$  for  $H_N$  amounts to the fact that the number of excitations remains finite (almost surely) for  $N \rightarrow \infty$ . Without loss of generality we set the integrals of  $V, W$  to zero here.

**Theorem 6.1.** *Let  $V, W \in L^2(T^3)$  be real-valued, even and satisfy  $\int V = 0 = \int W$ . Let  $\Psi_N \in L^2(T^3) \otimes L^2(T^3)^{\otimes_s N}$  be a sequence such that  $U_X \Psi_N$  converges to  $\Phi \in L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)$  for  $N \rightarrow \infty$ . Then*

$$\lim_{N \rightarrow \infty} \left\| U_X e^{-itH_N} \Psi_N - e^{-itH_{\text{BF}}} \Phi \right\|_{L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)} = 0$$

locally uniformly in  $t$ . If moreover  $\Phi \in D(-\Delta_x + d\Gamma(\omega))$ , there exist  $v, K > 0$  so that for all  $N \in \mathbb{N}$ ,  $t > 0$

$$\left\| U_X e^{-itH_N} U_X^* \Phi - e^{-itH_{\text{BF}}} \Phi \right\|_{L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)} \leq K e^{vt} N^{-1/4}.$$

The statement in [11] holds for any dimension  $d \in \mathbb{N}$ . We reproduce it here for  $d = 3$  to keep the notation consistent throughout the chapter.

To prove this theorem, it is sufficient to show the second, quantitative bound, which implies the first by a straightforward approximation argument. The key point is to control

$$\alpha(t) = \left\| (\mathcal{N}_+ + 1) U_X e^{-itH_N} U_X^* \Phi \right\|^2 \quad (6.17)$$

using a Grönwall argument. For this, the commutators  $[\mathcal{N}_+, U_X H_N U_X^*]$  need to be bounded by  $\mathcal{N}_+$ . For terms in  $U_X H_N U_X^*$  that are at most quadratic in the creation

and annihilation operators this is immediate, due to the commutation relations. For the higher-order terms  $\mathcal{L}_3, \mathcal{L}_4$ , one can exploit that  $U_X H_N U_X^*$  preserves the space with less than  $N$  excitations and bound any excess creation/annihilation operators using the factors  $N^{-1/2}$ . The bound on  $\alpha$  can then be used to bound the difference of  $H_{\text{BF}}$  and  $U_X H_N U_X^*$  acting on the solution, and thus the difference of the evolutions using Duhamel's formula.

### 6.1.2 Excitation spectrum of a dilute system

In the article [13], we study the Hamiltonian  $H_N$  from (6.1) in a scaling corresponding to a dilute system of bosons with density  $N^{-2}$ . In this case, we have

$$V_N(y) = N^2 V(Ny), \quad W_N(x) = NW(\sqrt{N}x), \quad (6.18)$$

for compactly supported, non-negative potentials  $V, W \in L^2(\mathbb{R}^3)$ , whose scaled versions have support in the unit square and thus define potentials on the torus. Note that  $NV_N$  and  $\sqrt{N}W_N$  tend weakly to the  $\delta$  distribution (multiplied by their integral) as  $N \rightarrow \infty$ , so one may think of this case as a mean-field limit with singular interaction.

In [13] we give an expansion of the ground state energy  $\inf \sigma(H_N)$  in  $N$ . We also relate the excitation spectrum, the difference of the eigenvalues to the ground state, of  $H_N$  to that of the corresponding Bogoliubov-Fröhlich Hamiltonian. The corresponding analysis in the mean-field situation of Section 6.1.1 was previously done by Myśliwi and Seiringer [20].

Bogoliubov theory for the dilute Bose gas was studied in [2, 8, 19, 17]. There, it was proved that the excitation spectrum can be described by the Bogoliubov Hamiltonian

$$H_{\text{Bog}} = d\Gamma(\omega(i\nabla)), \quad \omega(k) = \sqrt{k^4 + 16\pi\mathbf{a}_V k^2}, \quad (6.19)$$

where  $\mathbf{a}_V$  is the scattering length, defined for a potential  $U \in L^1(\mathbb{R}^3, \mathbb{R})$  by

$$4\pi\mathbf{a}_U := \inf_{\varphi \in H^1(\mathbb{R}^3)} \int (|\nabla\varphi(x)|^2 + \frac{1}{2}U(x)|1 + \varphi(x)|^2) dx. \quad (6.20)$$

For  $U \geq 0$  one observes that  $4\pi\mathbf{a}_U \leq \frac{1}{2} \int U$  by choosing  $\varphi = 0$ . Note that simply setting the potential  $V_N$  to  $N^{-1} \int V$  times  $\delta$  yields a different dispersion  $\omega$ , with  $16\pi\mathbf{a}_V$  replaced by  $2 \int V$ . The correct formula for  $\omega$  is the result of taking into account how the singularity affects the terms that could simply be treated as errors in the mean-field case. Representing the interaction in the excitation picture as in (6.10) and with the heuristics that  $\int W$  should be replaced by  $4\pi\mathbf{a}_W$ , the impurity-boson interaction becomes

$$\hat{v}(k) = 4\pi\mathbf{a}_W \sqrt{\frac{k^2}{\omega(k)}}, \quad (6.21)$$

where the  $k$ -dependence is due to the Bogoliubov transformation that relates the the quadratic Hamiltonian (6.15) to  $d\Gamma(\omega)$  (cf. [22]). The Bogoliubov-Fröhlich Hamiltonian

$$-\Delta_x + d\Gamma(\omega) + a^*(v_x) + a(v_x) \quad (6.22)$$

is thus precisely the periodic version of the one whose construction was discussed in [10] and Chapter 4.2.3. For given  $N$ , the actual interaction in the excitation representation is of the form

$$a^*(P_+ \sqrt{N} W_N) + a(P_+ \sqrt{N} W_N), \quad (6.23)$$

which corresponds to an ultraviolet cutoff at scale  $\sqrt{N}$ . From the construction in [10] we thus expect that the interaction gives a divergent contribution to the energy of the form (cf. (4.88))

$$E_N = e_1 \sqrt{N} + e_2 \log N + \mathcal{O}(1). \quad (6.24)$$

The first result of [13] is that this is indeed the case. The term of order  $\sqrt{N}$  is responsible for changing the term  $\int W \sqrt{N}$  from (6.10) to  $8\pi \mathfrak{a}_W \sqrt{N}$ , and the  $\log N$ -term gives a new contribution to the energy. This is universal in the sense that it depends only on the scattering length of  $W$  but not on the details of the interaction. The precise statement is:

**Theorem 6.2** (Expansion of the  $N$ -particle energy). *Let  $V, W \in L^2_{\text{comp}}(\mathbb{R}^3, \mathbb{R})$  be non-negative,  $W$  even and  $V$  radial. Then as  $N \rightarrow \infty$*

$$\inf \sigma(H_N) = 4\pi \mathfrak{a}_V N + 8\pi \mathfrak{a}_W \sqrt{N} - 32\pi(2\pi/3 - \sqrt{3}) \mathfrak{a}_W^4 \log N + \mathcal{O}(1).$$

The second result of [13] is that the excitation spectrum is given, in the limit  $N \rightarrow \infty$ , by that of the Bogoliubov-Fröhlich Hamiltonian on the torus, which is constructed using a version of Theorem 4.11.

**Theorem 6.3** (Excitation spectrum). *Let  $V, W \in L^2_{\text{comp}}(\mathbb{R}^3, \mathbb{R})$  be non-negative,  $W$  even and  $V$  radial. Let  $H_{\text{BF}}, D(H_{\text{BF}})$  be the self-adjoint operator associated to the expression (6.22) by Theorem 4.11. For  $n \in \mathbb{N}_0$  denote by  $e_n(H)$  the  $n$ -th min-max value of the operator  $H$ . Then*

$$\lim_{N \rightarrow \infty} (e_n(H_N) - e_0(H_N)) = e_n(H_{\text{BF}}) - e_0(H_{\text{BF}}).$$

The assumption that  $V$  be radial is used to obtain an a-priori bound on the number of excitations. The statements remain true for non-radial  $V$  if that bound holds (compare [13, Condition 4.1]).

As corollaries to the proof of Theorem 6.3, one also obtains estimates on the spectral projections of  $H_N$  and the dynamics. We give here the statement for the latter, which may be compared with Theorem 6.1.



**Corollary 6.4.** *Assume the hypothesis of Theorem 6.3 and let  $U_X$  be the excitation map defined in (6.8). There is a unitary  $U_B$  (the Bogoliubov transformation of the bosonic system) so that for any sequence  $\Psi_N$  such that  $U_X\Psi_N$  converges to  $\Phi \in L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)$  for  $N \rightarrow \infty$*

$$\lim_{N \rightarrow \infty} U_X e^{-it(H_N - e_0(H_N))} \Psi_N = U_B e^{-it(H_{BF} - e_0(H_{BF}))} U_B^* \Phi$$

in the norm of  $L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)$ .

The  $N$  boson Hamiltonian (6.1) can be related to a system in the thermodynamic limit by scaling. Consider a gas of bosons with density  $\rho$  in the thermodynamic limit. Assume that the boson-boson interaction has scattering length  $\mathfrak{a}$  and that the system is dilute, meaning that  $\rho\mathfrak{a}^3 \ll 1$ . The system also contains impurities with density  $\rho_I$  that interact with the bosons via a potential with scattering length  $\mathfrak{a}_I$ .

Now, consider a subsystem of the Gross-Pitaevski scale  $L = \mathfrak{a}(\rho\mathfrak{a}^3)^{-1/2}$ . The expected number of bosons in this system is  $N = (\rho\mathfrak{a}^3)^{-1/2}$ . If we choose

$$\rho_I/\rho = \sqrt{\rho\mathfrak{a}^3} \tag{6.25}$$

there is on average one impurity in a subsystem of this size. Assuming that there is exactly one impurity, the Hamiltonian for the subsystem becomes after rescaling by  $L$

$$L^2 \tilde{H}_L = -\Delta_x + \sum_{i=1}^n (-\Delta_{y_i}) + \sum_{1 \leq i < j \leq n} L^2 V(L(y_i - y_j)) + \sum_{i=1}^n L^2 W(L(x - y_i)). \tag{6.26}$$

The length scale of the boson-boson interaction is now  $\mathfrak{a}/L = \sqrt{\rho\mathfrak{a}^3} = N^{-1}$ . If we choose the relative range of the interactions as

$$\mathfrak{a}_I/\mathfrak{a} = (\rho\mathfrak{a}^3)^{-1/4}, \tag{6.27}$$

then  $\mathfrak{a}_I/L = (\rho\mathfrak{a}^3)^{1/4} = N^{-1/2}$ , i.e.,  $L^2 \tilde{H}_L$  can be written in the form of  $H_N$  from (6.1) with  $V_N, W_N$  as in (6.3). Assuming that the energy of every subsystem of size  $L$  behaves like  $\inf \sigma(H_N)$  gives a conjecture on the expansion of the energy per volume.

**Conjecture.** *The energy per volume has the following asymptotic expansion as  $\rho\mathfrak{a}^3 \rightarrow 0$*

$$e(\rho, \rho_B) = 4\pi\mathfrak{a}\rho^2 \left( 1 + 2(\rho\mathfrak{a}^3)^{1/4} - 4(2\pi/3 - \sqrt{3})(\rho\mathfrak{a}^3)^{1/2} \log(\rho\mathfrak{a}^3) + \mathcal{O}((\rho\mathfrak{a}^3)^{1/2}) \right),$$

Note that the last term in this expansion is larger than the well-known Lee-Huang-Yang correction to the energy of the dilute Bose gas [6, 7, 14], which is of the order of the error term.

**Remark 6.5.** The  $\log N$ -term in the expansion of the energy can be interpreted as a three-body effect. It is well known that potentials of the form (6.3) lead to important pair-correlations at short distances, where the potential is strongly repulsive and particles must avoid each other. For the case of the interaction  $W$ , the relevant length scale is  $N^{-1/2}$ , and on this scale the behaviour for a boson and the impurity is given by the minimiser  $\varphi$  in (6.20), i.e., the optimal wave function for a pair is approximately

$$1 + \varphi(\sqrt{N}(x - y)) \quad (6.28)$$

for  $|x - y| \lesssim N^{-1/2}$ . If we make the ansatz

$$\Psi(x, y_1, y_2) = (1 + \varphi(\sqrt{N}(x - y_1)))(1 + \varphi(\sqrt{N}(x - y_2)))\Phi(x, y_1, y_2) \quad (6.29)$$

for the three-particle wave-function of two bosons and the impurity, then the action of the Hamiltonian  $H_2$  gives rise to the term

$$N\nabla\varphi(\sqrt{N}(x - y_1))\nabla\varphi(\sqrt{N}(x - y_2))\Phi(x, y_1, y_2). \quad (6.30)$$

This can be interpreted as an effective three-body potential acting on  $\Phi$ , and the  $\log N$ -term in Theorem 6.2 is precisely the scattering length of this potential multiplied by the number of boson pairs  $\sim N^2/2$ .

A similar term in the energy expansion of the pure boson system was predicted in the physics literature [23, 9, 21], and recently established rigorously in the Gross-Pitaevski limit [3].

The proof of the results described above is quite involved, since one needs to perform both the analysis of the Gross-Pitaevski limit for the bosons and the construction of the Bogoliubov-Fröhlich Hamiltonian in the presence of additional terms coming from the interaction. A rough outline of the procedure is as follows.

- 1) Use  $U_X$  to transform  $H_N$  into  $U_X H_N U_X^*$  on  $L^2(T^3) \otimes \Gamma(\mathfrak{H}_+)$ .
- 2) Apply a Bogoliubov transformation  $U_q$ , whose generator is quadratic in boson creation and annihilation operators. This implements the idea that in low energy states the wave-function should behave like  $1 + \varphi_V(N(y_i - y_j))$  when a pair of bosons is close,  $|y_i - y_j| \lesssim N^{-1}$ , where  $\varphi_V$  is the minimiser of (6.20) with  $U = V$ . This transformation makes the scattering length  $\mathfrak{a}_V$  appear at the leading order of the energy.
- 3) Apply a Weyl-transformation  $U_W$ , which additionally depends on the impurity position  $x$ . This implements the behaviour as  $1 + \varphi_W(\sqrt{N}(x - y_i))$  for  $|x - y_i| \lesssim N^{-1/2}$  and makes the scattering length  $\mathfrak{a}_W$  appear in the energy asymptotics.

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- 4) Apply a transformation  $U_c$  to the boson Hamiltonian whose generator is cubic in creation and annihilation operators. This accounts for scattering processes that mix low and high energy bosons and is responsible for the scattering length  $\mathfrak{a}_V$  appearing in  $\omega$ , (6.19).
- 5) Apply Bogoliubov's transformation  $U_B$ , which transforms the remaining boson Hamiltonian into the simple expression  $d\Gamma(\omega)$  plus error terms.
- 6) After these transformations, one has, schematically

$$U^* H_N U \approx 4\pi\mathfrak{a}_V(N-1) + 8\pi\mathfrak{a}_W\sqrt{N} + e_N^{(U)} \\ + (H_{\text{BF},\Lambda_N} - e_1\Lambda_N) + N^{-1/2}d\Gamma(W_{N,x}),$$

where  $e_N^{(U)}$  is a scalar of order one and  $H_{\text{BF},\Lambda_N}$  is essentially the Bogoliubov–Fröhlich Hamiltonian with an  $N$ -dependent cutoff  $\Lambda_N$ . The final step is thus to take the limit  $\Lambda_N \rightarrow \infty$ , as explained in Chapter 4, which will make the  $\log N$ -term appear. However, there is an additional term  $N^{-1/2}d\Gamma(W_{N,x})$  present here, which does not make sense in the limit, but is also not negligible (a scaling argument suggests it is of order one). This difficulty is resolved by noticing that this term contributes only a constant at order one, plus smaller errors. Hence, it does not modify the Bogoliubov–Fröhlich Hamiltonian describing the excitation spectrum in the limit.

## 6.2 The mean-field Nelson model

In the article [4] we consider a system of many bosons, weakly coupled to a scalar quantum field. We derive the mean-field equations for the condensate and a classical field, and prove the validity of Bogoliubov's approximation for the excitations.

The formal expression of the Hamiltonian of the full system is

$$\sum_{j=1}^N -\Delta_{x_j} + d\Gamma(\omega(i\nabla)) + \frac{1}{\sqrt{N}} \sum_{j=1}^N (a(v_{x_j}) + a^*(v_{x_j})), \quad (6.31)$$

where  $\omega(k) = \sqrt{k^2 + 1}$  and  $\hat{v}(k) = \omega(k)^{-1/2}$  correspond to the Nelson model, cf. Section 4.2.2. This expression is ultraviolet singular, but one can associate it with a self-adjoint operator  $H_N$ ,  $D(H_N) \subset \mathcal{H}_N = L^2(\mathbb{R}^3)^{\otimes_s N} \otimes \Gamma(L^2(\mathbb{R}^3))$  by Nelson method (explained briefly in Section 4.2.2 and below), or a generalisation to  $N$ -particles of Theorem 4.10 (see [12]).

The results of [4] prove an approximation of the dynamics generated by this operator  $H_N$  on initial conditions that describe a condensate of particles with a coherent field. It had been shown in [1] that the time evolution of  $H_N$  can be approximated, in a certain weak sense, by the flow of the Schrödinger-Klein-Gordon equations for  $N \rightarrow \infty$ .

The dynamics of states describing a condensate, and fluctuations around them, were discussed for the model with an ultraviolet cutoff in [5]. The novelty of our work [4] consists in removing the ultraviolet cutoff, with the most interesting feature being the effect on the dynamics of excitations.

**Mean-field approximation.** For an initial state  $\Psi_N$  where the particles form a condensate with wave-function  $u_0$  and the field is in a coherent state with  $f = \sqrt{N}\alpha_0$  (meaning that there are on average  $N$  bosons, each with wave-function  $\alpha_0$ ), the time-evolution  $e^{-iH_N t}\Psi_N$  will be approximately of the same form, but with different functions  $(u_t, \alpha_t)$ . These are determined by solving the Schrödinger-Klein-Gordon equations

$$\begin{cases} i\partial_t u_t(x) = -\Delta u(x) + \varphi_{\alpha_t}(x)u(x) - \frac{1}{2}\langle u, \varphi_{\alpha_t} u \rangle u_t(x) \\ i\partial_t \alpha_t(k) = \omega(k)\alpha_t(k) + \omega^{-1/2}(k)|\widehat{u_t}|^2(k), \end{cases} \quad (6.32)$$

where  $\varphi_\alpha(x) = 2\text{Re}\langle \hat{v}_x, \alpha \rangle$ , with initial condition  $(u_0, \alpha_0)$ . This is a Hamiltonian system of equations with energy

$$\mathcal{E}(u, \alpha) = \langle u, (-\Delta + \varphi_\alpha)u \rangle + \langle \alpha, \omega \alpha \rangle. \quad (6.33)$$

In order to capture the corrections to this mean-field picture, we need a generalisation of the excitation map introduced in (6.8) to allow for a time-dependent condensate and accommodate the field. Let  $f \in L^2(\mathbb{R}^3)$  and define the associated Weyl transformation as

$$W(f) = \exp(a^*(f) - a(f)). \quad (6.34)$$

The coherent state generated by  $f$  is simply  $W(f)\Omega$ , where  $\Omega \in \Gamma(L^2(\mathbb{R}^3))$  is the vacuum. It is thus mapped back to the vacuum by  $W^*(f)$ , so  $W(f)^*\Phi$  describes the excitations of an arbitrary  $\Phi \in \Gamma(L^2(\mathbb{R}^3))$  relative to the coherent state generated by  $f$ . For the particles, we simply allow the condensate wave-function in (6.9) to be any normalised element  $u$  of  $L^2(\mathbb{R}^3)$ , and define

$$\begin{aligned} U_X(u, \alpha) : \mathcal{H}_N &\rightarrow \Gamma(L^2(\mathbb{R}^3)) \otimes \Gamma(L^2(\mathbb{R}^3)) \\ \Psi &\mapsto \left( \bigoplus_{j=0}^N P_{\{u\}^\perp}^{\otimes j} \frac{a(u)^{N-j}}{\sqrt{(N-j)!}} \otimes 1 \right) (1 \otimes W^*(\sqrt{N}\alpha)), \end{aligned} \quad (6.35)$$

with  $P_{\{u\}^\perp}$  the orthogonal projection to  $\{u\}^\perp$ . The image of this isometry is the subspace

$$U_X(u, \alpha)\mathcal{H}_N = \left( \bigoplus_{j=0}^N (\{u\}^\perp)^{\otimes_s N} \right) \otimes \Gamma(L^2(\mathbb{R}^3)) \subset \Gamma(\{u\}^\perp \oplus L^2(\mathbb{R}^3)). \quad (6.36)$$

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The operator

$$U_X(u_0, \alpha_0)^* d\Gamma(1_{\{u\}^\perp \oplus L^2}) U_X(u_0, \alpha_0) \quad (6.37)$$

thus corresponds to the number of excitations relative to the mean-field state defined by  $(u, \alpha)$ .

By the results of [1, 5], which are extended in [4] to give quantitative bounds without an UV cutoff, the functions  $u, \alpha$  should follow the flow of the equations (6.32). In [4, Theorem 1.1] we prove a quantitative version of this result, which can be summarised as follows.

**Theorem 6.6.** *Let  $(u_0, \alpha_0) \in H^3(\mathbb{R}^3) \oplus \mathcal{F}H^{5/2}(\mathbb{R}^3)$  and denote by  $(u_t, \alpha_t)$  the unique solution to (6.32) with initial condition  $(u_0, \alpha_0)$ . Let  $(\Psi_N)_{N \in \mathbb{N}}$  be a sequence in  $\mathcal{H}_N$  with*

$$\begin{aligned} N^{-1} \langle U_X(u_0, \alpha_0) \Psi_N, d\Gamma(1_{\{u\}^\perp \oplus L^2}) U_X(u_0, \alpha_0) \Psi_N \rangle &= \mathcal{O}(N^{-1}) \\ |N^{-1} \langle \Psi_N, H_N \Psi_N \rangle - \mathcal{E}(u_0, \alpha_0)| &= \mathcal{O}(N^{-1/2}), \end{aligned}$$

then

$$N^{-1} \langle U_X(u_t, \alpha_t) e^{-iH_N t} \Psi_N, d\Gamma(1_{\{u\}^\perp \oplus L^2}) U_X(u_t, \alpha_t) e^{-iH_N t} \Psi_N \rangle = \mathcal{O}(N^{-1/2})$$

locally uniformly in time.

This theorem means that if at an initial time the fraction of excitations is  $N^{-1}$  and the energy per particle is close to the mean-field energy up to order  $N^{-1/2}$ , then at later times the ratio of excitations with respect to the time-evolved condensate is still at most  $N^{-1/2}$ . Simply evolving the condensate functions  $u, \alpha$  thus accounts for the vast majority of particles and, e.g., the (normalised) one-particle density matrix of the time evolved state converges to the one of the evolved condensate for all time.

The apparent loss in the estimates of the particle number at time  $t$  compared to that at time zero stems from a bound on derivatives of  $U_X(u_0, \alpha_0) \Psi_N$  involving the mean-field energy  $\mathcal{E}$  and the square-root of the particle number. A result without such loss can be proved by adapting the hypothesis, but the condition on the energy difference seems more natural from a physical point of view.

Note that this theorem cannot be applied to the state

$$\Psi_N = u_0^{\otimes N} \otimes W(\sqrt{N} \alpha_0) \Omega \quad (6.38)$$

with no excitations, since it is not in the form domain of  $H_N$  (compare Section 4.2.2) and has infinite energy. However, slight modifications of this state do satisfy the hypothesis of the theorem, see [4, Proposition 1.2].

**Bogoliubov approximation.** In order to approximate the dynamics of the full system, and not only the majority of particles, one needs to include the dynamics of the excitations. Setting  $\Phi(t) = U_X(u_t, \alpha_t)e^{-iH_N t}\Psi_N$ , these are exactly given by the equation

$$i\partial_t\Phi(t) = U_X(u_t, \alpha_t)H_N U_X^*(u_t, \alpha_t) + i(\partial_t U_X(u_t, \alpha_t))U_X^*(u_t, \alpha_t)\Phi(t). \quad (6.39)$$

Evaluating the expression for the generator yields a sum of terms weighted by powers of  $\sqrt{N}$ . The term of order  $N$  is scalar, and the non-trivial terms of order  $\sqrt{N}$  are eliminated by using the mean-field equation (6.33). Dropping terms with negative powers of  $\sqrt{N}$  yields the generator of the Bogoliubov dynamics

$$\begin{aligned} d\Gamma(h_\alpha(t)) \otimes 1 + 1 \otimes d\Gamma(\omega) + \int (P_{\{u_t\}^\perp} \overline{\hat{v}(\cdot)(k)u_t}(x) a_k b_x^* + \text{adj.} \\ + \int (P_{\{u_t\}^\perp} \hat{v}(\cdot)(k)u_t(x) a_k^* b_x + \text{adj.}), \end{aligned} \quad (6.40)$$

where  $h_\alpha(t) = -\Delta + \varphi_{\alpha_t} - \frac{1}{2}\langle u_t, \varphi_{\alpha_t} u_t \rangle$ . We used here the representation of the excitation space as a tensor product (6.36) with creation/annihilation operators  $b^*, b$  for the first (particle) factor, and  $a^*, a$  for the field. However, this expression is singular. Since  $\hat{v}, \omega^{-1/2}\hat{v}$  are not square-integrable, the interaction term in the second line is not a (form) perturbation of the first line.

One could imagine giving a meaning to this expression using the techniques of chapter 4, but this is not straightforward since using  $h_\alpha$  to control the regularity of the interaction leads to a loss of control of the number of excitations of the field.

In order to give a meaning to the dynamics generated by the time-dependent expression (6.40), we used in [4] an approach that is inspired by Nelson's original construction of the Hamiltonian  $H_N$ . This construction relies on the use of the dressing transformation

$$W^D = \prod_{j=1}^N W(N^{-1/2}(-\Delta + \omega)^{-1}v_{x_j}). \quad (6.41)$$

This maps the form domain  $D(H_N^{1/2})$  to the one of the free operator  $\sum_{j=1}^N(-\Delta_{x_j}) + d\Gamma(\omega)$ , and the quadratic form of  $H_N$  to that of a dressed operator  $H_N^D$ , which is a form perturbation of the free operator. It is the product of exponentials of commuting operators, so we may think of it as the evaluation at “time”  $\theta = 1$  of a unitary group  $W^D(\theta)$ . The generator of this group inherits the mean-field scaling. In fact, it is very similar to the interaction term in (6.31) but with the new form factor  $w_x = i(-\Delta + \omega)^{-1}v_x$ . We can thus associate to  $W^D(\theta)$  a mean-field approximation, which is a flow acting on the condensate functions  $(u_0, \alpha_0)$ . At  $\theta = -1$ , this flow reaches a point  $\mathfrak{D}(u_0, \alpha_0)$ , which defines a non-linear transformation of  $(u_0, \alpha_0)$ . This can

## 6 Effective equations for many-boson systems

be seen as a dressed initial condition, and if  $U_X(u_0, \alpha_0)\Psi_N$  has few particles, then  $U_X(\mathfrak{D}(u_0, \alpha_0))W^D\Psi_N$  also has few particles, which are now excitations relative to the condensate given by the pair  $\mathfrak{D}(u_0, \alpha_0)$ . One can calculate the generator of the dynamics in the auxiliary time  $\theta$  of these excitations and its Bogoliubov approximation as above. Since the form factor  $w_x$  is more regular (it is an element of  $L^2(\mathbb{R}^6)$ ), it is not difficult to prove that the latter generates a two-parameter family of Bogoliubov transformations  $\mathbb{W}^D(\theta, \theta')$  that approximates  $W^D$ .

Now, the dressed Hamiltonian  $H_N^D = W^D H_N (W^D)^*$  is also more regular than  $H_N$ . It is associated to a mean-field equation whose solution is  $\mathfrak{D}(u_t, \alpha_t)$ , the dressed version of the solution to (6.32). Considering excitations with respect to this pair gives rise to a Bogoliubov Hamiltonian, which is well defined as a quadratic form and generates a two-parameter family  $\mathbb{U}^D(t, s)$  of Bogoliubov transformations (cf. (5.21)). One may thus define the dynamics formally associated with the singular expression (6.40) by  $\mathbb{U} = (\mathbb{W}^D)^* \mathbb{U}^D \mathbb{W}^D$  (where the time variables and the dependence on the mean-field solutions are suppressed).

The main results of [4] may be summarised as the commutativity of the following diagram for  $N \rightarrow \infty$ , with quantitative estimates for each cycle.

$$\begin{array}{ccccc}
 & & \Phi^D & \xrightarrow{\mathbb{U}^D} & \Phi^D(t) \\
 & \nearrow U_X(\mathfrak{D}(u_0, \alpha_0)) & \uparrow \mathbb{W}^D & \nearrow U_X(\mathfrak{D}(u_t, \alpha_t)) & \downarrow (\mathbb{W}^D)^* \\
 W^D \Psi_N & \xrightarrow{\quad} & e^{-itH_N^D} W^D \Psi_N & & \\
 \uparrow & & \downarrow & \downarrow & \\
 \Psi_N & \nearrow U_X(u_0, \alpha_0) & \Phi & \xrightarrow{\mathbb{U}} & \Phi(t) \\
 \downarrow & & \downarrow & \downarrow & \downarrow \\
 & \xrightarrow{\quad} & e^{-itH_N} \Psi_N & \nearrow U_X(u_t, \alpha_t) & 
 \end{array}$$

**Figure 6.1:** The diagram commutes up to small errors in  $N$ . The exact dynamics are represented in the front plane, with the Bogoliubov approximations in the second plane. Note the dependence of the excitation maps on the solutions to the mean-field equations.

The commutativity of the diagram is reasonable from a geometric point of view: The Bogoliubov approximation is essentially a projection of the dynamics to the manifold of quasi-free states. As long as this is performed in a unique way, the result of projecting after a unitary dynamics or projecting at the start and then following the induced dynamics must be equal.

For rather general initial conditions, and thus without an explicit rate of convergence, the result can be stated as follows.

**Theorem 6.7.** *Let  $(u_0, \alpha_0) \in H^3(\mathbb{R}^3) \oplus \mathcal{FH}^{5/2}$  with  $\|u_0\|_{L^2(\mathbb{R}^3)} = 1$  and let  $(u_t, \alpha_t)$  denote the solution to (6.32) for initial data  $(u_0, \alpha_0)$ . Let  $\Phi \in \Gamma(\{u_0\}^\perp) \otimes \Gamma(L^2(\mathbb{R}^3))$*

with  $\|\Phi\| = 1$  and let  $\Psi_N$ ,  $N \geq 1$ , be such that

$$\lim_{N \rightarrow \infty} \|\Psi_N - U_X^*(u_0, \alpha_0)\Phi\|_{\mathcal{H}_N} = 0.$$

Then for all  $T > 0$

$$\lim_{N \rightarrow \infty} \sup_{|t| \leq T} \|e^{-itH_N}\Psi_N - U_X^*(u_t, \alpha_t)\mathbb{U}(t)\Phi\|_{\mathcal{H}_N} = 0.$$

By imposing restrictions on the initial conditions  $\Phi = U_X(u_0, \alpha_0)\Psi_N$ , one obtains a rate of convergence of  $N^{-1/4} \log N e^{p(t)}$  for a polynomial  $p$ . Note that this is similar to the rate in Section 6.1.1, with an additional  $\log N$  reflecting the singularity of the model.

The proof of this theorem makes use of the dynamics with ultraviolet cutoff, i.e., where the interaction form factor is replaced by  $v_\Lambda(k) = \omega(k)^{-1/2} 1_{|k| \leq \Lambda}$ . For this interaction, the Bogoliubov Hamiltonian (6.40) is easily shown to be essentially self-adjoint on the domain of the non-interacting Hamiltonian  $d\Gamma(h_\alpha + \omega)$  and generate a two-parameter family of Bogoliubov transformations. As a byproduct, we obtain a characterisation of the Bogoliubov dynamics  $\mathbb{U}$  as the limit of the regularised Bogoliubov dynamics  $\mathbb{U}_\Lambda$ .

**Proposition 6.8.** *The Bogoliubov transformation  $\mathbb{U}(t, s) = (\mathbb{W}^D)^* \mathbb{U}^D(t, s) \mathbb{W}^D$  satisfies*

$$\mathbb{U}(t, s) = \text{s-lim}_{\Lambda \rightarrow \infty} \mathbb{U}_\Lambda(t, s) e^{-iE_\Lambda(t, s)} \quad (6.42)$$

for a family  $E_\Lambda(t, s) = -4\pi(t - s) \log \Lambda + \mathcal{O}(1)$ .

The divergence of the numbers  $E_\Lambda$  is exactly the same as in Nelson's construction of  $H_N$ , so, in a sense, the singularity is already fully captured at the level of the Bogoliubov approximation.

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## Notation

Symbol	Explanation
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$\mathbb{N}$	Natural numbers (not including zero!)
$\mathbb{N}_0$	$\mathbb{N} \cup \{0\}$
$\mathbb{R}_+$	Non-negative real numbers, $\mathbb{R}_+ = [0, \infty)$
$\mathcal{S}(\mathbb{R}^d)$	Space of Schwartz functions on $\mathbb{R}^d$
$\mathcal{S}'(\mathbb{R}^d)$	Space of tempered distributions on $\mathbb{R}^d$
$C^k(U)$	Space of $k$ -times continuously differentiable functions $U \rightarrow \mathbb{C}$
$C_0^k(U)$	Functions in $C^k(U)$ with compact support, $\text{supp } f \Subset U$
$C_b^k(U)$	Bounded functions in $C^k(U)$ with bounded derivatives
$H^s(\mathbb{R}^d)$	$L^2$ -Sobolev space of order $s \in \mathbb{R}$
$H_0^s(U)$	Closure of $C_0^k(U)$ in $H^s(\mathbb{R}^d)$
$B(X, Y)$	Space of bounded linear operators from $X$ to $Y$
$B(X)$	Space of bounded linear operators on $X$ , $B(X, X)$
$X'$	Space of bounded linear functionals on $X$ , $B(X, \mathbb{C})$
$\mathfrak{S}^p(\mathcal{H})$	Schatten space of $p$ -summable operators on $\mathcal{H}$
$K(X)$	Space of compact linear operators on $X$ , $K(\mathcal{H}) = \mathfrak{S}^\infty(\mathcal{H})$
$\Gamma(\mathcal{H})$	Symmetric Fock space over $\mathcal{H}$ , $\Gamma(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}$
$a(f)$	Annihilation operator, $\langle \Phi^{(n-1)}, a(f)\Psi^{(n)} \rangle = \sqrt{n} \langle \Phi^{(n-1)} \otimes f, \Psi^{(n)} \rangle$
$a^*(f)$	Creation operator, $a^*(f)\Psi^{(n)} = \sqrt{n+1} P_{\text{sym}} f \otimes \Psi^{(n)}$
$\Gamma(T)$	Second quantisation of the transformation $T$ , $\Gamma(T) = \bigoplus_{n=0}^{\infty} T^{\otimes n}$
$d\Gamma(A)$	Second quantisation of the generator $A$ , $e^{d\Gamma(A)} = \Gamma(e^A)$
$\mathcal{N}$	Number operator, $\mathcal{N} = d\Gamma(1)$
$1_U$	Characteristic function of the set $U$ , or identity operator on the vector space $U$
$\mathcal{F}$	Fourier transform, $\mathcal{F}f(k) = \frac{1}{(2\pi)^{d/2}} \int e^{-ikx} f(x) dx$