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A global approach to the
Schrödinger-Poisson system:
An Existence result in the case
of infinitely many states

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Abstract

In this paper we prove the existence of a solution to a nonlinear Schrödinger–Poisson eigenvalue problem in dimension less than 3. Our proof is based on a global approach to the determination of eigenvalues and eigenfunctions which allows us to characterize the complete sequence of eigenvalues and eigenfunctions at once, via a variational approach, and thus differs from the usual and less general proofs developed for similar problems in the literature. Our approach seems to be new for the determination of the spectrum and eigenfunctions for compact and self-adjoint operators, even in a finite dimensional setting.

Keywords: Schrödinger–Poisson, variational methods, unitary operators, Palais–Smale condition.

2010 AMS Subject Classification: Primary: 49J35, 35A15, 35S15; Secondary: 47G20, 45G05.

1 Introduction

In this paper we are interested in the study of the following stationary Schrödinger system of equations: find an infinite sequence $(\lambda_m, u_m)_{m \geq 1}$ and a potential V satisfying

$$\begin{cases} -\Delta u_m + \tilde{V}_0 u_m + V u_m = \lambda_m u_m & \text{in } \Omega \\ -\Delta V = \sum_{m=1}^{\infty} \rho_m |u_m|^2 & \text{in } \Omega \end{cases} \quad (1a)$$

$$\quad (1b)$$

where, in addition, we require that

$$\begin{cases} u_m \in H_0^1(\Omega), & \text{for all } m \geq 1, \quad V \in H_0^1(\Omega), \\ (u_m)_{m \geq 1} & \text{is a Hilbert basis for } L^2(\Omega). \end{cases} \quad (2a)$$

$$\quad (2b)$$

Here we assume that the external potential \tilde{V}_0 and the positive numbers $(\rho_m)_{m \geq 1}$ are given.

The system (1a)-(1b) appears in the modeling of nanoscale semiconductor devices as part of the so-called “quantum-kinetic subband model”, which itself is a simplified model of the full evolution 3D-Schrödinger-Poisson equation N. Ben Abdallah & F. Méhats [1, 5]. In order to improve the cost of numerical simulation of the evolution 3D-Schrödinger-Poisson equation and taking advantage of the extreme confinement of the electrons in one direction transverse to the transport directions, one can perform a block diagonalisation of the electron Hamiltonian, thanks to a separation of the confinement and transport directions. This reduction process leads to replace the 3D-Schrödinger-Poisson equation by a system of 1D stationary Schrödinger equations (for the confinement) coupled to a 2D equation (for the transport). In that reduced model, the system of 1D stationary Schrödinger equations is nothing but (1a)-(1b) where the parameters $(\rho_m)_{m \geq 1}$ are the sequence of occupation numbers, which may depend on time and space, and which are given by the above mentioned 2D equation (for the transport).

On the other hand, as it is outlined in P. Zweifel [17], the Schrödinger-Poisson system of equations derives from a quantum transport equation, the Poisson-Wigner system. After, performing the Wigner transform to the former system one ends up with the following system of evolution equations

$$\begin{cases} i \partial_t \psi_m = -\Delta \psi_m + \tilde{V}_0 \psi_m + V \psi_m & (3a) \end{cases}$$

$$\begin{cases} \psi_m(0, x) = \psi_{0m}(x) & (3b) \end{cases}$$

$$\begin{cases} -\Delta V = \sum_{m=1}^{\infty} \rho_m |\psi_m|^2, & (3c) \end{cases}$$

with the condition $(\psi_{0m}|\psi_{0k})_{L^2} = \delta_{km}$ for any $k, m \geq 1$. Seeking standing-wave solutions of the form

$$\psi_m(t, x) := e^{-i\lambda_m t} u_m(x)$$

leads to the equations (1a)-(1b).

Existence of solutions to the system (1a)-(1b) has been proved in R. Illner, O. Kavian, H. Lange [2] in the case when $\rho_m = 0$ for any $m \geq 2$, and the same method extends to the case when $\rho_m = 0$ for any $m \geq M$ for a given $M \geq 2$. On the other hand, a different but similar eigenvalue problem has been considered by F. Nier [8, 10, 9].

In order to solve this system of equations, taking into account the fact that the family $(u_m)_{m \geq 1}$ must be contained in $H_0^1(\Omega)$ and, at the same time, has to be a Hilbert basis of $L^2(\Omega)$, we observe the following. Let us consider a fixed Hilbert basis of $L^2(\Omega)$, denoted by $(e_m)_{m \geq 1}$, such that $e_m \in H_0^1(\Omega)$ for all $m \geq 1$. For instance such a basis may be given by the eigenfunctions of the Laplace operator on $H_0^1(\Omega)$, that is a family satisfying

$$-\Delta e_m = \mu_m e_m, \quad e_m \in H_0^1(\Omega), \quad \int_{\Omega} e_\ell(x) e_m(x) dx = \delta_{\ell m}, \quad (4)$$

where the sequence of eigenvalues of the Laplace operator, with Dirichlet boundary conditions, is denoted by $(\mu_m)_{m \geq 1}$. Now, saying that the family $(u_m)_{m \geq 1}$ satisfies condition (2b) means that the linear operator U acting on $L^2(\Omega)$ and defined by

$$\text{for all } m \geq 1, \quad U e_m := u_m, \quad U f := \sum_{m \geq 1} (f|e_m) u_m \quad \text{for } f \in L^2(\Omega), \quad (5)$$

is a unitary operator, that is $U^*U = UU^* = I$. Therefore determining the whole family $(u_m)_{m \geq 1}$ satisfying equations (1a)–(2b) is equivalent to find a linear operator U defined on $L^2(\Omega)$ verifying

$$U^*U = UU^* = I, \quad U e_j \in H_0^1(\Omega) \quad \text{for } j \geq 1, \quad (6)$$

and such that the family $u_j := U e_j$ is the family of normalized eigenfunctions of (1a) where V is given by (1b).

In this paper we give a variational formulation of the system (1a)–(2b), yielding a solution in terms of critical points of a real valued functional defined on a subset of the group of unitary operators. More precisely we define a subset \mathbb{S} of unitary operators on $L^2(\Omega)$ as

$$\mathbb{S} := \{U : L^2(\Omega) \longrightarrow L^2(\Omega) ; U \text{ satisfies (6)}\}, \quad (7)$$

and then we define a functional J on \mathbb{S} by setting

$$J_0(U) := \sum_{m \geq 1} \rho_m \int_{\Omega} \left(|\nabla u_m(x)|^2 + \tilde{V}_0(x) u_m^2(x) \right) dx, \quad (8)$$

and then

$$J(U) := J_0(U) + \frac{1}{2} + \int_{\Omega} |\nabla V[U](x)|^2 dx, \quad (9)$$

where $u_m := Ue_m$ and $V[U]$ is the solution of (1b). The main purpose of this paper is to show that critical points of J on \mathbb{S} yield solutions of the Schrödinger–Poisson system and that the minimum of J is achieved on \mathbb{S} .

It is clear that in order to define the potential $V[U]$ and the functional J on the manifold \mathbb{S} some conditions must be imposed on the sequence $(\rho_m)_{m \geq 1}$.

Our main result concerning the system of equations (1a)–(2b) is the following:

Theorem 1 *Let $\Omega \subset \mathbb{R}^N$ be a bounded domain and $N \leq 3$. Assume that the sequence $(\rho_m)_{m \geq 1}$ satisfies*

$$\rho_m > 0, \quad \sum_{m \geq 1} m^{2/N} \rho_m < \infty, \quad (10)$$

and

$$\tilde{V}_0^+ \in L^1(\Omega), \quad \tilde{V}_0^- \in L^{p_0}(\Omega),$$

for some $p_0 > N/2$ (or $p_0 = 1$ if $N = 1$). Then the Schrödinger–Poisson system of equations (1a)–(2b) has a solution obtained as the minimum of the functional J defined in (9).

In order to give a clear exposition of our global approach to the determination of a system of eigenvectors in terms of unitary operators U , in this introduction we give an outline of our approach, getting rid of technicalities inherent to an infinite dimensional Hilbert space and to nonlinear problems. Thus, in a first step, assume that we are given a finite dimensional (complex)

Hilbert space H of dimension $n \geq 2$, its scalar product being denoted by $(\cdot|\cdot)$. If $A : H \rightarrow H$ is a self-adjoint, nonnegative operator (matrix), our aim is to define a procedure in which all the eigenvectors of A are determined at once, to compare with a step by step construction of eigenvalues

(and eigenvectors) through the construction of critical values of the Rayleigh quotient

$$\frac{(Au|u)}{(u|u)}, \quad u \neq 0,$$

by a min-max procedure. To this end, for $u_1, \dots, u_n \in H$ let us define the functional

$$F(u_1, \dots, u_n) := \sum_{j=1}^n \rho_j(Au_j|u_j),$$

where, as above, we assume that the coefficients ρ_j verify $\rho_j > 0$, and also, for the sake of simplicity of exposition (see below for the general case), here assume moreover that

$$\rho_i \neq \rho_j \quad \text{for } i \neq j.$$

Define the subset (or manifold) $S \subset H^n$ by

$$S := \{ (u_1, \dots, u_n) \in H^n ; (u_i|u_j) = \delta_{ij} \}$$

We claim that upon maximizing or minimizing F on the manifold $S \subset H^n$, all the eigenvectors of A can be determined (as a matter of fact, any critical point of F yields such a result).

We begin by observing that an orthonormal basis e_1, \dots, e_n of H being given once and for all, the manifold S can be identified with the set of unitary matrices U such that $U^*U = UU^* = I$, where I is the identity operator on H : indeed it is enough to see u_j as the j -th column of U , that is to set $u_j := Ue_j$. Then we see that $(Au_j|u_j) = (U^*AUe_j|e_j)$, and denoting by D the diagonal matrix $D := \text{diag}(\rho_1, \dots, \rho_n)$, that is the matrix defined by $De_j = \rho_j e_j$, we check easily that

$$F(u_1, \dots, u_n) = \sum_{j \geq 1} \rho_j(Au_j|u_j) = \sum_{j \geq 1} \rho_j(U^*AUe_j|e_j) = \text{tr}(DU^*AU),$$

where $\text{tr}(B)$ denotes the trace of the operator (or matrix) B . Finally, considering for instance the minimization of F , this can be reformulated in the following way:

$$\text{minimize } J(U) := \text{tr}(DU^*AU) \text{ under the constraint } U^*U = I.$$

Clearly J is C^∞ (in fact analytic) and positive on the set

$$\mathbf{SL}(n) := \{U : H \longrightarrow H ; U^*U = I\},$$

which is a smooth and compact manifold: therefore J achieves its minimum at some point $U_0 \in \mathbf{SL}(n)$. Now we have to show that the vectors $u_j := U_0 e_j$ are indeed the eigenvectors of A .

Let $M : H \rightarrow H$ be skew-adjoint (that is $M^* = -M$) and consider the one parameter group $U(t) = \exp(tM)U_0$ for $t \in \mathbb{R}$; note that since $M^* = -M$, one has $\exp(tM)^* = \exp(-tM)$ and thus one checks easily that having $U_0^* U_0 = I$, then for all $t \in \mathbb{R}$ one has $U(t) \in \mathbf{SL}(n)$, and consequently $J(U_0) \leq J(U(t))$ for all $t \in \mathbb{R}$. Now

$$J(U(t)) = \operatorname{tr}(DU_0^* \exp(-tM)A \exp(tM)U_0) \quad \text{and} \quad \left. \frac{dJ(U(t))}{dt} \right|_{t=0} = 0,$$

so that, after a straightforward calculation, we obtain

$$\begin{cases} \text{for all } M \text{ such that } M^* = -M, \text{ we have} \\ \operatorname{tr}(DU_0^* M A U_0) = \operatorname{tr}(DU_0^* A M U_0). \end{cases}$$

Setting

$$B := U_0 D U_0^*,$$

and using the fact that for two given matrices K, L we have $\operatorname{tr}(KL) = \operatorname{tr}(LK)$, we observe that $\operatorname{tr}(DU_0^* M A U_0) = \operatorname{tr}(MAB)$, and that

$$\operatorname{tr}(DU_0^* A M U_0) = \operatorname{tr}(BAM) = \operatorname{tr}(MBA).$$

Summing up, we conclude that

$$\text{for all } M \text{ such that } M^* = -M, \quad \text{we have} \quad \operatorname{tr}(M(AB - BA)) = 0.$$

Taking $M := (AB - BA)^*$, we conclude that $BA = AB$, that is

$$U_0 D U_0^* A = A U_0 D U_0^*.$$

Applying this equality to the vector $u_j := U_0 e_j$, and taking into account the definition of the diagonal operator D , we obtain (recall that $U_0^* U_0 = I$)

$$(U_0 D U_0^*) A u_j = A U_0 D U_0^* u_j = A U_0 D e_j = \rho_j A U_0 e_j = \rho_j A u_j,$$

that is $(U_0 D U_0^*) A u_j = \rho_j A u_j$, which means that $A u_j$ is an eigenvector of $U_0 D U_0^*$. This implies that $D(U_0^* A u_j) = \rho_j (U_0^* A u_j)$, and we see that $U_0^* A u_j$ is an eigenvector of D for the eigenvalue ρ_j , which is a simple eigenvalue of

D , corresponding to the eigenvector e_j . This means that there exists $\lambda_j \in \mathbb{C}$ such that $U_0^* A u_j = \lambda_j e_j$, that is

$$A u_j = \lambda_j u_j.$$

As a matter of fact one sees that $\lambda_j \in \mathbb{R}$, while u_j is an eigenvector of A and U_0 is a diagonalization operator for A , which consists in the matrix whose columns are the eigenvectors u_j . Actually this procedure allows us to construct all the eigenvectors of A through the minimization of a unique functional defined on the group $\mathbf{SU}(n)$. Also, since $F(U_0) = \sum_{j \geq 1} \lambda_j \rho_j$, one easily sees that different choices in ordering the numbers ρ_j yield different ordering of eigenvalues and eigenvectors of A : for instance one may check that if the ρ_j 's are decreasing, that is if $\rho_j > \rho_{j+1}$ for $1 \leq j \leq n-1$, then one obtains the eigenvalues of A in a non decreasing order, that is $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$. While if $\rho_j < \rho_{j+1}$ for $1 \leq j \leq n-1$, then one obtains the eigenvalues in a non increasing order, that is $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. (Had we began by maximizing J , the conclusion would be somehow reversed but analogous: if the ρ_j 's are decreasing then the λ_j 's would be non increasing).

In the next section of this paper we will show that, for a certain class of self-adjoint operators A , the eigenvectors and eigenvalues of A can be obtained through the minimization of the functional

$$J_0(U) := \text{tr}(DU^*AU)$$

on an appropriate subset of unitary operators U : this is precisely stated and proved in section 2. In section 3 we gather a certain number of preliminary results used in section 4, after stating the assumptions on the domain Ω and on the sequence $(\rho_m)_m$, we prove theorem 1, as well as slightly more general variants of the Schrödinger–Poisson systems (see theorem 12 in section 4). In section 5 we shall discuss some generalizations and state a few remarks about the results presented here.

2 Global determination of eigenvectors and eigenvalues

In this section we consider an infinite dimensional, separable, complex Hilbert space whose scalar product is denoted by $(\cdot|\cdot)$ and its norm by $\|\cdot\|$. We shall make the following assumptions:

Hypothesis 1 We assume that $(A, D(A))$ is a densely defined, selfadjoint positive operator acting on the Hilbert space H , and that the domain $D(A)$ equipped with its graph norm is compactly imbedded in H , so that A has a compact resolvent and A possesses a sequence of eigenvalues $(\mu_j)_{j \geq 1}$ such that $0 \leq \mu_j < \mu_{j+1}$, each eigenvalue having finite multiplicity $m_j \geq 1$, and $\mu_j \rightarrow +\infty$ as $j \rightarrow \infty$, H being infinite dimensional.

Denoting by $D(A^{1/2})$ the domain of $A^{1/2}$, that is the subspace of H obtained upon the completion of $D(A)$ with the scalar product $(u, v) \mapsto (u|v) + (Au|v)$, we recall that $D(A^{1/2})$ is dense in H . Hence we can introduce the next assumption:

Hypothesis 2 We consider a fixed Hilbert basis of H , denoted by $(e_j)_{j \geq 1}$, such that $e_j \in D(A^{1/2})$ for each $j \geq 1$.

With the Hilbert basis $(e_j)_{j \geq 1}$ given by hypothesis 2, we consider a sequence $(\rho_j)_{j \geq 1}$ of real numbers such that

$$\rho_j > 0, \quad \sum_{j \geq 1} \rho_j \|e_j\|_{D(A^{1/2})}^2 < \infty, \quad (11)$$

and we denote by D the diagonal operator defined by

$$De_j := \rho_j e_j, \quad \text{for } j \geq 1. \quad (12)$$

Note that since H is infinite dimensional and A has a compact resolvent, while $e_j \in D(A^{1/2})$, we have $\|e_j\|_{D(A^{1/2})} \rightarrow \infty$ as $j \rightarrow \infty$. Indeed, otherwise, the sequence $(e_j)_j$ would be bounded in $D(A^{1/2})$, and the imbedding $D(A^{1/2}) \subset H$ being compact, one would extract a subsequence $(e_{j_k})_{k \geq 1}$ such that $e_{j_k} \rightharpoonup f$ in $D(A^{1/2})$ and $e_{j_k} \rightarrow f$ strongly in H ; in particular $\|f\| = 1$, since $(e_j)_j$ is a Hilbert basis of H . But we have also $e_j \rightarrow 0$ in H , and thus we should have $f = 0$. This contradiction shows that $(e_j)_j$ cannot contain any bounded sequence in $D(A^{1/2})$. As a consequence we have $\rho_j \rightarrow 0$ and D is a compact operator.

Next we shall consider unitary operators $U : H \rightarrow H$ which satisfy the following condition (this expresses the fact that the operator DU^*AU is of trace class, see M. Reed & B. Simon [14], volume 1, section VI.6)

$$\begin{cases} U^*U = UU^* = I, & Ue_j \in D(A^{1/2}) \text{ for } j \geq 1, \\ \sum_{j \geq 1} \rho_j (U^*AUe_j|e_j) < \infty. \end{cases} \quad (13)$$

and we define the set \mathbb{S} through

$$\mathbb{S} := \{U : H \rightarrow H ; U \text{ satisfies (13)}\}. \quad (14)$$

Remark 2 Let us point out that such operators U exist, that is \mathbb{S} is not empty: indeed, not only for $t \in \mathbb{R}$ we have $e^{itA} \in \mathbb{S}$, but also for any $\lambda > 0$, the operator U_λ (the so-called Cayley transform of λA , see K. Yosida [16]) defined by

$$U_\lambda := (I + i\lambda A)(I - i\lambda A)^{-1}$$

is a bounded operator on H and one checks easily that

$$U_\lambda^* = (I - i\lambda A)(I + i\lambda A)^{-1},$$

so that $U_\lambda^* U_\lambda = I$. Moreover, for any $f \in D(A^{1/2})$ we have $(I + i\lambda A)^{-1} f \in D(A^{3/2})$, and thus $U_\lambda f \in D(A^{1/2})$. As a matter of fact, not only U_λ is a unitary operator on H , but one has also $\|U_\lambda f\|_{D(A^{1/2})} = \|f\|_{D(A^{1/2})}$. Therefore, since the sequence $(\rho_j)_j$ satisfies (11), one sees that U_λ satisfies (13) and $U_\lambda \in \mathbb{S}$.

For a unitary operator $U : H \rightarrow H$ satisfying (13), we define $J_0(U)$ by

$$J_0(U) := \text{tr}(DU^*AU) := \sum_{j \geq 1} \rho_j(U^*AUe_j|e_j) \quad (15)$$

The following result concerns eigenvectors of A :

Theorem 3 Assume that the hypotheses 1 and 2, as well as condition (11) are satisfied. Then the functional J_0 defined in (15) achieves its minimum on \mathbb{S} defined by (14). Then there exists $\widehat{U}_0 \in \mathbb{S}$ such that

$$J_0(\widehat{U}_0) = \min_{U \in \mathbb{S}} J_0(U),$$

and \widehat{U}_0 is a diagonalization operator for A ; more precisely, for each $j \geq 1$, the vector $\varphi_j := \widehat{U}_0 e_j$ is an eigenvector of A corresponding to the eigenvalue $\lambda_j := (A\varphi_j|\varphi_j)$.

Remark 4 It is clear that the eigenvalues $(\lambda_j)_{j \geq 1}$ are independent of the choice of the sequence $(\rho_j)_{j \geq 1}$. However, as pointed out in the introduction, if one assumes that the sequence $(\rho_j)_{j \geq 1}$ is decreasing, then the eigenvalues $(\lambda_j)_{j \geq 1}$ are ordered in a non decreasing order, that is $\lambda_j \leq \lambda_{j+1}$ for $j \geq 1$.

We split the proof of this result into a couple of lemmas.

Lemma 5 The functional J_0 achieves its minimum on \mathbb{S} at a certain $U_0 \in \mathbb{S}$.

Proof. Indeed consider the infimum $\alpha := \inf_{U \in \mathbb{S}} J_0(U)$. Since $\mathbb{S} \neq \emptyset$, we have $0 \leq \alpha < \infty$. Consider a minimizing sequence $(U_n)_{n \geq 1} \in \mathbb{S}$, such that for instance $\alpha \leq J(U_n) \leq \alpha + 1/n$. Then for each fixed $j \geq 1$, setting $u_j^n := U_n e_j$, we have for all $n \geq 1$

$$\|u_j^n\|_{D(A^{1/2})}^2 = 1 + (Au_j^n | u_j^n) \leq 1 + \frac{\alpha + 1}{\rho_j}.$$

Thus, since the inclusion $D(A^{1/2}) \subset H$ is compact, upon extracting subsequences through Cantor's diagonal scheme, and denoting again this diagonal subsequence by $(u_j^n)_n$, we may assume that for all $j \geq 1$ there exist a family $(u_j)_j$ such that for $j \geq 1$ fixed

$$u_j^n \rightharpoonup u_j \quad \text{weakly in } D(A^{1/2}), \quad u_j^n \rightarrow u_j \quad \text{strongly in } H$$

as $n \rightarrow \infty$. Setting $U_0 e_j := u_j$, one checks easily that U_0 can be extended by linearity to the subspace $\text{span}\{e_j ; j \geq 1\}$, and that for $f \in \text{span}\{e_j ; j \geq 1\}$ we have

$$\|U_0 f\|^2 = \lim_{n \rightarrow \infty} \|U_n f\|^2 = \|f\|^2.$$

In other words U_0 is a unitary operator on (the algebraic) $\text{span}\{e_j ; j \geq 1\}$, and therefore can be extended as such to the whole space H . Since for any $m \geq 1$ we have

$$\sum_{j=1}^m \rho_j (Au_j | u_j) \leq \liminf_{n \rightarrow \infty} \sum_{j=1}^m \rho_j (Au_j^n | u_j^n) \leq \liminf_{n \rightarrow \infty} J_0(U_n) = \alpha,$$

upon letting $m \rightarrow \infty$ we conclude that $J_0(U_0) \leq \alpha$. Thus, having $U_0^* U_0 = I$ and $U_0 e_j \in D(A^{1/2})$ for all $j \geq 1$, and $J_0(U_0) < \infty$, we have $U_0 \in \mathbb{S}$ and $J_0(U_0) = \alpha$. \square

Next we show that U_0 , given by lemma 5 is a diagonalization operator for A .

Lemma 6 *Under the assumptions of theorem 3, let U_0 be given by lemma 5, and set $u_j := U_0 e_j$, for $j \geq 1$.*

(i) *Assume that $k \geq 1$ is such that*

$$\rho_\ell \neq \rho_k \quad \text{for } \ell \neq k. \tag{16}$$

Then there exist $\lambda_k \in \mathbb{R}_+$ such that $Au_k = \lambda_k u_k$.

(ii) Assume that $k \geq 1$ is such that for some $m \geq 2$

$$\begin{cases} \rho_k = \rho_{k+\ell} & \text{for } 0 \leq \ell \leq m-1, \\ \rho_k \neq \rho_n & \text{for } n \notin \{k+\ell; 0 \leq \ell \leq m-1\}. \end{cases} \quad (17)$$

Then there exists a unitary transformation U_k of the m -dimensional space $H_k := \text{span}\{U_0 e_{k+\ell}; 0 \leq \ell \leq m-1\}$ such that if

$$\widehat{u}_{k+\ell} := U_k U_0 e_{k+\ell},$$

then there exists $\lambda_{k+\ell} \in \mathbb{R}_+$ such that $A\widehat{u}_{k+\ell} = \lambda_{k+\ell}\widehat{u}_{k+\ell}$ for $0 \leq \ell \leq m-1$.

Proof. First let $M : H \rightarrow H$ be a bounded skewadjoint operator such that $M : D(A^{1/2}) \rightarrow D(A^{1/2})$ is also bounded. Indeed such operators do exist (consider for instance $i(I + \lambda A)^{-1}$ for $\lambda > 0$). Setting $U(t) := \exp(-tM)U_0$ for $t \in \mathbb{R}$, one checks easily that, since $M^* = -M$, one has $U(t) \in \mathbb{S}$ for all t , and thus the function $g(t) := J_0(U(t))$ is well defined, is of class C^1 and achieves its minimum at $t = 0$. However since

$$g(t) = \text{tr}(DU_0^* \exp(tM)A \exp(-tM)U_0),$$

one concludes that

$$g'(0) = \text{tr}(DU_0^* M A U_0) - \text{tr}(DU_0^* A M U_0) = 0 \quad (18)$$

for all bounded operators $M : H \rightarrow H$ such that $M^* = -M$ and M is also bounded from $D(A^{1/2})$ into itself. In the same way, if we consider a bounded operator $L : H \rightarrow H$ such that $L = L^*$ and L is also bounded from $D(A^{1/2})$ into itself, upon setting $M := iL$, we conclude that (18) yields

$$\text{tr}(DU_0^* L A U_0) = \text{tr}(DU_0^* A L U_0), \quad (19)$$

for all such operators L .

Note that the above relation (18) yields that

$$\begin{aligned} \sum_{j \geq 1} \rho_j(U_0^* M A U_0 e_j | e_j) - \sum_{j \geq 1} \rho_j(U_0^* A M U_0 e_j | e_j) &= 0 \\ \sum_{j \geq 1} \rho_j(M A u_j | u_j) - \sum_{j \geq 1} \rho_j(A M u_j | u_j) &= 0, \end{aligned}$$

that is, since $M^* = -M$,

$$-\sum_{j \geq 1} \rho_j(Au_j|Mu_j) - \sum_{j \geq 1} \rho_j(AMu_j|u_j) = 0 \iff \operatorname{Re} \sum_{j \geq 1} \rho_j(Au_j|Mu_j) = 0. \quad (20)$$

Analogously using (19) one obtains in the same way

$$\sum_{j \geq 1} \rho_j(Au_j|Lu_j) = \sum_{j \geq 1} \rho_j(ALu_j|u_j) \iff \operatorname{Im} \sum_{j \geq 1} \rho_j(Au_j|Lu_j) = 0. \quad (21)$$

At this point, in a first step, assume that the integer k is such that condition (16) is fulfilled. Consider an integer $n \neq k$, so that $\rho_n \neq \rho_k$, and define the operators M and L in the following way

$$\begin{cases} Mu_k := u_n, & Mu_n := -u_k, \\ Lu_k := u_n, & Lu_n := u_k, \\ Lu_j = Mu_j = 0 & \text{for } j \notin \{k, n\}. \end{cases} \quad (22)$$

Clearly M and L satisfy the required conditions above, and using (20), with our choice of the operator M , we get $(\rho_n - \rho_k)\operatorname{Re}(Au_k|u_n) = 0$, that is, since $\rho_k - \rho_n \neq 0$,

$$\operatorname{Re}(Au_k|u_n) = 0.$$

Upon using (21), with our above choice of the operator L and the fact that $\rho_n - \rho_k \neq 0$, analogously we have that

$$\operatorname{Im}(Au_k|u_n) = 0.$$

So, from the above two relations, we infer that $(Au_k|u_n) = 0$ for all n such that $\rho_n \neq \rho_k$, that is

$$Au_k \in \operatorname{span}\{u_n ; n \neq k\}^\perp = \operatorname{span}\{u_k\},$$

where we use the fact that the family $(u_j)_j$ is a Hilbert basis of H , being the image of the Hilbert basis $(e_j)_j$ under the unitary operator U_0 . This means that $Au_k = \lambda_k u_k$ for some $\lambda_k \in \mathbb{C}$, but since A is a nonnegative self-adjoint operator, as a matter of fact we have $\lambda_k \geq 0$.

Next assume that the integer k is such that the coefficient ρ_k has multiplicity $m \geq 2$, that is condition (17) is satisfied. Arguing as above, we consider the following operators M and L : for $n \notin \{k + j ; 0 \leq j \leq m - 1\}$ and $0 \leq \ell \leq (m - 1)$ fixed, set

$$\begin{cases} Mu_{k+\ell} := u_n, & Mu_n := -u_{k+\ell}, \\ Lu_{k+\ell} := u_n, & Lu_n := u_{k+\ell} \\ Lu_j = Mu_j = 0 & \text{for all } j \notin \{n, k + \ell\}. \end{cases} \quad (23)$$

Then, proceeding as above, we conclude that $(Au_{k+\ell}|u_n) = 0$ for all $n \notin \{k+j; 0 \leq j \leq m-1\}$, that is:

$$Au_{k+\ell} \in (\text{span}\{u_n; n \neq k+j, 0 \leq j \leq m-1\})^\perp$$

that is

$$Au_{k+\ell} \in \text{span}\{u_{k+i}; 0 \leq i \leq m-1\}.$$

This means that if we set $H_k := \text{span}\{u_{k+i}; 0 \leq i \leq m-1\}$, then $A : H_k \rightarrow H_k$ is a self-adjoint operator on the finite dimensional space H_k . Therefore there exists a unitary operator U_k , acting on this space, such that if for $0 \leq \ell \leq m-1$ we set $\hat{u}_{k+\ell} = U_k u_{k+\ell} = U_k U_0 e_{k+\ell}$, we have $A\hat{u}_{k+\ell} = \lambda_{k+\ell}\hat{u}_{k+\ell}$ for some $\lambda_{k+\ell} \geq 0$. \square

As we may see from the above analysis, when all the ρ_j 's are distinct, then U_0 , any unitary operator which minimizes J_0 , is a diagonalization operator for A . However in the general case, when some of the coefficients ρ_k have multiplicity $m_k \geq 2$, it is possible that one has to impose a unitary transformation U_k in the space

$$H_k := \text{span}\{U_0 e_{k+\ell}; 0 \leq \ell \leq m_k - 1\}$$

in order to have the operator A diagonalized. In other words, one may find a unitary operator U_k on H_k such that if $A_k := A|_{H_k}$ is the trace of A on H_k , the operator $U_k^* A_k U_k$ is diagonal. Thus since $\rho_k = \rho_{k+\ell}$ for $0 \leq \ell \leq m-1$, if we denote by \hat{U} the unitary operator obtained through the composition of all such operators U_k and U_0 , one has $J_0(\hat{U}) = J_0(U_0)$. More precisely, we can state the following corollary, which ends the proof of theorem 3:

Corollary 7 *Under the assumptions of theorem 3, let U_k be given by lemma 6 when $k \geq 1$ is such that (17) is satisfied. Then the operator \hat{U}_0 defined by $\hat{U}_0 e_k = U_0 e_k$ when k satisfies (16), and*

$$\hat{U}_0 e_{k+\ell} := U_k U_0 e_{k+\ell}, \quad \text{for } 0 \leq \ell \leq m-1, \quad \text{when (17) is satisfied,}$$

belongs to \mathbb{S} , while $J_0(\hat{U}_0) = J_0(U_0)$ and $\hat{U}_0^ A \hat{U}_0$ is diagonal. Setting $\varphi_j := \hat{U}_0 e_j$ for $j \geq 1$, then there exists $\lambda_j \geq 0$ such that $A\varphi_j = \lambda_j \varphi_j$.*

Remark 8 *Regarding the finite dimensional case, R.V. Kohn (private communication) mentioned to us a result due to J. von Neumann [7] which states that for two $n \times n$ matrices A and B*

$$|\text{tr}(AB)| \leq \sum_{j=1}^n \sigma_j(A) \sigma_j(B)$$

where $(\sigma_j(A))_{1 \leq j \leq n}$ and $(\sigma_j(B))_{1 \leq j \leq n}$ denote the decreasing singular values of A and B respectively. From this L. Mirsky [6] points out that one can conclude another result due to J. von Neumann, stating that:

$$\sup_{U, V} |\operatorname{tr}(BUAV)| = \sum_{j=1}^n \sigma_j(A)\sigma_j(B).$$

Our result in the finite dimensional case, specialized to self-adjoint matrices, can be interpreted as another proof of the above result in that particular case, and also characterizes the diagonalization matrix by a variational method.

3 Preliminary results for Schrödinger–Poisson system

In this section we prove an existence result regarding the system of equations (1a)–(2b). We shall assume that

$$\Omega \subset \mathbb{R}^N \text{ is a bounded domain and that } N \leq 3, \quad (24)$$

and we endow the (complex) space $L^2(\Omega)$ with its scalar product denoted by $(\cdot | \cdot)$ and its norm $\|\cdot\|$. Let \tilde{V}_0 be a real valued potential such that

$$\tilde{V}_0^+ \in L^1(\Omega), \quad \tilde{V}_0^- \in L^{p_0}(\Omega) \text{ for some } p_0 > \frac{N}{2} \text{ and } p_0 \geq 1. \quad (25)$$

Then we define an unbounded operator $(A, D(A))$ by setting

$$D(A) := \left\{ u \in H_0^1(\Omega) ; -\Delta u + \tilde{V}_0 u \in L^2(\Omega) \right\}, \quad Au := -\Delta u + \tilde{V}_0 u. \quad (26)$$

This operator is self-adjoint, has a compact resolvent, and there exists a Hilbert basis of eigensystem denoted by $(\lambda_m, \varphi_m)_{m \geq 1}$, that is (here δ_{mn} being the Kronecker symbol)

$$-\Delta \varphi_m + \tilde{V}_0 \varphi_m = \lambda_m \varphi_m, \quad \varphi_m \in H_0^1(\Omega), \quad \int_{\Omega} \varphi_m(x) \varphi_n(x) dx = \delta_{mn}.$$

It is well-known that by Weyl's theorem there exist two positive constants c_1, c_2 , depending on Ω and \tilde{V}_0 , such that for all integers $m \geq 1$ one has

$$c_1 m^{2/N} \leq \lambda_m \leq c_2 m^{2/N}.$$

(See for instance [3], chapter 5, § 3, where the case of Neumann boundary conditions is also treated). For this reason, as far as the sequence $(\rho_m)_{m \geq 1}$

is concerned, in order to ensure the finiteness of the functionals we are going to minimize, we assume that the growth condition (10) is satisfied.

For a given unitary operator $U : L^2(\Omega) \rightarrow L^2(\Omega)$ we shall denote by $V := V[U]$ the potential defined by the Poisson equation (here $|U\varphi_j|$ denotes the modulus of the function $U\varphi_j$)

$$-\Delta V = \sum_{j \geq 1} \rho_j |U\varphi_j|^2 \quad \text{in } \Omega, \quad V \in H_0^1(\Omega). \quad (27)$$

It is noteworthy to recall that, thanks to the Sobolev imbedding theorem we have $H_0^1(\Omega) \subset L^{2^*}(\Omega)$, where $2^* = 2N/(N-2)$ when $N \geq 3$, while 2^* can be any finite exponent if $N = 2$, and $2^* = \infty$ if $N = 1$: thus, when $N \leq 3$, the right hand side of the above equation belongs to some $L^q(\Omega)$ with $q > N/2$, and more precisely a classical regularity result (see for instance [4]) states that there exists a constant $c > 0$ such that if $V \in H_0^1(\Omega)$ satisfies $-\Delta V = f$ and $f \in L^q(\Omega)$, then

$$\|V\|_\infty \leq c \|f\|_q. \quad (28)$$

Therefore, if $V := V[U]$ is given by (27) we have $V \in L^\infty(\Omega)$ when $N \leq 3$ (see below lemma 11). Note also that by the maximum principle we have $V[U] > 0$ in Ω .

It is useful to consider the Sobolev space \mathbb{H}_1 endowed with the norm $\|\cdot\|_{\mathbb{H}_1}$:

$$\mathbb{H}_1 := \left\{ u \in H_0^1(\Omega) ; \|u\|_{\mathbb{H}_1}^2 := \|\nabla u\|^2 + \int_\Omega \tilde{V}_0^+(x) |u(x)|^2 dx < \infty \right\}.$$

The imbedding $\mathbb{H}_1 \subset L^2(\Omega)$ is compact. Note that since the eigenfunctions φ_m belong to $L^\infty(\Omega)$, we have $\varphi_m \in \mathbb{H}_1$.

Regarding the manifold \mathbb{S} defined in (7), we have to modify it slightly, as we did in section § 2. More precisely we shall consider unitary operators $U : L^2(\Omega) \rightarrow L^2(\Omega)$ such that

$$U^*U = UU^* = I, \quad U\varphi_j \in \mathbb{H}_1 \quad \text{for } j \geq 1, \quad \sum_{j \geq 1} \rho_j (U^*AU\varphi_j | \varphi_j) < \infty, \quad (29)$$

and we consider the manifold defined by

$$\mathbb{S} := \{U : L^2(\Omega) \rightarrow L^2(\Omega) ; U \text{ satisfies (29)}\}. \quad (30)$$

We denote by D the diagonal operator acting on $L^2(\Omega)$ defined by $D\varphi_j = \rho_j\varphi_j$, and for $U \in \mathbb{S}$ we define the functionals J_0 and J_1 as follows:

$$J_0(U) := \text{tr}(DU^*AU) = \sum_{j \geq 1} \rho_j \int_\Omega \left(|\nabla U\varphi_j|^2(x) + \tilde{V}_0(x) |U\varphi_j|^2(x) \right) dx \quad (31)$$

and

$$\begin{aligned}
J_1(U) &:= \frac{1}{2} \int_{\Omega} |\nabla V[U]|^2(x) dx \\
&= \left\langle -\frac{1}{2} \Delta V[U], V[U] \right\rangle \\
&= \frac{1}{2} \sum_{j \geq 1} \rho_j (V[U] U \varphi_j |U \varphi_j) = \frac{1}{2} \text{tr}(DU^* V[U] U),
\end{aligned} \tag{32}$$

where, in the last equality of (32), by an abuse of notation, we denote by $V[U]$ the (linear) multiplication operator $f \mapsto V[U]f$. Since we assume $N \leq 3$, we know that $V[U] \in L^\infty(\Omega)$ as seen above, so that this operator acts boundedly on $L^2(\Omega)$.

Note that here the potential \tilde{V}_0 may have a negative part, so at some point we will need to ensure that the functional J_0 is bounded below, and that is *coercive* in some sense. More precisely we have:

Lemma 9 *There exists $C \geq 0$ such that for any $U \in \mathbb{S}$ one has*

$$J_0(U) \geq \frac{1}{2} \sum_{j \geq 1} \rho_j \int_{\Omega} \left(|\nabla U \varphi_j|^2 + 2\tilde{V}_0^+ |U \varphi_j|^2 \right) dx - C.$$

Proof. Assume that $N = 3$ (the case $N \leq 2$ can be handled in a similar way). For $t > 0$ and $u \in H_0^1(\Omega)$ such that $\|u\| = 1$ we have

$$\begin{aligned}
\int_{\Omega} \tilde{V}_0^- |u|^2 dx &= \int_{[\tilde{V}_0^- > t]} \tilde{V}_0^- |u|^2 dx + \int_{[\tilde{V}_0^- \leq t]} \tilde{V}_0^- |u|^2 dx \\
&\leq \int_{\Omega} 1_{[\tilde{V}_0^- > t]} \tilde{V}_0^- |u|^2 dx + t \int_{\Omega} |u|^2 dx \\
&\leq \|1_{[\tilde{V}_0^- > t]} \tilde{V}_0^-\|_{L^{N/2}} \|u\|_{L^{2^*}}^2 + t \\
&\leq C_1(N) \text{meas}([\tilde{V}_0^- > t])^\theta \|\tilde{V}_0^-\|_{L^{p_0}} \|\nabla u\|^2 + t
\end{aligned}$$

where we have used Hölder's inequality twice (once with $N/(N-2)$ and $(N/(N-2))' = N/2$, once with p_0 and $N/2$, where $\theta = (2/N) - (1/p_0) = (2/3) - (1/p_0) > 0$). We used also Sobolev's inequality $\|u\|_{2^*} \leq C \|\nabla u\|$. Now, since $\tilde{V}_0^- \in L^{p_0}(\Omega)$, we know that $\text{meas}([\tilde{V}_0^- > t]) \rightarrow 0$ as $t \rightarrow +\infty$. We choose $t > 0$ large enough to ensure that

$$C_1(N) \text{meas}([\tilde{V}_0^- > t])^\theta \|\tilde{V}_0^-\|_{L^{p_0}} \leq \frac{1}{2}.$$

Then we have for all $u \in \mathbb{H}_1$

$$\int_{\Omega} |\nabla u|^2 dx + \int_{\Omega} \tilde{V}_0 |u|^2 dx \geq \frac{1}{2} \|\nabla u\|^2 + \int_{\Omega} \tilde{V}_0^+ |u|^2 dx - t.$$

Applying this to $u := U\varphi_j$, multiplying by $\rho_j > 0$ and calculating the sum over j yields the inequality claimed by our lemma, with $C := t \sum_{j \geq 1} \rho_j$. \square

It is well known that the fact that the functional $u \mapsto \|\nabla u\|^2$ is weakly sequentially lower semi-continuous (l.s.c.) on $H_0^1(\Omega)$ plays a crucial role in many, if not all, minimization problems. Regarding the functional J_0 we need an analogous property which is stated below:

Lemma 10 *The functional J_0 is “weakly sequentially lower semi-continuous” in the following sense: let $(U_n)_{n \geq 1}$ be a sequence in \mathbb{S} such that for some $R > 0$ and all $n \geq 1$ one has $J_0(U_n) \leq R$. Then there exists a subsequence $(U_{n_k})_k$ such that for any fixed $j \geq 1$ one has $U_{n_k}\varphi_j \rightharpoonup u_j$ in \mathbb{H}_1 as $k \rightarrow +\infty$, and if we set $u_j^{n_k} := U_{n_k}\varphi_j$ and we define a linear operator U by setting $U\varphi_j := u_j$ we have $u_j^{n_k} \rightarrow u_j$ strongly in $L^2(\Omega)$ and*

$$\lim_{k \rightarrow \infty} \int_{\Omega} \tilde{V}_0^- |u_j^{n_k}|^2 dx = \int_{\Omega} \tilde{V}_0^- |u_j|^2 dx, \quad U \in \mathbb{S}, \quad J_0(U) \leq \liminf_{k \rightarrow \infty} J_0(U_{n_k}).$$

Proof. Assume $N = 3$. Thanks to lemma 9, we know that

$$\sum_{j \geq 1} \rho_j \int_{\Omega} (|\nabla U_n \varphi_j|^2 + 2\tilde{V}_0^+ |U_n \varphi_j|^2) dx \leq 2R + 2C =: C_1.$$

This implies that for each $j \geq 1$ fixed the sequence $(u_j^n)_n := (U_n \varphi_j)_n$ is bounded in \mathbb{H}_1 , more precisely $\|u_j^n\|_{\mathbb{H}_1}^2 \leq C/\rho_j$. By using Cantor’s diagonal scheme and the compactness of the imbedding $\mathbb{H}_1 \subset L^2(\Omega)$, we may extract a subsequence denoted by $(u_j^{n_k})_{k \geq 1}$ such that

$$\begin{cases} u_j^{n_k} \rightharpoonup u_j & \text{weakly in } \mathbb{H}_1, \\ u_j^{n_k} \rightarrow u_j & \text{strongly in } L^2(\Omega), \\ u_j^{n_k} \rightarrow u_j & \text{a.e. in } \Omega, \end{cases}$$

as $k \rightarrow \infty$. For any $m \geq 1$ fixed, we have

$$\sum_{j=1}^m \rho_j \|u_j\|_{\mathbb{H}_1}^2 \leq \liminf_{k \rightarrow \infty} \sum_{j=1}^m \rho_j \|u_j^{n_k}\|_{\mathbb{H}_1}^2 \leq \liminf_{k \rightarrow \infty} \sum_{j=1}^{\infty} \rho_j \|u_j^{n_k}\|_{\mathbb{H}_1}^2 \leq C.$$

and finally

$$\sum_{j=1}^{\infty} \rho_j \|u_j\|_{\mathbb{H}_1}^2 \leq \liminf_{k \rightarrow \infty} \sum_{j=1}^{\infty} \rho_j \|u_j^{n_k}\|_{\mathbb{H}_1}^2 \leq C, \quad (33)$$

Setting $U\varphi_j := u_j$, one checks easily that U can be extended by linearity to the subspace $\text{span}\{\varphi_j ; j \geq 1\}$, and that for $f \in \text{span}\{\varphi_j ; j \geq 1\}$ we have

$$\|Uf\|^2 = \lim_{n \rightarrow \infty} \|U_n f\|^2 = \|f\|^2.$$

In other words U is a unitary operator on (the algebraic) $\text{span}\{\varphi_j ; j \geq 1\}$, and therefore can be extended as such to the whole space $L^2(\Omega)$. Then (33) shows that $U \in \mathbb{S}$.

We note also that in particular we have

$$\sum_{j \geq 1} \rho_j \int_{\Omega} \tilde{V}_0^-(x) |u_j(x)|^2 dx < \infty. \quad (34)$$

Since we assume $N = 3$, the strong convergence of $u_j^{n_k} \rightarrow u_j$ in $L^2(\Omega)$ implies (through Hölder's inequality, or interpolation between $L^2(\Omega)$ and $L^6(\Omega)$) that for any fixed $p < 3$, and any $j \geq 1$ we have that $u_j^{n_k} \rightarrow u_j$ strongly in $L^{2p}(\Omega)$ and a.e. in Ω , and thus $|u_j^{n_k}|^2 \rightarrow |u_j|^2$ strongly in $L^p(\Omega)$. Since $\tilde{V}_0^- \in L^{p_0}(\Omega)$ and $p_0 > 3/2$, taking $p := p'_0 = p_0/(p_0 - 1)$ we conclude first that

$$\lim_{k \rightarrow \infty} \int_{\Omega} \tilde{V}_0^- |u_j^{n_k}|^2 dx = \int_{\Omega} \tilde{V}_0^- |u_j|^2 dx,$$

and then thanks to (34) and the monotone convergence theorem,

$$\lim_{k \rightarrow \infty} \sum_{j \geq 1} \rho_j \int_{\Omega} \tilde{V}_0^- |u_j^{n_k}|^2 dx = \sum_{j \geq 1} \rho_j \int_{\Omega} \tilde{V}_0^- |u_j|^2 dx.$$

From this and (33) it is clear that

$$\begin{aligned} \sum_{j=1}^{\infty} \rho_j \int_{\Omega} \left(|\nabla u_j|^2 + \tilde{V}_0^+(x) |u_j| \right) dx &\leq \liminf_{k \rightarrow \infty} J_0(U_{n_k}) \\ &\quad + \lim_{k \rightarrow \infty} \sum_{j \geq 1} \rho_j \int_{\Omega} \tilde{V}_0^- |u_j^{n_k}|^2 dx \\ &\leq \liminf_{k \rightarrow \infty} J_0(U_{n_k}) \\ &\quad + \sum_{j \geq 1} \rho_j \int_{\Omega} \tilde{V}_0^- |u_j|^2 dx, \end{aligned}$$

which means that $J_0(U) \leq \liminf_{k \rightarrow \infty} J_0(U_{n_k})$, as claimed. \square

Regarding the functional J_1 we have the following result:

Lemma 11 *The functional J_1 is “weakly sequentially continuous” in the following sense: let $(U_n)_{n \geq 1}$ be a sequence in \mathbb{S} such that for some $R > 0$ and all $n \geq 1$ one has*

$$\sum_{j \geq 1} \rho_j \|U_n \varphi_j\|_{\mathbb{H}_1}^2 \leq R,$$

and such that for any fixed $j \geq 1$ one has $U_n \varphi_j \rightharpoonup u_j$ in \mathbb{H}_1 as $n \rightarrow +\infty$. If we set $u_j^n := U_n \varphi_j$ and we define a linear operator U by setting $U \varphi_j := u_j$ we have $V[U^n] \rightarrow V[U]$ strongly in $L^\infty(\Omega) \cap H_0^1(\Omega)$ and $J_1(U^n) \rightarrow J_1(U)$ as $n \rightarrow \infty$.

Proof. Let us assume $N = 3$, as the cases $N \leq 2$ is easily handled analogously. Since $u_j^n \rightharpoonup u_j$ in \mathbb{H}_1 , we have $u_j^n \rightarrow u_j$ strongly in $L^2(\Omega)$. By Sobolev imbedding theorem we conclude that for $3 < p < 6$ for some constants $c > 0$ and $\theta := 3(p-2)/(2p)$ we have

$$\| |u_j^n|^2 \|_{p/2} = \|u_j^n\|_p^2 \leq c \|u_j^n\| \cdot \|u_j^n\|_6^{2\theta} \leq c \|u_j^n\| \cdot \|\nabla u_j^n\|^{2\theta} = c \|\nabla u_j^n\|^{2\theta}.$$

From this we infer first that $|u_j^n|^2 \rightarrow |u_j|^2$ in $L^{p/2}(\Omega)$ as $n \rightarrow \infty$, and next that for any $m \geq 1$ fixed, and setting $q_0 := 1/\theta > 1$ and $q'_0 = q_0/(q_0-1) < \infty$ we have

$$\begin{aligned} \left\| \sum_{j>m} \rho_j |u_j^n|^2 \right\|_{p/2} &\leq \sum_{j>m} \rho_j \|u_j^n\|_p^2 \leq c \sum_{j>m} \rho_j \|\nabla u_j^n\|^{2\theta} \\ &\leq c \left(\sum_{j>m} \rho_j \right)^{1/q'_0} \left(\sum_{j>m} \rho_j \|\nabla u_j^n\|^2 \right)^{1/q_0} \leq c R^{1/q} \left(\sum_{j>m} \rho_j \right)^{1/q'} \end{aligned}$$

From this it follows that

$$\sum_{j \geq 1} \rho_j |u_j^n|^2 \rightarrow \sum_{j \geq 1} \rho_j |u_j|^2 \quad \text{strongly in } L^{p/2}(\Omega),$$

for any $p \in (3, 6)$. Therefore thanks to (28) we have that $V[U_n] \rightarrow V[U]$ strongly in $L^\infty(\Omega)$ and finally

$$\sum_{j \geq 1} \rho_j \int_{\Omega} V[U_n] |u_j^n|^2 dx \rightarrow \sum_{j \geq 1} \rho_j \int_{\Omega} V[U] |u_j|^2 dx,$$

as $n \rightarrow \infty$, which means that $J_1(U_n) \rightarrow J_1(U)$. □

4 Existence of solutions for the Schrödinger–Poisson system

In this section we solve the following Schrödinger–Poisson problem:

$$\begin{cases} -\Delta u_m + \tilde{V}_0 u_m + V u_m = \lambda_m u_m & \text{in } \Omega \\ -\Delta V = \sum_{m=1}^{\infty} \rho_m |u_m|^2 & \text{in } \Omega \end{cases} \quad (35a)$$

$$(35b)$$

and moreover

$$\begin{cases} u_m \in H_0^1(\Omega), \text{ for all } m \geq 1, & V \in H_0^1(\Omega), \\ (u_m)_{m \geq 1} \text{ is a Hilbert basis for } L^2(\Omega). \end{cases} \quad (36a)$$

$$(36b)$$

The main result of this section is:

Theorem 12 *Assume that the hypotheses (24)–(25), as well as condition (10) are satisfied. The functionals J_0 and J_1 being defined in (31)–(32), we set $J(U) := J_0(U) + J_1(U)$ for $U \in \mathbb{S}$ given by (30). Then J achieves its minimum on \mathbb{S} and there exists $\hat{U}_0 \in \mathbb{S}$ such that $J_0(\hat{U}_0) = \min_{U \in \mathbb{S}} J_0(U)$, and the family $u_j := \hat{U}_0 \varphi_j$ is solution to (35a)–(36b). Moreover if $V \in H_0^1(\Omega)$ satisfies by $-\Delta V = \sum_{m \geq 1} \rho_m |u_m|^2$, then the eigenvalues λ_j are given by*

$$\lambda_j := (-\Delta u_j + \tilde{V}_0 u_j + V u_j |u_j|) = \int_{\Omega} |\nabla u_j|^2 dx + \int_{\Omega} (\tilde{V}_0 + V) u_j(x)^2 dx.$$

We split the proof of this theorem into several lemmas. First we show that J achieves indeed its minimum.

Lemma 13 *The functional J achieves its minimum on \mathbb{S} at a certain $U_0 \in \mathbb{S}$.*

Proof. Since $\mathbb{S} \neq \emptyset$ and J_0 is bounded below (see lemma 9), so is J and the infimum

$$\alpha := \inf_{U \in \mathbb{S}} J(U)$$

is finite. Consider a minimizing sequence $(U_n)_{n \geq 1} \in \mathbb{S}$, such that for instance $\alpha \leq J(U_n) \leq \alpha + 1/n$. In particular $J_0(U_n) \leq 1 + \alpha$, and thanks to lemma 10, there exists a subsequence (which denote again by U_n) such that if we set setting $u_j^n := U_n \varphi_j$ for each fixed $j \geq 1$, we have, for all $2 \leq p < 2^*$,

$$\begin{cases} u_j^n \rightharpoonup u_j & \text{weakly in } \mathbb{H}_1, \\ u_j^n \rightarrow u_j & \text{strongly in } L^p(\Omega), \\ u_j^n \rightarrow u_j & \text{a.e. in } \Omega, \end{cases}$$

and the operator U_0 being defined by $U_0\varphi_j := u_j$, we have $U_0 \in \mathbb{S}$ and

$$J_0(U_0) \leq \liminf_{n \rightarrow \infty} J_0(U_n).$$

On the other hand, thanks to lemma 11, we know that $V[U_n] \rightarrow V[U_0]$ in $L^\infty(\Omega)$ and that $J_1(U_n) \rightarrow J_1(U_0)$. Thus

$$\alpha = \liminf_{n \rightarrow \infty} J(U_n) = \liminf_{n \rightarrow \infty} J_0(U_n) + \lim_{n \rightarrow \infty} J_1(U_n) \geq J_0(U_0) + J_1(U_0) = J(U_0),$$

that is, since $U_0 \in \mathbb{S}$, we have $J_0(U_0) = \alpha = \inf_{U \in \mathbb{S}} J(U)$. \square

Lemma 14 *Let U_0 be given by lemma 13, and let $M : H \rightarrow H$ be a bounded skewadjoint operator such that $M : \mathbb{H}_1 \rightarrow \mathbb{H}_1$ is also bounded. Set $U(t) := \exp(-tM)U_0$ for $t \in \mathbb{R}$, and $g_0(t) := J_0(U(t))$. Then g_0 is of class C^1 and*

$$g'_0(0) = -2\operatorname{Re} \sum_{j \geq 1} \rho_j(AU_0\varphi_j | MU_0\varphi_j). \quad (37)$$

Proof. First one checks easily that, since $M^* = -M$, one has $U(t) \in \mathbb{S}$ for all t , and thus the function

$$g_0(t) := J_0(U(t)) = \sum_{j \geq 1} \rho_j(AU(t)\varphi_j | U(t)\varphi_j)$$

is well defined and is of class C^1 . Since $U'(t) := dU(t)/dt = -M \exp(-tM)U_0$, one sees that

$$g'_0(t) = \sum_{j \geq 1} \rho_j(AU'(t)\varphi_j | U(t)\varphi_j) + \sum_{j \geq 1} \rho_j(AU(t)\varphi_j | U'(t)\varphi_j),$$

and finally,

$$g'_0(0) = - \sum_{j \geq 1} \rho_j(AMU_0\varphi_j | U_0\varphi_j) - \sum_{j \geq 1} \rho_j(AU_0\varphi_j | MU_0\varphi_j),$$

which yields our claim since $A^* = A$. \square

We have an analogous result concerning the functional J_1 : before showing this, we need to show that the mapping $U \mapsto V[U]$ is smooth.

Lemma 15 *Let U_0 be given by lemma 13, and let $M : H \rightarrow H$ be a bounded skewadjoint operator such that $M : \mathbb{H}_1 \rightarrow \mathbb{H}_1$ is also bounded. Set $U(t) := \exp(-tM)U_0$ for $t \in \mathbb{R}$. Denoting by $V(t)$ the mapping $t \mapsto V[U(t)]$,*

then $t \mapsto V(t)$ is of class C^1 from \mathbb{R} into $L^\infty(\Omega) \cap H_0^1(\Omega)$ and denoting by W the solution of

$$-\Delta W = -2\operatorname{Re} \sum_{j \geq 1} \rho_j (MU_0 \varphi_j) \overline{U_0 \varphi_j}, \quad W \in H_0^1(\Omega),$$

we have $V'(0) = W$.

Proof. The fact that for all $T > 0$ and $t \in [-T, T]$ we have

$$\|M \exp(-tM)U_0 \varphi_j\|_{\mathbb{H}_1} \leq \|M\|_{\mathcal{L}(\mathbb{H}_1)} \exp(T\|M\|_{\mathcal{L}(\mathbb{H}_1)}) \|U_0 \varphi_j\|_{\mathbb{H}_1},$$

shows that for any $p \in (3, 6)$ (see the proof of lemma 11) the mapping

$$t \mapsto \sum_{j \geq 1} \rho_j |U(t) \varphi_j|^2$$

is of class C^1 from $(-T, T) \rightarrow L^{p/2}(\Omega) \subset H^{-1}(\Omega)$, and thus using (28), the mapping $t \mapsto V(t) := V[U(t)]$ is of class C^1 from $(-T, T)$ into $L^\infty(\Omega) \cap H_0^1(\Omega)$. The calculation of $V'(0)$ is straightforward. \square

Now we can state the following result, which will allow us to characterize U_0 given by lemma 13.

Lemma 16 *Let U_0 be given by lemma 13, and let $M : H \rightarrow H$ be a bounded skewadjoint operator such that $M : \mathbb{H}_1 \rightarrow \mathbb{H}_1$ is also bounded. Set $U(t) := \exp(-tM)U_0$ for $t \in \mathbb{R}$, and $g_1(t) := J_1(U(t))$. Then g_1 is of class C^1 and*

$$g_1'(0) = -2 \operatorname{Re} \sum_{j \geq 1} \rho_j (V[U_0]U_0 \varphi_j | MU_0 \varphi_j). \quad (38)$$

Proof. Thanks to lemma 15 one checks easily that the function

$$g_1(t) := J_1(U(t)) = \frac{1}{2} \int_{\Omega} |\nabla V[U(t)]|^2 dx = \frac{1}{2} (-\Delta V[U(t)] | V[U(t)])$$

is C^1 , and that denoting by $W := V'(0)$, we have (with $V_0 := V[U_0]$)

$$\begin{aligned} g_1'(0) &= (-\Delta W | V_0) = -2 \operatorname{Re} \sum_{j \geq 1} \rho_j \int_{\Omega} (MU_0 \varphi_j) \overline{U_0 \varphi_j} V_0 dx \\ &= -2 \operatorname{Re} \sum_{j \geq 1} \rho_j (MU_0 \varphi_j | V_0 U_0 \varphi_j), \end{aligned}$$

where we use the fact that $V_0 := V[U_0]$ is real valued. \square

The following result is analogous to lemma 6: the only difference is that due to the presence of the nonlinear term we have to check that when some ρ_k has multiplicity $m \geq 2$, we can still proceed as before.

Lemma 17 *Under the assumptions of theorem 12, let U_0 be given by lemma 13, and set $u_j := U_0\varphi_j$, for $j \geq 1$. Then the conclusions of lemma 6 hold.*

Proof. The proof is very much the same as in lemma 6, so we give only the outline and the changes to be made. With the notations of lemmas 14 and 16, we set $g(t) := J(U(t)) = g_0(t) + g_1(t)$. Since $g(0) \leq g(t)$ for all $t \in \mathbb{R}$, we have $g'(0) = 0$, that is

$$\operatorname{Re} \sum_{j \geq 1} \rho_j (AU_0\varphi_j | MU_0\varphi_j) + \operatorname{Re} \sum_{j \geq 1} \rho_j (V[U_0]U_0\varphi_j | MU_0\varphi_j) = 0 \quad (39)$$

for all bounded skew-adjoint operators M such that $M : \mathbb{H}_1 \rightarrow \mathbb{H}_1$ is also bounded.

In the same way, if we consider a bounded adjoint operator L such that $L : \mathbb{H}_1 \rightarrow \mathbb{H}_1$ is also bounded, we may set $M := iL$ and conclude that (39) yields

$$\operatorname{Im} \sum_{j \geq 1} \rho_j (AU_0\varphi_j | LU_0\varphi_j) + \operatorname{Im} \sum_{j \geq 1} \rho_j (V[U_0]U_0\varphi_j | LU_0\varphi_j) = 0 \quad (40)$$

for all such operators L .

At this point, in a first step, assume that the integer k is such that condition (16) is fulfilled. Choosing M and L as in (22), and proceeding exactly as in the proof of lemma 6, using the fact that $\rho_k - \rho_n \neq 0$, we conclude that

$$(Au_k + V[U_0]u_k | u_n) = 0,$$

that is

$$Au_k + V[U_0]u_k \in \operatorname{span}\{u_n ; n \neq k\}^\perp = \operatorname{span}\{u_k\}.$$

This means that

$$Au_k + V[U_0]u_k = \lambda_k u_k$$

for some $\lambda_k \in \mathbb{C}$, but since $A + V[U_0]$ is a self-adjoint operator, as a matter of fact we have $\lambda_k \in \mathbb{R}$.

Next assume that the integer k is such that the coefficient ρ_k has multiplicity $m \geq 2$, that is condition (17) is satisfied. Arguing as above, we choose the operators M and L as in (23), and conclude that

$$(Au_{k+\ell} + V[U_0]u_{k+\ell}|u_n) = 0$$

for all $n \notin \{k+j; 0 \leq j \leq m-1\}$, that is:

$$Au_{k+\ell} + V[U_0]u_{k+\ell} \in (\text{span}\{u_n; n \neq k+j, 0 \leq j \leq m-1\})^\perp.$$

This means that if we set $H_k := \text{span}\{u_{k+i}; 0 \leq i \leq m-1\}$, and

$$A_0 u := -\Delta u + (\tilde{V}_0 + V[U_0]) u$$

then $A_0 : H_k \rightarrow H_k$ is a self-adjoint operator on the finite dimensional space H_k . Therefore there exists a unitary operator U_k , acting on this space, such that if for $0 \leq \ell \leq m-1$ we set $\hat{u}_{k+\ell} = U_k u_{k+\ell} = U_k U_0 \varphi_{k+\ell}$, we have $A_0 \hat{u}_{k+\ell} = \lambda_{k+\ell} \hat{u}_{k+\ell}$ for some $\lambda_{k+\ell} \in \mathbb{R}$.

However, since U_k is a unitary operator on H_k we have

$$\sum_{\ell=0}^{m-1} |U_0 \varphi_{k+\ell}|^2 = \sum_{\ell=0}^{m-1} |U_k U_0 \varphi_{k+\ell}|^2$$

and thus

$$\sum_{j=k}^{k+m-1} \rho_j |U_0 \varphi_j|^2 = \rho_k \sum_{\ell=0}^{m-1} |U_0 \varphi_{k+\ell}|^2 = \rho_k \sum_{\ell=0}^{m-1} |U_k U_0 \varphi_{k+\ell}|^2.$$

This means that if we set $\tilde{U}_k \varphi_j := U_0 \varphi_j$ if $j \notin \{k+\ell; 0 \leq \ell \leq m-1\}$ and $\tilde{U}_j = U_k U_0 \varphi_j$ if $k \leq j \leq k+m-1$, we have $V[U_0] = V[\tilde{U}_k]$, and finally this implies that

$$A_0 \hat{u}_{k+\ell} = -\Delta \hat{u}_{k+\ell} + (\tilde{V}_0 + V[\tilde{U}_k]) \hat{u}_{k+\ell} = \lambda_{k+\ell} \hat{u}_{k+\ell}.$$

□

As we may see from the above analysis, when all the ρ_j 's are distinct, then U_0 , any unitary operator which minimizes J_0 , yields a solution to the Schrödinger–Poisson system. However in the general case, when some of the coefficients ρ_k have multiplicity $m_k \geq 2$, it is possible that one has to impose a unitary transformation U_k in the space

$$H_k := \text{span}\{U_0 \varphi_{k+\ell}; 0 \leq \ell \leq m_k - 1\}$$

in order to obtain a solution (note that these unitary transformations do not change the value of $V[U_0]$).

In other words, one may find a unitary operator U_k on H_k such that if $A_k := A|_{H_k}$ is the trace of A on H_k , the operator $U_k^* A_k U_k$ is diagonal. Thus since $\rho_k = \rho_{k+\ell}$ for $0 \leq \ell \leq m-1$, if we denote by \widehat{U} the unitary operator obtained through the composition of all such operators U_k and U_0 , one has $J_0(\widehat{U}) = J_0(U_0)$. More precisely, we can state the following corollary, which ends the proof of theorem 17:

Corollary 18 *Under the assumptions of theorem 12, let U_k be given by lemma 17 when $k \geq 1$ is such that (17) is satisfied. Define the operator \widehat{U}_0 by $\widehat{U}_0 \varphi_k = U_0 \varphi_k$ when k satisfies (16), and*

$$\widehat{U}_0 \varphi_{k+\ell} := U_k U_0 \varphi_{k+\ell}, \quad \text{for } 0 \leq \ell \leq m-1, \quad \text{when (17) is satisfied.}$$

Then \widehat{U}_0 belongs to \mathbb{S} , while $J_0(\widehat{U}_0) = J_0(U_0)$ and $V[\widehat{U}_0] = V[\widehat{U}_0]$. Moreover setting $u_j := \widehat{U}_0 \varphi_j$ for $j \geq 1$, there exists $\lambda_j \in \mathbb{R}$ such that

$$-\Delta u_j + \left(\widetilde{V}_0 + V[\widehat{U}_0] \right) u_j = \lambda_j u_j, \quad u_j \in \mathbb{H}_1, \quad (u_j | u_k) = \delta_{jk}$$

and moreover $V := V[\widehat{U}_0]$ satisfies

$$-\Delta V = \sum_{j \geq 1} \rho_j |u_j|^2, \quad V \in H_0^1(\Omega).$$

5 Further remarks

The one dimensional case $d = 1$ is particularly simple to handle, using a completely different method. Indeed we point out that for a given potential $V \in C([0, 1])$ the spectral sequence $(\lambda_k, \varphi_k)_{k \geq 1}$

$$-\varphi_k'' + (V + \widetilde{V})\varphi_k = \lambda_k \varphi_k, \quad \varphi_k(0) = \varphi_k(1) = 0, \quad \varphi_k'(0) > 0,$$

is well defined, and $\int_0^1 \varphi_k \varphi_j dx = \delta_{kj}$, each eigenvalue λ_k being simple. Using the simplicity of the eigenvalues, it is known that the mapping $V \mapsto \varphi_k$ is continuous from $C([0, 1])$ into $L^2(0, 1)$ (see J. Pöschel & E. Trubowitz [11]). If the coefficients $(\rho_j)_{j \geq 1}$ satisfy

$$\rho_j > 0, \quad \sum_{j \geq 1} \rho_j =: M < \infty$$

one can easily see that the mapping $F : C([0, 1]) \longrightarrow L^1(0, 1)$

$$V \mapsto F(V) := \sum_{k \geq 1} \rho_k |\varphi_k|^2$$

is continuous.

Now consider the mapping $B : L^1(0, 1) \longrightarrow L^1(0, 1)$ defined by $Bf := v$ where $v \in C^1([0, 1])$ is given by

$$-v'' = f \quad \text{in } (0, 1), \quad v(0) = v(1) = 0.$$

Clearly B can also be considered as a linear mapping on $C([0, 1])$, and B is compact. Also observe that the second equation in (1b) is equivalent to find $V \in C([0, 1])$ such that

$$V - BF(V) = 0.$$

Denoting by $T(V) := BF(V)$, we know that $I - T$ is a compact perturbation of the identity on $C([0, 1])$ and one can check easily that there exists $R > 0$ such that for any $\theta \in [0, 1]$

$$V - \theta T(V) = 0 \implies \|V\|_\infty < R.$$

Thus the invariance by homotopy of the Leray–Schauder topological degree implies that for all $\theta \in [0, 1]$ we have

$$\deg(I - \theta T, B(0, R), 0) = \deg(I, B(0, R), 0) = 1,$$

which means in particular that $\deg(I - T, B(0, R), 0) = 1$. Therefore there exists at least one $V \in C([0, 1])$ such that $V - T(V) = 0$, that is the system (1a)–(1b) has at least one solution, when $\Omega = (0, 1)$.

We point out also that in the case in which ρ_m is a function of λ_m , for instance $\rho_m := \exp(-\lambda_m)$ (see F. Nier [10]), the same approach can be applied. In dimensions $N \geq 1$, J.Ph. Solovej [15] considers a *one-particle density matrix* defined by $f \mapsto \gamma f := \sum_{m \geq 1} \rho_m(u_m | f) u_m$ and minimizes a functional depending on γ under the constraint $\text{spectrum}(\gamma) = \{\rho_m ; m \geq 1\}$. See also E. Prodan [12], E. Prodan & P. Nordlander [13] where Hartree-Fock approximations are considered.

[6]

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