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The self-energy of an impurity in an ideal Fermi gas to second order in the interaction strength

Christian Trefzger and Yvan Castin

*Laboratoire Kastler Brossel, École normale supérieure, CNRS,
UPMC, 24 rue Lhomond, 75231 Paris Cedex 05, France*

We study in three dimensions the problem of a spatially homogeneous zero-temperature ideal Fermi gas of spin-polarized particles of mass m perturbed by the presence of a single distinguishable impurity of mass M . The interaction between the impurity and the fermions involves only the partial s -wave through the scattering length a , and has negligible range b compared to the inverse Fermi wave number $1/k_F$ of the gas. Through the interactions with the Fermi gas the impurity gives birth to a quasi-particle, which will be here a Fermi polaron (or more precisely a *monomeron*). We consider the general case of an impurity moving with wave vector $\mathbf{K} \neq \mathbf{0}$: Then the quasi-particle acquires a finite lifetime in its initial momentum channel because it can radiate particle-hole pairs in the Fermi sea. A description of the system using a variational approach, based on a finite number of particle-hole excitations of the Fermi sea, then becomes inappropriate around $\mathbf{K} = \mathbf{0}$. We rely thus upon perturbation theory, where the small and negative parameter $k_F a \rightarrow 0^-$ excludes any branches other than the monomeric one in the ground state (as e.g. the dimeronic one), and allows us a systematic study of the system. We calculate the impurity self-energy $\Sigma^{(2)}(\mathbf{K}, \omega)$ up to second order included in a . Remarkably, we obtain an analytical explicit expression for $\Sigma^{(2)}(\mathbf{K}, \omega)$ allowing us to study its derivatives in the plane (K, ω) . These present interesting singularities, which in general appear in the third order derivatives $\partial^3 \Sigma^{(2)}(\mathbf{K}, \omega)$. In the special case of equal masses, $M = m$, singularities appear already in the physically more accessible second order derivatives $\partial^2 \Sigma^{(2)}(\mathbf{K}, \omega)$; using a self-consistent heuristic approach based on $\Sigma^{(2)}$ we then regularise the divergence of the second order derivative $\partial_K^2 \Delta E(\mathbf{K})$ of the complex energy of the quasi-particle found in reference [C. Trefzger, Y. Castin, Europhys. Lett. **104**, 50005 (2013)] at $K = k_F$, and we predict an interesting scaling law in the neighborhood of $K = k_F$. As a by product of our theory we have access to all moments of the momentum of the particle-hole pair emitted by the impurity while damping its motion in the Fermi sea, at the level of Fermi's golden rule.

I. INTRODUCTION AND MOTIVATIONS

In this work we study, in a three dimensional space, the problem of a mobile distinguishable impurity of mass M undergoing elastic scattering with an ideal Fermi gas of fermions of mass m , all in the same spin-state, at zero temperature and in the thermodynamic limit. The solution of this problem is a fundamental step in the microscopic comprehension of the concept of quasi-particle, which lays at the heart of the Fermi liquid theory developed by Landau [1]. It allows us to show the expected effects resulting from the coupling of the impurity with the Fermi sea reservoir: From reactive effects shifting the real energy of the impurity and changing its effective mass, to dissipative effects, appearing when the impurity is moving, inducing a finite lifetime of the impurity in its initial momentum channel $\hbar \mathbf{K}$ due to emission of particle-hole pairs in the Fermi sea that lower the impurity momentum. These two effects may be summarized by the notion of complex energy $\Delta E(\mathbf{K})$, counted from the energy of the unperturbed Fermi sea.

From the formalism perspective this leads naturally to the introduction of the impurity self-energy $\Sigma(\mathbf{K}, \omega)$, a function of the wave vector \mathbf{K} and of an angular frequency ω , that enters into the Dyson equation satisfied by the space-time Fourier transform $\mathcal{G}(\mathbf{K}, \omega)$ of the two-points Green's function, which constitutes a building block of the diagrammatic methods for the N -body problem [2]. Indeed, the complex energy $\Delta E(\mathbf{K})$ mentioned above, after division by \hbar , must be a pole of the analytic continuation of the function $\omega \mapsto \mathcal{G}(\mathbf{K}, \omega)$ to the lower complex half-plane.

Our single impurity-problem has of course a long history. It emerged in a nuclear physics context, in the case of a Λ -particle interacting with a Fermi sea of nucleons [3, 4] via a spherical hard-core potential of radius $a > 0$. The results, obtained by resummation of diagrams in the T -matrix formalism, are limited to $\mathbf{K} = \mathbf{0}$ but the expansion in powers of $k_F a$ was remarkably pushed up to the order four [5], k_F being here the Fermi wave number.

Recently the problem shows a renewed interest thanks to cold atoms experiments, where the impurity is an atom of the same chemical species as the fermions but in a different spin state [6–8], or even an atom of a different chemical species [9]. The experiments of reference [7] can then be very well interpreted by the fact that the fraction of atoms in the minority spin-state, when sufficiently small, constitutes a Fermi “liquid”, that is an almost ideal gas of fermionic quasi-particles whose internal energy and effective mass have been modified by the interaction with the Fermi sea of the atoms in the majority spin-state, in agreement with the theory of [10, 11] and as confirmed by the precise measurement of the equation of state of a spin-polarized gas [12, 13].

From a theoretical point of view, the model interactions appropriate to cold atoms strongly differ from those based

on hard-spheres of the first references [3–5]. Indeed, for cold atoms and for the previously cited experiments, the interaction between the impurity and a fermion is resonant in the s -wave and negligible in the other partial waves. This means that the s -wave scattering length a is much larger, in absolute value, than the range b of the interaction and it can have an arbitrary sign, two features that are missing in the hard-spheres model. One can even experimentally tend to the unitary limit $1/a = 0$ thanks to the amazing tool of Feshbach resonances [14]. In this resonant regime $|a| \gg b$, one expects the interacting potential to be characterized only by the scattering length to the exclusion of any other microscopic details (as e.g. its position dependence); in such a case we speak of *one-parameter universality* and theoretically we are led to make the range of the potential b tend to zero with a fixed scattering length, for any convenient model. In reality, this one-parameter universality has not to be taken for granted. It breaks down when the mass ratio m/M is too large so that the effective attractive interaction induced by the impurity between the fermions leads to the three-body Efimov effect, at the critical mass ratio $m/M \simeq 13.607$ [15–17], or also to the four-body Efimov effect, at the critical mass ratio $m/M \simeq 13.384$ [18]. In the presence of such Efimov effects, additional three-body and four-body parameters must be introduced to characterize the interaction, and in the limit of zero true range and effective range the energy spectrum is not bounded from below, which constitutes the Thomas effect [19]. Up to now, a necessary and sufficient condition on the mass ratio excluding all possible Efimov effects, even at the thermodynamic limit, is unknown [20] but we will suppose it to be satisfied in this work.

In this cold-atoms context, an important conceptual progress was to realize that our single impurity problem belongs to the general class of polaronic systems [21]. By analogy with solid-state physics, in which the polaron is an electron dressed by the (bosonic) phonons describing quantum-mechanically the deformation of the crystal induced by the electromagnetic interaction with the electron charge, the impurity constitutes a Fermi polaron because it is dressed by the particle-hole pairs induced by its now short-ranged interaction, with the fermions. The picture is indeed very rich since many classes of polarons may exist, depending on whether the quasi-particle is constructed by particle-hole pair dressing of the bare impurity [10, 11], or by dressing a two-body bound state (dimer) between the impurity and a fermion, that preexists in free space [21–24], or even by dressing a three-body bound state (trimer) between the impurity and two fermionic particles [25]. By systematically extend the terminology of reference [26], we can then refer to monomeron, dimeron or trimeron to underline the quasi-particle character of the considered object, as done by Lobo in [27]; we can also refer to dressed atom, dressed dimer or dressed trimer as in the review article [27]. The advantage of the former terminology appears in the more surprising case where the binding between the impurity and a small number of fermions does not preexist in vacuum but is itself induced by the presence of the Fermi sea. This is the case of the trimerons of reference [25], and of the dimerons at $a < 0$ on a narrow Feshbach resonance [26, 28, 29]; in the latter case see the conclusion of [26] for a physical interpretation.

Let us restrict ourselves here and in what follows to the monomeric branch, and let us consider the case of a negative scattering length $a < 0$ on a broad Feshbach resonance (therefore of negligible true and effective ranges); the dimeronic branch is then an excited branch [21] that is unstable [30]¹. Up to now the single impurity problem with resonant interaction has been treated analytically, essentially at zero wave vector $\mathbf{K} = \mathbf{0}$, using a non-perturbative variational approach that truncates the Hilbert space by keeping at most n particle-hole pairs, but without any constraint on their possible states. This approach was initiated by reference [10] (see also [31]), with $n = 1$; at $\mathbf{K} = \mathbf{0}$ the energy $\Delta E(\mathbf{0})$ is real and the predicted approximate value $\Delta E^{[1]}(\mathbf{0})$ gives an upper bound to $\Delta E(\mathbf{0})$, which was sufficient to establish the existence of a Fermi “liquid” phase in a strongly polarized gas at the unitary limit $1/a = 0$ [10]. In this rather spectacular strongly interacting case, there is *a priori* no small parameter allowing us to control the precision of the variational ansatz [10]; the fact that the result is identical to the one obtained with the non-perturbative (therefore non-systematic) use of the T -matrix formalism (in the ladder approximation) [31, 32] does not prove that the result is reliable. However, it was finally understood that a semi-analytical systematic study for increasing n (in practice limited to $n = 2$) is a winning strategy, allowing one to explicitly verify the rapid convergence of the series $\Delta E^{[n]}(\mathbf{0})$ [32, 33] towards the numerical diagrammatic quantum Monte Carlo results of reference [21].

We shall devote this work to the more original case of a non zero total momentum, $\mathbf{K} \neq \mathbf{0}$, still not fully understood (see however reference [34] at large K). The problem then changes nature and the monomeron becomes a resonance of complex energy $\Delta E(\mathbf{K})$ [4]; the moving quasi-particle is indeed unstable with respect to particle-hole pairs emission [35] since the kinetic energy and the momentum carried away by the pairs can be, let us recall it, as close to zero as we want. The variational approach also changes status: Not only it no longer provides an upper bound to the real part of the energy $\Re \Delta E(\mathbf{K})$, but it also predicts a non-physical interval of K -values, starting at 0, within which the imaginary part of the energy $\Im \Delta E(\mathbf{K})$ is exactly zero [36]². This explicitly contradicts the perturbative result of

¹ We recall that the energy of the dimer tends to $-\infty$ as $-\hbar^2/(2\mu a^2)$ when $a \rightarrow 0^+$, μ being the reduced mass of the impurity and a fermion, and that there is no dimer for $a < 0$.

² The same phenomenon occurs for the dimeron in two dimensions [37].

reference [4] obtained for $M = m$ up to second order included in $k_F a$, which gives an $\Im \Delta E(\mathbf{K})$ continuously vanishing as K^4 when $\mathbf{K} \rightarrow \mathbf{0}$, and more generally it disagrees with the Fermi “liquid” theory of [35].

This failure of the variational approach at $\mathbf{K} \neq \mathbf{0}$ is readily understood if one considers the one-impurity problem in the general context of a discrete state coupled to a continuum [38], as it was done in reference [26]. The discrete state corresponds to the impurity with wave vector \mathbf{K} in the presence of the unperturbed Fermi sea; its energy (counted from the Fermi sea energy) is thus the impurity kinetic energy $\hbar^2 K^2/(2M)$. The continuum is made of particle-hole pairs of any momenta in the Fourier space, in the presence of the impurity in the suitable wave vector state (such as to conserve the total momentum). (i) Within an exact treatment of the problem, it is clear that the continuum contains in particular a monomeron of arbitrarily small total momentum, thus of energy $\simeq \Delta E(\mathbf{0})$, that may be thought of as a relatively localized perturbation of the fermions gas in the neighborhood of a point in real space [39], in the presence of particle-hole pairs that are radiated at infinity and that carry away the missing momentum, without necessarily costing a significant amount of energy. A particle and a hole respectively of wave vector \mathbf{k} and \mathbf{q} can indeed carry away momentum of modulus up to $2k_F$ with a positive kinetic energy $\hbar^2(k^2 - q^2)/(2m)$ that is negligible when $k \rightarrow k_F^+$ and $q \rightarrow k_F^-$. The lower bound of the continuum then corresponds to the exact (here negative) energy $\Delta E(\mathbf{0})$. The coupling between the discrete state and the continuum leads in general the former to dilute into the latter to give birth to a resonance, and $\Im \Delta E(\mathbf{K}) < 0$ at $K > 0$. (ii) Within the variational treatment of the problem, limited to n particle-hole pairs, one expects the continuum to start at the energy $\Delta E^{[n-1]}(\mathbf{0})$, since at least one pair must be radiated at infinity to bring the monomeron at rest. Now this is strictly larger than $\Delta E^{[n]}(\mathbf{0})$, according to the usual variational reasoning; at $\mathbf{K} = \mathbf{0}$, the coupling of the discrete state to the continuum then seems to give rise to a discrete state of energy $\Delta E^{[n]}(\mathbf{0})$ separated from the continuum by an artificial energy gap of width $\Delta E^{[n-1]}(\mathbf{0}) - \Delta E^{[n]}(\mathbf{0})$. If this is the case $\Delta E^{[n]}(\mathbf{K})$ should remain exactly real in a region around $\mathbf{K} = \mathbf{0}$, that shrinks at larger n but that has no physical meaning. This plausible scenario is confirmed by the explicit calculation made for $n = 1$ in reference [26], provided the interaction is sufficiently weak: For fixed and finite M/m , we find indeed that the continuum starts at the energy $\Delta E^{[0]}(\mathbf{0}) = 0$, if $k_F a$ (negative) is sufficiently close to zero not to satisfy equation (24) of that reference. This has been used to estimate the non-physical value of the modulus of \mathbf{K} below which $\Im \Delta E^{[1]}(\mathbf{K}) = 0$ [36].

With the variational approach being disqualified at $\mathbf{K} \neq \mathbf{0}$, the theory toolbox apart from numerics is rather empty. Thus, we shall use the only reliable and systematic method, the perturbative approach, here up to the second order included in $k_F a$, in the spirit of the pioneering articles [3–5]. However, instead of a hard-sphere interaction we will use a Hubbard-type cubic lattice model of lattice spacing b , with a (here attractive) on-site interaction of bare coupling constant g_0 adjusted, as a function of b , to reproduce exactly the desired scattering length. This model was initially introduced for the case of a weakly interacting bosonic gas, in a tentative form in [40] then in its final form in [41], and since then it has witnessed some success for the case of spin 1/2 fermions, even in the strongly interacting regime [42–44]. For a fixed b we expand the self-energy $\Sigma(\mathbf{K}, \omega)$ up to order two in $k_F a$, then we take the continuous space limit $b \rightarrow 0$ in the coefficients of the expansion. The key point is that all the corresponding integrals in the Fourier space can be calculated analytically so that explicit expressions can be obtained for $\Sigma^{(2)}(\mathbf{K}, \omega)$. We shall give these expressions for any ω and for any impurity-to-fermion mass ratio M/m . The opposite order of taking limits ($b \rightarrow 0$ for a fixed scattering length, then $k_F a \rightarrow 0^-$) would lead to the same result by virtue of the one-parameter universality mentioned above and of the absence at $a < 0$ of essentially non-perturbative effects (as e.g. the emergence of a dimer at the zero-range limit for $a > 0$), but one would have to resort to the non-perturbative resummation of ladder diagrams as in [5].

To *second* order in $k_F a$, we find for $\Delta E(\mathbf{0})$ in the zero range limit exactly the same results as the ones of Bishop [5] for the hard-sphere interaction, after their direct transposition from the case $a > 0$ to the case $a < 0$. This is without too much of surprise, since it is well known that the non-zero range (of order a) of the hard-sphere interaction appears only at the next order: The two-body scattering amplitude $f_k = -1/[a^{-1} + ik - k^2 r_e/2 + O(k^3 a^2)]$ for the hard-sphere potential, of effective range $r_e = 2a/3$, differs from the one $f_k = -1/(a^{-1} + ik)$ of the zero range interaction by terms at least of order *three*, in $O(a^3 k^2)$, when $a \rightarrow 0$ for a fixed relative wave number k between a fermion and the impurity.

On the other hand, at $\mathbf{K} \neq \mathbf{0}$ our expressions of $\Delta E^{(2)}(\mathbf{K})$ are new. They were already briefly presented in reference [36], which shows their experimental observability by radio-frequency spectroscopy of cold atoms [9] but gives no detail of derivation, contrarily to this work in which this is one of the motivations. The knowledge of $\Sigma^{(2)}(\mathbf{K}, \omega)$ as a function of ω even allows us also to go further and, thanks to a heuristic self-consistent equation for the complex energy $\Delta E(\mathbf{K})$, to regularise the logarithmic divergence of the second order derivative with respect to K of $\Delta E(\mathbf{K})$, predicted by the perturbative theory for equal masses ($M = m$) at the Fermi surface ($K = k_F$) [36]. Note that to second order in $k_F a$ our expressions of $\Delta E^{(2)}(\mathbf{K})$ obtained for $a < 0$ can be directly extended to the case of the repulsive monomeron [45] where $a > 0$ ³.

³ In the case $a > 0$ the repulsive monomeron is an excited branch which can decay to the dimeronic and to the attractive monomeron

This long article is organized as follows. After a formal and maybe unusual writing of the self-energy $\Sigma(\mathbf{K}, \omega)$ in terms of the resolvent of the Hamiltonian in section II, we shall expand it up to second order included in the coupling constant g and we will readily express the result as a single integral, see section III, that we are able to calculate explicitly at the end of a rather technical section IV. We shall then reap rather formal benefits in section V, by identifying in the plane (K, ω) the singularities of the third order derivatives of the self-energy (truncated to second order in g), which are the counterparts at $\omega \neq 0$ to the singularities of the derivatives with respect to K of the complex energy (truncated to second order in g) of reference [36]. We have kept the physical applications for section VI: After having recovered the perturbative results of reference [36], we explicitly implement the aforementioned self-consistent approach and we predict a non-perturbative scaling law for the behavior of $\frac{d^2}{dK^2}\Delta E(\mathbf{K})$ in the neighborhood of the Fermi surface for equal masses and when $g \rightarrow 0^-$. En passant, we check in subsection VID that the impurity complex energy $\Delta E^{(2)}(\mathbf{K})$ is a smooth function of K at non-zero temperature. In another perspective, we will show how our techniques of integral calculus allow us to access all moments of the momentum of the particle-hole pair emitted by the impurity into the Fermi sea within Fermi's golden rule approximation; this gives not only the damping rate of the impurity momentum in the spirit of [35], but also its diffusion coefficient in the spirit of [47]. Our results are of course limited to second order in g but, contrarily to references [35, 47], they apply for any momentum. We shall conclude in section VII.

II. DEFINITION OF $\Sigma(\mathbf{K}, \omega)$ AND RELATION WITH THE RESOLVENT OF THE HAMILTONIAN

We start here with a few general reminders on the well known N -body Green's function approach [2], for a spatially homogeneous system with periodic boundary conditions, independently on the interaction model, then we establish the relation, maybe less well known, of this formalism with the resolvent and the notions of effective Hamiltonian and displacement operator, more usual in atomic physics [38]. Variables and operators of the impurity will be distinguished from those of fermions by the use of capital letters for the former, and small letters for the latter.

The case considered here is the one at zero temperature. The single impurity Feynman Green's function is then defined by [2]

$$\mathcal{G}(\mathbf{R}, t; \mathbf{R}', t') \equiv (i\hbar)^{-1} \langle \phi_0 | \hat{T} [\hat{\Psi}(\mathbf{R}, t) \hat{\Psi}^\dagger(\mathbf{R}', t')] | \phi_0 \rangle \quad (1)$$

where the state vector $|\phi_0\rangle$ is the ground state of N fermions in the absence of impurity (a simple Fermi sea), $\hat{\Psi}(\mathbf{R}, t)$ is the impurity field operator at position \mathbf{R} and time t in the Heisenberg picture, and the operator \hat{T} , called T-product, orders the factors in the chronological order from right to left, with the multiplication by the sign of the corresponding permutation if the field $\hat{\Psi}$ is fermionic. Since there is only one impurity, it is clear that its quantum statistic is irrelevant and that the Green's function is zero for $t < t'$, so that it is both a Feynman and a retarded Green's function:

$$\mathcal{G}(\mathbf{R}, t; \mathbf{R}', t') = (i\hbar)^{-1} Y(t - t') \langle \phi_0 | \hat{\Psi}(\mathbf{R}, t) \hat{\Psi}^\dagger(\mathbf{R}', t') | \phi_0 \rangle \quad (2)$$

with Y the usual Heaviside step function. As the second member depends only on $\mathbf{R} - \mathbf{R}'$ and $t - t'$, by virtue of spatial homogeneity and stationarity of the Fermi sea under free evolution, we take its spatiotemporal Fourier transform⁴ with respect to $\mathbf{R} - \mathbf{R}'$ and $t - t'$, with the usual regularisation $\exp[-\epsilon(t - t')/\hbar]$, $\epsilon \rightarrow 0^+$, to obtain the propagator $\mathcal{G}(\mathbf{K}, \omega)$. By definition of the self-energy Σ , called proper self-energy in [2], on one hand we have the Dyson equation

$$\mathcal{G}(\mathbf{K}, \omega) = [\hbar\omega + i\epsilon - E_{\mathbf{K}} - \Sigma(\mathbf{K}, \omega)]^{-1} \quad (3)$$

with the impurity kinetic energy function,

$$E_{\mathbf{K}} = \frac{\hbar^2 K^2}{2M} \quad (4)$$

On the other hand, the evolution operator during t of the full system of Hamiltonian \hat{H} is $\exp(-i\hat{H}t/\hbar)$, so that we obtain from an explicit calculation

$$\mathcal{G}(\mathbf{K}, \omega) = \langle \psi_{\mathbf{K}}^0 | \hat{G}(\hbar\omega + i\epsilon + e_0(N)) | \psi_{\mathbf{K}}^0 \rangle \quad \text{where} \quad |\psi_{\mathbf{K}}^0\rangle = \hat{C}_{\mathbf{K}}^\dagger |\phi_0\rangle \quad (5)$$

branches as discussed in reference [46].

⁴ Our convention is that the spatiotemporal Fourier transform of $f(x, t)$ defined on \mathbb{R}^2 is $\tilde{f}(k, \omega) = \int dt \int dx f(x, t) \exp[-i(kx - \omega t)]$.

with $e_0(N)$ the ground state energy of the unperturbed N fermions, $\hat{C}_{\mathbf{K}}^\dagger$ the creation operator of one impurity with wave vector \mathbf{K} and $\hat{G}(z) \equiv (z\hat{1} - \hat{H})^{-1}$ the resolvent operator of the full Hamiltonian \hat{H} .

The link established by equations (3,5) between the self-energy and the resolvent is a link between two worlds, the N -body problem in condensed matter physics and the one of atomic physics, where we rather speak about effective Hamiltonians and complex energy shifts. This link is made explicit by the method of projectors [38]. Let \hat{P} be the orthogonal projector on $|\psi_{\mathbf{K}}^0\rangle$, that is on the unperturbed state of the impurity with wave vector \mathbf{K} and the Fermi sea. In the corresponding subspace of dimension one we define the non-hermitian effective Hamiltonian, that parametrically depends, as the resolvent, on a complex energy z , by the general exact relations

$$\hat{P}\hat{G}(z)\hat{P} = \frac{\hat{P}}{z\hat{P} - \hat{H}_{\text{eff}}(z)} \text{ and } \hat{H}_{\text{eff}}(z) \equiv \hat{P}\hat{H}\hat{P} + \hat{P}\hat{H}\hat{Q} \frac{\hat{Q}}{z\hat{Q} - \hat{Q}\hat{H}\hat{Q}} \hat{Q}\hat{H}\hat{P} \quad (6)$$

where $\hat{Q} = \hat{1} - \hat{P}$ is the complementary projector to \hat{P} . Here, $\hat{H} = \hat{H}_0 + \hat{V}$, where \hat{H}_0 , the kinetic Hamiltonian of the particles, commutes with \hat{P} , and \hat{V} is the impurity-fermion interaction Hamiltonian. We finally obtain an explicit operator-expression of the self-energy, in terms of the displacement operator \hat{R} of reference [38] readily replaced here by its definition:

$$\Sigma(\mathbf{K}, \omega) = \langle \psi_{\mathbf{K}}^0 | \hat{V} | \psi_{\mathbf{K}}^0 \rangle + \langle \psi_{\mathbf{K}}^0 | \hat{V} \hat{Q} \frac{\hat{Q}}{\hbar\omega + i\epsilon + e_0(N) - \hat{Q}\hat{H}\hat{Q}} \hat{Q}\hat{V} | \psi_{\mathbf{K}}^0 \rangle \quad (7)$$

This will allow us to expand $\Sigma(\mathbf{K}, \omega)$ in powers of \hat{V} without using a diagrammatic representation.

III. EXPRESSION OF $\Sigma(\mathbf{K}, \omega)$ UP TO SECOND ORDER IN g AS A SINGLE INTEGRAL

A. The lattice model and the result as a multiple integral

To describe a zero-range interaction of fixed scattering length a between the impurity and a fermion, it is not possible in three dimensions to directly take the usual Dirac delta model, $V_\delta = g\delta(\mathbf{R} - \mathbf{r})$, of effective coupling constant

$$g = \frac{2\pi\hbar^2 a}{\mu}, \quad (8)$$

$\mu = mM/(m+M)$ being the reduced mass, except for a treatment limited to the Born approximation. Typically one makes this model meaningful by introducing a cutoff on the relative wave vectors of the two colliding particles (not on the wave vectors of each particle [48]), and then one takes the infinite cutoff limit [32]. However, we shall adopt here a more physical approach: We replace the Dirac delta by the Kronecker symbol, the latter also noted δ , that is we use the cubic lattice model described in detail in reference [49], the space being discretised along each Cartesian direction with a lattice spacing b , submultiple of the period L setting the periodic boundary conditions. The wave vectors of the particles then have a meaning modulo $2\pi/b$ in each direction, which allows us to restrict them to the first Brillouin zone of the lattice, $\text{FBZ} = [-\pi/b, \pi/b]^3$, and which provides a natural cutoff; thus the wave vectors span the set $\mathcal{D} = \text{FBZ} \cap (2\pi/L)\mathbb{Z}^3$. The full Hamiltonian \hat{H} is the sum of the kinetic energy of the particles \hat{H}_0 and of the on-site interaction \hat{V} . On one hand,

$$\hat{H}_0 = \sum_{\mathbf{k} \in \mathcal{D}} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + \sum_{\mathbf{K} \in \mathcal{D}} E_{\mathbf{K}} \hat{C}_{\mathbf{K}}^\dagger \hat{C}_{\mathbf{K}} \quad (9)$$

where the kinetic energy of a fermion of wave vector \mathbf{k} ,

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} \quad (10)$$

and the annihilation operator $\hat{c}_{\mathbf{k}}$ of a fermion, subject to the canonical anticommutation relations $\{\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}^\dagger\} = \delta_{\mathbf{k}, \mathbf{k}'}$, are the fermionic counterpart of the energy $E_{\mathbf{K}}$ and of the operator $\hat{C}_{\mathbf{K}}$ introduced for the impurity in the previous section. On the other hand,

$$\hat{V} = \sum_{\mathbf{r} \in [0, L]^3 \cap b\mathbb{Z}^3} b^3 g_0 \hat{\Psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{K}, \mathbf{K}' \in \mathcal{D}} \frac{b^3 g_0}{L^3} \delta_{\mathbf{k}+\mathbf{K}, \mathbf{k}'+\mathbf{K}'} \hat{C}_{\mathbf{K}'}^\dagger \hat{C}_{\mathbf{K}}^\dagger \hat{c}_{\mathbf{k}'} \hat{c}_{\mathbf{k}} \hat{C}_{\mathbf{K}} \quad (11)$$

where the field operator $\hat{\psi}(\mathbf{r})$, such that $\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \delta_{\mathbf{r},\mathbf{r}'}/b^3$, is the fermionic counterpart of the impurity field $\hat{\Psi}(\mathbf{R})$, δ^{mod} is a Kronecker δ modulo a vector of the reciprocal lattice $(2\pi/b)\mathbb{Z}^3$, and the bare coupling constant g_0 is adjusted so that the scattering length of the impurity on a fermion, defined of course for the infinite lattice ($L = \infty$), has the arbitrary desired value in \mathbb{R} [49]:

$$g_0^{-1} = g^{-1} - \int_{\text{FBZ}} \frac{d^3k}{(2\pi)^3} \frac{2\mu}{\hbar^2 k^2} \quad (12)$$

Let us determine the self-energy $\Sigma(\mathbf{K}, \omega)$ perturbatively up to second order included in g , for $g < 0$, as explained in the introduction. For a fixed lattice spacing b , we shall make g tend to zero from negative values. Thus g_0 tends to zero,

$$g_0 \stackrel{a/b \rightarrow 0}{=} g + g^2 \int_{\text{FBZ}} \frac{d^3k}{(2\pi)^3} \frac{2\mu}{\hbar^2 k^2} + O(g^3) \quad (13)$$

In the relation (7), at this order we can neglect \hat{V} in the denominator. The action of \hat{V} on the non-perturbed state $|\psi_{\mathbf{K}}^0\rangle$ creates a hole of wave vector \mathbf{q} in the Fermi sea by promoting a fermion to the wave vector \mathbf{k} ; the impurity takes the momentum change and acquires the wave vector $\mathbf{K} - \mathbf{k} + \mathbf{q}$ (modulo a vector of the reciprocal lattice). In the obtained expression of $\Sigma(\mathbf{K}, \omega)$, we replace g_0 with its expansion (13) then we take the continuous space limit $b \rightarrow 0$ for a fixed g . It remains to take the thermodynamic limit to obtain the exact perturbative expansion:

$$\Sigma(\mathbf{K}, \omega) = \Sigma^{(1)}(\mathbf{K}, \omega) + \Sigma^{(2)}(\mathbf{K}, \omega) + O(g^3) \quad (14)$$

with, up to second order:

$$\Sigma^{(1)}(\mathbf{K}, \omega) = \rho g \quad (15)$$

$$\Sigma^{(2)}(\mathbf{K}, \omega) = g^2 \int_{q < k_F} \frac{d^3q}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \left[\frac{2\mu}{\hbar^2 k^2} - \frac{Y(k - k_F)}{F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega)} \right] \quad (16)$$

This writing was made more compact as in [36] thanks to the notation

$$F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega) \equiv E_{\mathbf{K} - \mathbf{k} + \mathbf{q}} + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}} - \hbar\omega - i\epsilon \quad (17)$$

Unsurprisingly, the contribution of order one reduces to the mean-field shift, which involves the average density of fermions ρ or their Fermi wave number k_F :

$$\rho = \int_{q < k_F} \frac{d^3q}{(2\pi)^3} = \frac{k_F^3}{6\pi^2} \quad (18)$$

Remarkably, hereafter we will show that the sextuple integral in the second order contribution can be evaluated analytically in an explicit way.

As a side remark, one may further expand g_0 and $\Sigma(\mathbf{K}, \omega)$ in powers of g , at the cost of obtaining integrals that may be difficult to calculate analytically. We give here as an example the result at order three:

$$\begin{aligned} \Sigma^{(3)}(\mathbf{K}, \omega) &= g^3 \int_{q < k_F} \frac{d^3q}{(2\pi)^3} \left\{ \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \left[\frac{2\mu}{\hbar^2 k^2} - \frac{Y(k - k_F)}{F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega)} \right] \right\}^2 \\ &\quad - g^3 \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \left[\int_{q < k_F} \frac{d^3q}{(2\pi)^3} \frac{Y(k - k_F)}{F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega)} \right]^2 - \frac{\rho g}{\hbar} \partial_\omega \Sigma^{(2)}(\mathbf{K}, \omega) \end{aligned} \quad (19)$$

resulting from a triple action of \hat{V} on the non-perturbed state $|\psi_{\mathbf{K}}^0\rangle$, with forced return to $|\psi_{\mathbf{K}}^0\rangle$. The first action of \hat{V} creates a particle-hole pair of wave vectors \mathbf{k} and \mathbf{q} . The second action of \hat{V} can bring neither back to the initial state [due to the projector \hat{Q} into equation (7)], nor forth to the state with two particle-hole pairs (since the third action of \hat{V} cannot destroy two pairs). It then (i) scatters the excited fermion from \mathbf{k} to \mathbf{k}' with an amplitude g_0 , or (ii) it scatters the hole from \mathbf{q} to \mathbf{q}' with an amplitude $-g_0$, by collision with the impurity, or (iii) it does not change anything at all [term $\mathbf{k}' = \mathbf{k}$ and $\mathbf{K}' = \mathbf{K}$ in equation (11)]. This gives rise respectively to the first, the second and the third term of equation (19); the integrals over \mathbf{k} and \mathbf{k}' , or over \mathbf{q} and \mathbf{q}' , which have a symmetric integrand with respect to the exchange of wave vectors, lead to a square of an integral over \mathbf{k} , or over \mathbf{q} .

B. From a sextuple integral to a single integral for $\Sigma^{(2)}(\mathbf{K}, \omega)$

We detail here, step by step, the reduction of the multidimensional integral giving $\Sigma^{(2)}(\mathbf{K}, \omega)$ in equation (16).

First of all it is convenient to use dimensionless quantities, by expressing wave vectors in units of the Fermi wave number, the energy difference between $\hbar\omega$ and the impurity kinetic energy $E_{\mathbf{K}}$ in units of the Fermi energy $\epsilon_F \equiv \hbar^2 k_F^2 / (2m)$ of the fermions,

$$\bar{\mathbf{K}} \equiv \frac{\mathbf{K}}{k_F}, \quad \bar{\mathbf{q}} \equiv \frac{\mathbf{q}}{k_F}, \quad \bar{\mathbf{k}} \equiv \frac{\mathbf{k}}{k_F}, \quad \varepsilon \equiv \frac{E_{\mathbf{K}} - \hbar\omega}{\epsilon_F} \quad (20)$$

and the g^2 -component of the self-energy in units of $(\rho g)^2 / \epsilon_F$:

$$\Sigma^{(2)}(\mathbf{K}, \omega) \equiv \frac{(\rho g)^2}{\epsilon_F} \bar{\Sigma}^{(2)}(\bar{\mathbf{K}}, \varepsilon) \quad (21)$$

Regarding the impurity mass, we express it in units of the mass of a fermion by the dimensionless number

$$r \equiv \frac{M}{m} \quad (22)$$

Then, the rotational invariance of $\mathbf{K} \mapsto \Sigma^{(2)}(\mathbf{K}, \omega)$, already taken into account in the writing (21), allows us to average equation (16) on the direction $\hat{\mathbf{K}}$ of the impurity wave vector. At fixed \mathbf{k} and \mathbf{q} , the expansion of $F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega)$ in powers of \mathbf{K} leads us to introduce spherical coordinates of polar axis given by the direction of $\mathbf{k} - \mathbf{q}$; then the integrand depends only on the cosine w of the polar angle of $\hat{\mathbf{K}}$, so that:

$$\left\langle \frac{\hbar^2 k_F^2 / (2M)}{F_{\mathbf{k}, \mathbf{q}}(\mathbf{K}, \omega)} \right\rangle_{\hat{\mathbf{K}}} = \int_{-1}^1 \frac{dw}{2} \frac{1}{x - yw - i\epsilon} \quad (23)$$

$$\xrightarrow{\epsilon \rightarrow 0^+} \frac{1}{2y} \ln \frac{|x+y|}{|x-y|} + \frac{i\pi}{2y} [Y(x+y) - Y(x-y)] \equiv f(x, y) \quad (24)$$

where

$$\lambda \equiv |\bar{\mathbf{k}} - \bar{\mathbf{q}}|, \quad x \equiv \lambda^2 + r(\bar{k}^2 - \bar{q}^2 + \varepsilon) \in \mathbb{R}, \quad y \equiv 2\bar{K}\lambda \in \mathbb{R}^+ \quad (25)$$

and we used the primitive $\frac{1}{2} \ln(v^2 + \epsilon^2) + i \arctan(v/\epsilon)$ of the function $v \mapsto (v - i\epsilon)^{-1}$ on \mathbb{R} .

Similarly, in the integration over \mathbf{k} at fixed \mathbf{q} we choose the polar axis of direction \mathbf{q} , so that the integrand depends only on the polar angle θ between \mathbf{k} and \mathbf{q} , not on the azimuthal angle. In the polar integral, we use the variable λ of equation (25) rather than θ itself, with

$$\sin \theta d\theta = \frac{\lambda d\lambda}{k\bar{q}} \quad (26)$$

Finally, in the integral over \mathbf{q} , that is the most external one, the integrand does not depend anymore on the direction of \mathbf{q} , which brings out the usual 4π solid angle factor. At this point we are easily reduced to a triple integral:

$$\bar{\Sigma}^{(2)}(\bar{\mathbf{K}}, \omega) = \frac{9r}{2} \int_0^1 \bar{q} d\bar{q} \int_0^{+\infty} \bar{k} d\bar{k} \int_{|\bar{k}-\bar{q}|}^{\bar{k}+\bar{q}} \lambda d\lambda \left[\frac{1}{(1+r)\bar{k}^2} - Y(\bar{k}-1)f(x, y) \right] \quad (27)$$

where the function f is the one of equation (24). The integration over λ , although feasible, is tricky since λ appears in $f(x, y)$ under a trinomial form, and the complexity of the result compromises further integration; instead, \bar{k} and \bar{q} appear only by their square. Hence the idea to reverse the order of integration as in reference [39]: We perform separately the complete integration over the domain $\bar{k} < 1$, and otherwise we use

$$\int_0^1 d\bar{q} \int_1^{+\infty} d\bar{k} \int_{|\bar{k}-\bar{q}|}^{\bar{k}+\bar{q}} d\lambda = \int_0^{+\infty} d\lambda \int_{\max(1-\lambda, 0)}^1 d\bar{q} \int_{\max(\lambda-\bar{q}, 1)}^{\lambda+\bar{q}} d\bar{k} \quad (28)$$

All this leads to

$$\bar{\Sigma}^{(2)}(\bar{\mathbf{K}}, \varepsilon) = \frac{3r}{1+r} - \frac{9r}{2} \int_0^{+\infty} d\lambda \left[\frac{\psi^+(\lambda) - \psi^-(\lambda)}{4\bar{K}} - \chi(\lambda) \right] \quad (29)$$

in terms of the auxiliary functions

$$\psi^\pm(\lambda) \equiv \int_{\max(1-\lambda, 0)}^1 \bar{q} d\bar{q} \int_{\max(\lambda-\bar{q}, 1)}^{\lambda+\bar{q}} \bar{k} d\bar{k} u[\lambda^2 \pm 2\bar{K}\lambda + r(\bar{k}^2 - \bar{q}^2 + \varepsilon)] \quad (30)$$

$$\chi(\lambda) \equiv \int_{\max(1-\lambda, 0)}^1 \bar{q} d\bar{q} \int_{\max(\lambda-\bar{q}, 1)}^{\lambda+\bar{q}} \bar{k} d\bar{k} \frac{\lambda}{(1+r)\bar{k}^2} \quad (31)$$

where $\psi^-(\lambda)$ is obtained from $\psi^+(\lambda)$ simply by changing \bar{K} to $-\bar{K}$, and the useful function

$$u(X) \equiv \ln|X| + i\pi Y(X), \quad (32)$$

naturally introduced by the property $2yf(x, y) = u(x+y) - u(x-y)$, will also intervene via its primitives $u^{[n]}(X)$ of order n , which vanish at zero as well as all their derivatives up to order $n-1$:

$$u^{[n]}(X) = \frac{X^n}{n!} \left[u(X) - \sum_{s=1}^n \frac{1}{s} \right] \quad (33)$$

$u(X)$ is actually the limit of the usual branch of the complex logarithm $\ln z$ when z tends to $-X \in \mathbb{R}$ from the upper half of the complex plane.

Let us outline how to compute $\psi^\pm(\lambda)$. The integration over \bar{k} is trivial provided we take \bar{k}^2 as the integration variable. It directly leads to the primitive $u^{[1]}$, evaluated at points of the form $A\bar{q}^2 + B$ or $A\bar{q} + B$, where the coefficients A and B do not depend on \bar{q} . The integration over \bar{q} is then either of the form $\int d\bar{q} \bar{q} u^{[1]}(A\bar{q}^2 + B)$, in which case we take \bar{q}^2 as the integration variable and $u^{[2]}$ appears, or of the form $\int d\bar{q} \bar{q} u^{[1]}(A\bar{q} + B)$, in which case we use the integration by parts (taking the derivative of the factor \bar{q}) that leads to $u^{[2]}$ and to $u^{[3]}$. In practice, we are led to distinguish between the case (i) $0 < \lambda < 1$, of lower boundaries $1-\lambda$ and 1 in the integrals over \bar{q} and over \bar{k} respectively, (ii) $1 < \lambda < 2$, of lower boundaries 0 for \bar{q} and $\lambda-\bar{q}$ (or 1) for \bar{k} depending on \bar{q} being lower (or higher) than $\lambda-1$, and (iii) $\lambda > 2$, of lower boundaries 0 and $\lambda-\bar{q}$. However, we note that the first two cases lead to the same expressions⁵, so that it is sufficient to distinguish the interval $[0, 2]$, over which

$$\psi^\pm(\lambda) = \frac{u^{[2]}[P_\gamma^\pm(\lambda)]}{4r^2} + \frac{u^{[2]}[P_\alpha^\pm(\lambda)] - u^{[2]}[P_\beta^\pm(\lambda)]}{4r^2\lambda} - \frac{u^{[3]}[P_\alpha^\pm(\lambda)] - u^{[3]}[P_\beta^\pm(\lambda)]}{8r^3\lambda^2} \quad (34)$$

and the interval $[2, +\infty[$, over which

$$\psi^\pm(\lambda) = \frac{u^{[2]}[P_\alpha^\pm(\lambda)] + u^{[2]}[P_\delta^\pm(\lambda)]}{4r^2\lambda} - \frac{u^{[3]}[P_\alpha^\pm(\lambda)] - u^{[3]}[P_\delta^\pm(\lambda)]}{8r^3\lambda^2} \quad (35)$$

We have introduced here the trinomials appearing in the expression of $\psi^\pm(\lambda)$:

$$P_\alpha^\pm(\lambda) = (1+r)\lambda^2 + 2(r \pm \bar{K})\lambda + r\varepsilon \quad (36)$$

$$P_\beta^\pm(\lambda) = (1-r)\lambda^2 + 2(r \pm \bar{K})\lambda + r\varepsilon \quad (37)$$

$$P_\gamma^\pm(\lambda) = \lambda^2 \pm 2\bar{K}\lambda + r\varepsilon \quad (38)$$

$$P_\delta^\pm(\lambda) = (1+r)\lambda^2 + 2(\pm\bar{K} - r)\lambda + r\varepsilon \quad (39)$$

The four trinomials corresponding to the function $\psi^-(\lambda)$ are deduced of course from those associated to $\psi^+(\lambda)$ by changing \bar{K} to $-\bar{K}$. They obey the duality relations that we use later in this paper:

$$P_\alpha^-(\lambda) = P_\delta^+(-\lambda) \quad \text{and} \quad P_\delta^-(\lambda) = P_\alpha^+(-\lambda) \quad (40)$$

Notice that $P_\beta^\pm(\lambda)$ is actually of degree one in the special case ($r=1$) where the impurity and the fermions have the same mass, $M=m$.

⁵ When $\lambda \in [1, 2]$, after integration over \bar{k} we obtain for $\psi^\pm(\lambda)$ an expression of the form $\int_0^{\lambda-1} d\bar{q}[f(\bar{q}) + f(-\bar{q})] + \int_{\lambda-1}^1 d\bar{q}[f(\bar{q}) - g(\bar{q})]$, which we transform by the change of variable $\bar{q} \rightarrow -\bar{q}$ in the parts containing $f(-\bar{q})$ and $g(\bar{q})$. After collecting the different pieces and using the odd parity of $g(\bar{q})$, which implies that $\int_{-1}^{+1} d\bar{q} g(\bar{q}) = 0$, we end up with the expression $\int_{1-\lambda}^1 d\bar{q}[f(\bar{q}) - g(\bar{q})]$ which is exactly the same one as $\psi^\pm(\lambda)$ over $[0, 1]$.

As for the integral (31), an elementary calculation leads to⁶

$$\chi(\lambda) = \frac{\lambda}{2(1+r)} \left[(1-\lambda^2) \ln(1+\lambda) + \lambda \left(\frac{3}{2}\lambda - 1 \right) \right] \quad \forall \lambda \in [0, 2] \quad (41)$$

$$\chi(\lambda) = \frac{\lambda}{2(1+r)} \left[(1-\lambda^2) \ln \frac{\lambda+1}{\lambda-1} + 2\lambda \right] \quad \forall \lambda \in [2, +\infty[\quad (42)$$

IV. EXPLICIT CALCULATION OF $\Sigma^{(2)}(\mathbf{K}, \omega)$ IN THE GENERAL CASE

In the previous section we expressed the contribution of order g^2 to the impurity self-energy as a single integral, see the integral of $\psi^+(\lambda) - \psi^-(\lambda)$ over λ in equation (30), in which we now temporarily introduce a finite upper bound $\Lambda > 2$. The evaluation of this integral can be done explicitly. Let us give here the main steps.

A. Expression in terms of two functionals $I[P]$ and $J[P]$

The first step consists in reducing the number of types of terms in the integrand. In equations (34) and (35) there are *a priori* three distinct types, according to the power 0, 1 or 2 of λ in the denominator. However, it suffices to integrate the terms of the third type by parts (integrating the factor $1/\lambda^2$), to transform them into terms of the first two types; this holds over each interval of integration $[0, 2]$ and $[2, \Lambda]$. Also, the all-integrated terms in $\lambda = 2$ cancel exactly since $P_\beta^\pm(2) = P_\delta^\pm(2)$, and the all-integrated term in $\lambda = 0$ is zero since in addition $\frac{d}{d\lambda}P_\alpha^\pm(0) = \frac{d}{d\lambda}P_\beta^\pm(0)$. Writing the integrals over $[2, \Lambda]$ as the difference of the integrals over $[0, \Lambda]$ and over $[0, 2]$ with the same integrand, we are reduced to zero lower integration bounds, and finally to the only two functionals

$$I[P](\lambda) \equiv \int_0^\lambda dt u^{[2]}[P(t)] \quad (43)$$

$$J[P](\lambda) \equiv \int_0^\lambda dt \frac{u^{[2]}[P(t)] - u^{[2]}[P(0)]}{t} \quad (44)$$

where the polynomial $P(\lambda)$ is in practice one of the eight trinomials $P_\sigma^\pm(\lambda)$, $\sigma \in \{\alpha, \beta, \gamma, \delta\}$. The term subtracted in the numerator of the integrand in $J[P]$ assures the convergence of the integral in its lower bound without introducing any remainder in the final result since all the trinomials have the same value in zero. We finally get

$$\begin{aligned} \int_0^\Lambda d\lambda \psi^\pm(\lambda) = & C^\pm(\Lambda) - \frac{(1+r)\{I_\alpha^\pm(\Lambda) - I_\delta^\pm(\Lambda)\} \pm \bar{K}\{J_\alpha^\pm(\Lambda) - J_\delta^\pm(\Lambda)\}}{4r^3} \\ & + \frac{I_\gamma^\pm(2) - I_\beta^\pm(2) - I_\delta^\pm(2)}{4r^2} + \frac{I_\beta^\pm(2) - I_\delta^\pm(2) \pm \bar{K}\{J_\beta^\pm(2) - J_\delta^\pm(2)\}}{4r^3} \end{aligned} \quad (45)$$

with the shorthand notations

$$I_\sigma^\pm(\lambda) \equiv I[P_\sigma^\pm](\lambda) \quad \text{and} \quad J_\sigma^\pm(\lambda) \equiv J[P_\sigma^\pm](\lambda) \quad (46)$$

for the functionals I and J evaluated at the eight trinomials. The contribution of the all-integrated term in Λ resulting from the integration by parts is

$$C^\pm(\Lambda) = \frac{u^{[3]}[P_\alpha^\pm(\Lambda)] - u^{[3]}[P_\delta^\pm(\Lambda)]}{8r^3\Lambda} \quad (47)$$

B. Explicit value of the functionals

The second step consists in calculating the functionals $I[P]$ and $J[P]$, where P is a polynomial. We usefully write it in its factorised form,

$$P(\lambda) = A_P \prod_{\lambda_0 \in \text{Root } P} (\lambda - \lambda_0) \quad (48)$$

⁶ This allows us to verify that the integrand of (29) is $O(1/\lambda^2)$ and that the integral converges at large λ .

where A_P is the leading coefficient and $\text{Root } P$ is the set of roots of $P(\lambda)$ counted with their multiplicity. According to equations (36,37,38,39), it is sufficient here to restrict to the polynomials $P(\lambda)$ of degree at most two with real coefficients, which includes the special case $P_\beta^\pm(\lambda)$ (of degree one) for a mass ratio $r = 1$. Then we need to consider two distinct cases, the one where all roots of $P(\lambda)$ are real, and the one where the two roots are complex conjugate.

Let us first tackle with the **evaluation of the functional** $I[P]$. In order to make notations more compact and the result reusable in the calculation of $J[P]$, we introduce the auxiliary polynomial Q_I of P for the functional $I[P]$:

$$Q_I(\lambda) = \frac{1}{2}[P(\lambda)]^2 \quad (49)$$

Thus, taking into account (33) and (43), we get the useful rewriting

$$I[P](\lambda) = \int_0^\lambda dt Q_I(t) \left[\ln |P(t)| + i\pi Y[P(t)] - \frac{3}{2} \right] \quad (50)$$

In this integral, the contribution of the logarithm is obtained by simply proposing a primitive $\mathcal{F}(t)$ of the function $t \mapsto Q_I(t) \ln |P(t)|$, which the reader may check by calculating the derivative $\mathcal{F}'(t)$. If P has real roots we choose

$$\mathcal{F}(t) = Q_I^{[1]}(t) \left[\ln |A_P| - \frac{3}{2} \right] + \sum_{\lambda_0 \in \text{Root } P} \left\{ \left[Q_I^{[1]}(t) - Q_I^{[1]}(\lambda_0) \right] \ln |t - \lambda_0| - \int_0^t d\tau \frac{Q_I^{[1]}(\tau) - Q_I^{[1]}(\lambda_0)}{\tau - \lambda_0} \right\} \quad (51)$$

where the polynomial $Q_I^{[1]}(t)$ is the primitive of the polynomial $Q_I(t)$ vanishing in $t = 0$, in agreement with the notation introduced previously for the function u . The only potential singularities of the function $\mathcal{F}(t)$, located in the values of the roots λ_0 , come from the second contribution, which remains, however, continuous since the polynomial prefactor of $\ln |t - \lambda_0|$ vanishes in $t = \lambda_0$; the other contributions are polynomials in t . If P has complex roots, we take instead the primitive

$$\mathcal{F}(t) = Q_I^{[1]}(t) \left[\ln |P(t)| - \frac{3}{2} \right] + \sum_{\lambda_0 \in \text{Root } P} \left\{ Q_I^{[1]}(\lambda_0) [\ln(-\lambda_0) - \ln(t - \lambda_0)] - \int_0^t d\tau \frac{Q_I^{[1]}(\tau) - Q_I^{[1]}(\lambda_0)}{\tau - \lambda_0} \right\} \quad (52)$$

where the logarithm $\ln z$ in the complex plane is defined with its principal branch $\Im \ln z \in]-\pi, \pi[$ corresponding to a branch cut on the real negative half-axis. The function $\mathcal{F}(t)$ is smooth (infinitely differentiable) on the real axis. As it vanishes in $t = 0$ and as its derivative is real, since Q_I has real coefficients, it is real-valued. Moreover, we notice that it can be deduced from (51) up to an additive constant by changing $|t - \lambda_0|$ to $(t - \lambda_0)$ in the logarithm.

Let us now consider the contribution of the Heaviside function to the integral (50). If P has complex roots, we can replace $Y[P(t)]$ with $Y[P(\lambda)]$ in the integrand, since $P(t)$ has a constant sign on the real axis; the contribution $i\pi Y[P(\lambda)]Q_I^{[1]}(\lambda)$ appears after integration. If P has real roots, we integrate by parts according to the theory of distributions, by integrating the polynomial factor $Q_I(t)$ and by taking the derivative of the factor containing the Heaviside function:

$$\frac{d}{dt} Y[P(t)] = P'(t) \delta[P(t)] = \sum_{\lambda_0 \in \text{Root } P} \frac{P'(\lambda_0)}{|P'(\lambda_0)|} \delta(t - \lambda_0) \quad (53)$$

according to the well-known properties of Y and of the Dirac δ distribution. The all-integrated term contains the already mentioned contribution $i\pi Y[P(\lambda)]Q_I^{[1]}(\lambda)$, and the remaining integral is elementary, given that $\int_0^\lambda dt \delta(t - \lambda_0) = Y(\lambda - \lambda_0) - Y(-\lambda_0)$. Note that the prefactor of δ in (53) is a pure sign, which is the one of the leading coefficient A_P for the largest of the roots and its opposite for the smallest of the roots⁷.

It remains to give the **final expression** of $I[P](\lambda)$ on the real axis, valid, let us stress it, for P of degree at most two with real coefficients, but for any value of the polynomial Q_I , not at all limited to (49), as it is apparent in the description of our calculations. If P has real roots,

$$I[P](\lambda) = Q_I^{[1]}(\lambda) \left\{ u[P(\lambda)] - \frac{3}{2} \right\} + \sum_{\lambda_0 \in \text{Root } P} \left\{ - \int_0^\lambda dt \frac{Q_I^{[1]}(t) - Q_I^{[1]}(\lambda_0)}{t - \lambda_0} - Q_I^{[1]}(\lambda_0) \left[\ln |\lambda - \lambda_0| - \ln |\lambda_0| + i\pi \frac{P'(\lambda_0)}{|P'(\lambda_0)|} [Y(\lambda - \lambda_0) - Y(-\lambda_0)] \right] \right\} \quad (54)$$

⁷ In the case where P has actually a double root, which can be seen as the convergence of two single roots towards a common value λ_0 , the contributions of the two roots to the remaining integral cancel out and only the all-integrated term survives.

If P has complex roots,

$$I[P](\lambda) = Q_I^{[1]}(\lambda) \left\{ u[P(\lambda)] - \frac{3}{2} \right\} + \sum_{\lambda_0 \in \text{Root } P} \left\{ - \int_0^\lambda dt \frac{Q_I^{[1]}(t) - Q_I^{[1]}(\lambda_0)}{t - \lambda_0} - Q_I^{[1]}(\lambda_0) [\ln(\lambda - \lambda_0) - \ln(-\lambda_0)] \right\} \quad (55)$$

bearing in mind that if $Q_I(\lambda)$ has real coefficients the imaginary part of $I[P](\lambda)$ originates only from the one of $u[P(\lambda)]$, therefore from the first term.

Let us now tackle with the **evaluation of the functional** $J[P]$, under the same hypothesis of a polynomial $P(\lambda)$ of degree at most two with real coefficients. The auxiliary polynomial has to be defined as follows:

$$Q_J(\lambda) = \frac{Q_I(\lambda) - Q_I(0)}{\lambda} = \frac{[P(\lambda)]^2 - [P(0)]^2}{2\lambda} \quad (56)$$

to lead to the useful splitting in two sub-functionals,

$$J[P](\lambda) = J_1[P](\lambda) + \frac{[P(0)]^2}{2} J_2[P](\lambda), \quad (57)$$

with

$$J_1[P](\lambda) = \int_0^\lambda dt Q_J(t) \left\{ u[P(t)] - \frac{3}{2} \right\} \quad (58)$$

$$J_2[P](\lambda) = \int_0^\lambda dt \frac{u[P(t)] - u[P(0)]}{t} \quad (59)$$

As the expressions (54) and (55) are valid for any polynomial Q_I , the functional $J_1[P](\lambda)$ is obtained by replacing Q_I with Q_J , and thus $Q_I^{[1]}$ with $Q_J^{[1]}$. In the functional $J_2[P](\lambda)$, the imaginary part of $u[P(t)] - u[P(0)]$ in the numerator of the integrand is zero if P has complex roots since P has then a constant sign. Otherwise its contribution is evaluated by integrating by parts as for $I[P]$. In the real part of $u[P(t)] - u[P(0)]$, one uses the factorization (48) for P ; dividing by t , one obtains the function $t \mapsto \ln[|t - \lambda_0|/|\lambda_0|]/t$ for each real root λ_0 of $P(\lambda)$, or $t \mapsto \ln[(t - \lambda_0)/\lambda_0]/t$ for each complex root, whose integral is expressible in terms of the dilogarithm Li_2 . Note that Li_2 is also called polylogarithm of order two or Jonquière's function of parameter equal to two, and it satisfies $\text{Li}_2'(z) = -\ln(1-z)/z$ and $\text{Li}_2(0) = 0$. If P has real roots we finally find

$$J_2[P](\lambda) = i\pi \{Y[P(\lambda)] - Y[P(0)]\} \ln|\lambda| + \sum_{\lambda_0 \in \text{Root } P} \left\{ -\bar{\text{Li}}_2(\lambda/\lambda_0) - i\pi \ln|\lambda_0| \frac{P'(\lambda_0)}{|P'(\lambda_0)|} [Y(\lambda - \lambda_0) - Y(-\lambda_0)] \right\} \quad (60)$$

where the function $\bar{\text{Li}}_2$ is real-valued on the real axis,

$$\bar{\text{Li}}_2(\lambda) = \lim_{\epsilon \rightarrow 0^+} \frac{\text{Li}_2(\lambda + i\epsilon) + \text{Li}_2(\lambda - i\epsilon)}{2} = - \int_0^\lambda \frac{dt}{t} \ln|t - 1| \quad (61)$$

it coincides with Li_2 for $\lambda < 1$ but gives for $\lambda > 1$ the average of the values of Li_2 just above and just below its branch cut $[1, +\infty[$. If P has complex roots, we obtain the real-valued result

$$J_2[P](\lambda) = - \sum_{\lambda_0 \in \text{Root } P} \text{Li}_2(\lambda/\lambda_0) \quad (62)$$

C. For an infinite cutoff

The third step consists in taking the infinite cutoff limit, $\Lambda \rightarrow +\infty$. The various terms depending on Λ in (45) and the integral of $\chi(\lambda)$ over $[0, \Lambda]$ in (29) diverge if they are considered individually. However, their divergent contributions have to cancel exactly in the final result for $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$, since the integral in (29) is convergent, and it

is useless to evaluate them one by one. To eliminate them in a simple but systematic way, let us write each term of (45) asymptotically in the canonical form:

$$\mathcal{I}(\Lambda) \stackrel{\Lambda \rightarrow +\infty}{=} \sum_{(i,j) \in \mathbf{N}^2} a_{i,j} \Lambda^i (\ln \Lambda)^j + o(1) \quad (63)$$

with a finite number of nonzero coefficients $a_{i,j}$. The unicity of writing of this form allows us to uniquely define the *partie finie* of $\mathcal{I}(\Lambda)$ in $+\infty$:

$$\text{Pf } \mathcal{I}(+\infty) \equiv a_{0,0} = \lim_{\Lambda \rightarrow +\infty} \left[\mathcal{I}(\Lambda) - \sum_{(i,j) \in \mathbf{N}^{2*}} a_{i,j} \Lambda^i (\ln \Lambda)^j \right] \quad (64)$$

An explicit calculation of the integral of $\chi(\lambda)$ over $[0, 2]$ and over $[2, \Lambda]$, starting from (41,42) and using the integration by parts to eliminate the logarithm, leads to only one divergent term, linear in Λ thus of the form (63), and finally to

$$\text{Pf} \int_0^{+\infty} d\lambda \chi(\lambda) = -\frac{2}{3(1+r)} \quad (65)$$

This, by the way, cancels exactly the constant term $\frac{3r}{1+r}$ in equation (29). Also, it is clear from equations (54) and (55) that the functional $I[P](\Lambda)$ obeys the form (63): $u[P(\Lambda)]$ and $\ln|\Lambda - \lambda_0|$ or $\ln(\Lambda - \lambda_0)$ give contributions in $\ln \Lambda + O(1)$, and the other factors or terms give purely polynomial divergent contributions. The calculation of its *partie finie* is then trivial if we realize that, for all polynomials $R(\lambda) = \sum_{n \geq 1} b_n \lambda^n$ vanishing in zero thus of zero *partie finie* in $+\infty$, such as the polynomial $Q_I(\lambda)$ or the contribution of \int_0^λ in (54) and (55), we have

$$\text{Pf} [R(\lambda) \ln(\Lambda - \lambda_0)]_{\Lambda \rightarrow +\infty} = - \sum_{n \geq 1} b_n \frac{\lambda_0^n}{n} = - \int_0^{\lambda_0} d\lambda \frac{R(\lambda)}{\lambda} \quad (66)$$

given the asymptotic expansion of $\ln(\lambda - \lambda_0) = \ln \lambda - \sum_{n \geq 1} (\lambda_0/\lambda)^n/n$ in $+\infty$. This gives for $P(\lambda)$ with real roots:

$$\text{Pf } I[P](+\infty) = \sum_{\lambda_0 \in \text{Root } P} \left\{ Q_I^{[1]}(\lambda_0) \left[\ln |\lambda_0| - i\pi Y(\lambda_0) \frac{P'(\lambda_0)}{|P'(\lambda_0)|} \right] - \int_0^{\lambda_0} d\lambda \frac{Q_I^{[1]}(\lambda)}{\lambda} \right\} \quad (67)$$

and for $P(\lambda)$ with complex roots:

$$\text{Pf } I[P](+\infty) = \sum_{\lambda_0 \in \text{Root } P} \left\{ Q_I^{[1]}(\lambda_0) \ln(-\lambda_0) - \int_0^{\lambda_0} d\lambda \frac{Q_I^{[1]}(\lambda)}{\lambda} \right\} \quad (68)$$

These considerations and expressions extend directly to the functional $J_1[P](\Lambda)$, since it is sufficient to replace the polynomial $Q_I^{[1]}(\lambda)$ with the polynomial $Q_J^{[1]}(\lambda)$. As for the functional $J_2[P](\lambda)$, the properties of the dilogarithm function, or simply a direct reasoning on the integrals that led to it⁸, give for $P(\lambda)$ with real roots a result that may be complex

$$\text{Pf } J_2[P](+\infty) = \sum_{\lambda_0 \in \text{Root } P} \left[\frac{(\ln |\lambda_0|)^2}{2} - \frac{\pi^2}{3} Y(\lambda_0) + \frac{\pi^2}{6} Y(-\lambda_0) - i\pi \ln |\lambda_0| Y(\lambda_0) \frac{P'(\lambda_0)}{|P'(\lambda_0)|} \right] \quad (69)$$

and for $P(\lambda)$ with complex roots a real result

$$\text{Pf } J_2[P](+\infty) = \frac{\pi^2}{3} + \sum_{\lambda_0 \in \text{Root } P} \frac{1}{2} [\ln(-\lambda_0)]^2 \quad (70)$$

⁸ We obtain on the real axis $\text{Li}_2(x) = \frac{\pi^2}{12} - \frac{1}{2}(\ln |x|)^2 + \frac{\pi^2}{4} \frac{x}{|x|} - \frac{1}{x} + O(\frac{1}{x^2})$ for $x \rightarrow \pm\infty$, and out of the real axis, $\text{Li}_2(z) = -\frac{1}{2}[\ln(-z)]^2 - \frac{\pi^2}{6} + O(\frac{1}{z})$, with the principal branch of the complex logarithm.

It remains to deal with the quantity $C^\pm(\Lambda)$ in equation (45). For our usual generic polynomial $P(\lambda)$ of degree at most two with real coefficients, we find, independently on the fact that its roots are real or complex, the expression

$$\text{Pf} \left[\frac{u^{[3]}[P(\Lambda)]}{\Lambda} \right]_{\Lambda \rightarrow +\infty} = Q_C(0) [\ln |A_P| - \frac{11}{6} + i\pi Y(A_P)] - \sum_{\lambda_0 \in \text{Root } P} \int_0^{\lambda_0} d\lambda \frac{Q_C(\lambda) - Q_C(0)}{\lambda} \quad (71)$$

in terms of the leading coefficient A_P of P and of the auxiliary polynomial $Q_C(\lambda) \equiv \{[P(\lambda)]^3 - [P(0)]^3\}/(3!\lambda)$ which is *a priori* nonzero in zero. We have used (66) with $R(\lambda) = [Q_C(\lambda) - Q_C(0)]/\lambda$.

Fortunately, the obtained results for the *partie finie* when the cutoff $\Lambda \rightarrow +\infty$ can be largely simplified thanks to the duality relations (40). Indeed, only the polynomials $P_\alpha^\pm(\lambda)$ and $P_\delta^\pm(\lambda)$ appear in the Λ -dependent terms of equation (45), and only the difference $\psi^+(\lambda) - \psi^-(\lambda)$ matters in the final result (29). To the generic polynomial $P(\lambda)$ of degree two we then associate its dual

$$\check{P}(\lambda) \equiv P(-\lambda) \quad (72)$$

Of course, the roots of $\check{P}(\lambda)$ are the opposite of the roots of $P(\lambda)$, while the two polynomials have the same value in zero and the same leading coefficient. One simply substitutes the polynomial $P(\lambda)$ and its roots λ_0 , its auxiliary polynomials $Q_I(\lambda)$, $Q_J(\lambda)$ defined by (49) and (56), and their primitives $Q_I^{[1]}(\lambda)$, $Q_J^{[1]}(\lambda)$ (that appear in the expression of the *partie finie* of the functionals $I[P](\Lambda)$ and $J[P](\Lambda)$ in $\Lambda = +\infty$), with the dual polynomial $\check{P}(\lambda) \equiv P(-\lambda)$ and its roots $\check{\lambda}_0 = -\lambda_0$, its auxiliary polynomials $\check{Q}_I(\lambda) = Q_I(-\lambda)$, $\check{Q}_J(\lambda) = -Q_J(-\lambda)$ and their primitives $\check{Q}_I^{[1]}(\lambda) = -Q_I^{[1]}(-\lambda)$, $\check{Q}_J^{[1]}(\lambda) = Q_J^{[1]}(-\lambda)$. One then obtains the expression of the *partie finie* of $I[\check{P}](\Lambda)$ and $J[\check{P}](\Lambda)$ in $\Lambda = +\infty$. Moreover, in equation (71), replacing $P(\lambda)$ with $\check{P}(\lambda)$ amounts to replacing $Q_C(\lambda)$ with $\check{Q}_C(\lambda) = -Q_C(-\lambda)$.

Thus we obtain a series of simplified relations. First, $\text{Pf} \{ [u^{[3]}[P(\Lambda)] + u^{[3]}[\check{P}(\Lambda)]]/\Lambda \} = 0$ in $\Lambda = +\infty$ so that

$$\text{Pf} [C^+ - C^-](+\infty) = 0 \quad (73)$$

and the terms $C^\pm(\Lambda)$ of equation (45) give no contribution to $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$. Then, for the functional I , whose values at P and \check{P} have to be summed up, in the case realized in practice of a coefficient $A_P > 0$ in $P(\lambda)$, we have

$$\text{Pf} \{ I[P] + I[\check{P}] \}(+\infty) \stackrel{A_P > 0}{=} -i\pi [Q_I^{[1]}(\lambda_2) - Q_I^{[1]}(\lambda_1)] = -\frac{i\pi A_P^2}{60} (\lambda_2 - \lambda_1)^5 \quad (74)$$

where the roots λ_1, λ_2 of $P(\lambda)$ are sorted by increasing order if they are real, and by increasing order of their imaginary part if they are complex, so that

$$\lambda_2 - \lambda_1 = \frac{\Delta_P^{1/2}}{|A_P|} \text{ (real roots) } \text{ or } \frac{i(-\Delta_P)^{1/2}}{|A_P|} \text{ (complex roots)}, \quad (75)$$

Δ_P being the discriminant of the polynomial $P(\lambda)$ ⁹. We proceed in a similar way for the functional J , whose values at P and \check{P} have to be subtracted since J is multiplied by \bar{K} in equation (45). Taking into account the splitting (57), let us first writ, here also for $A_P > 0$,

$$\begin{aligned} & \text{Pf} \{ J_1[P] - J_1[\check{P}] \}(+\infty) \stackrel{A_P > 0}{=} -i\pi [Q_J^{[1]}(\lambda_2) - Q_J^{[1]}(\lambda_1)] \\ & = -\frac{i\pi A_P^2}{24} (\lambda_2 - \lambda_1)(\lambda_1 + \lambda_2)[(\lambda_1 + \lambda_2)^2 - 10\lambda_1\lambda_2] \end{aligned} \quad (76)$$

where we recall that the sum $\lambda_1 + \lambda_2$ and the product $\lambda_1\lambda_2$ of the roots are respectively the coefficients of the terms of order one in λ and of order zero in λ of the normalized dual polynomial $\check{P}(\lambda)/A_P$. Then, to give the remaining term, let us consider first the case of $P(\lambda)$ with real roots:

$$\text{Pf} \{ J_2[P] - J_2[\check{P}] \}(+\infty) \stackrel{A_P > 0}{=} -\pi^2 Y(\lambda_1\lambda_2) \frac{\lambda_1 + \lambda_2}{|\lambda_1 + \lambda_2|} - i\pi \ln \frac{|\lambda_2|}{|\lambda_1|}, \quad (77)$$

where we have used $A_P > 0$, $Y(x) - Y(-x) = \text{sgn } x$, $\text{sgn } x + \text{sgn } y = 2Y(xy) \text{sgn } (x + y)$ for any real x and y . In the case of $P(\lambda)$ with complex roots, without any hypothesis on the sign of A_P , it reads

$$\text{Pf} \{ J_2[P] - J_2[\check{P}] \}(+\infty) = -i\pi \ln \left(\frac{-\lambda_2}{\lambda_1} \right) = -2\pi \arcsin \frac{\lambda_1 + \lambda_2}{2|\lambda_1\lambda_2|^{1/2}} \quad (78)$$

This concludes our calculation of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$.

⁹ In the case of complex roots, we use the property $\ln(\lambda_2) - \ln(-\lambda_2) = \ln(-\lambda_1) - \ln(\lambda_1) = i\pi$.

D. A compact form of the final result

To conclude this section, let us give (under a compact form as in [36]) the contribution of order g^2 to the self-energy of the impurity, in dimensionless units as in (21):

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) = \frac{9}{32r^2\bar{K}}[\mathcal{S}^+ - \mathcal{S}^-] \quad (79)$$

where the quantities \mathcal{S}^\pm defined as

$$\mathcal{S}^\pm \equiv (1+r)[i_\alpha^\pm + I_\delta^\pm(2)] - (1-r)I_\beta^\pm(2) - rI_\gamma^\pm(2) \pm \bar{K}[j_\alpha^\pm - J_\beta^\pm(2) + J_\delta^\pm(2)] \quad (80)$$

are mutually interchanged by changing \bar{K} to $-\bar{K}$, which does not cause any problem since the property $\bar{K} > 0$ was never used in the two previous subsections. In equation (80), the quantities $I_\sigma^\pm(\lambda)$ and $J_\sigma^\pm(\lambda)$, related to the trinomials (36,37,38,39) by equation (46), can be evaluated explicitly for $\lambda = 2$ thanks to the expressions (54,55) and (60,62), given the splitting (57) and the link between the functionals $J_1[P]$ and $I[P]$ indicated just below equation (59); the new quantities introduced in (80),

$$i_\alpha^\pm \equiv \text{Pf}(I_\alpha^\pm + I_\delta^\mp)(+\infty) \quad \text{and} \quad j_\alpha^\pm \equiv \text{Pf}(J_\alpha^\pm - J_\delta^\mp)(+\infty) \quad (81)$$

are deduced from the results (74), (76) and (77,78) by setting $P(\lambda) = P_\alpha^\pm(\lambda)$ since we have the duality (40), and by bearing in mind also the splitting (57).

V. SINGULARITIES OF THE DERIVATIVES OF $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$

The self-energy of the impurity to second order in the interaction, $(\bar{K}, \varepsilon) \mapsto \bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ in its dimensionless form, calculated explicitly in section IV, is a smooth function on $\mathbb{R}^+ \times \mathbb{R}$ except on certain singularity curves that we are going to study here. To see it, it is sufficient to remark that each of the terms in the splitting (79,80) is a function of the leading coefficients A_P and of the roots λ_0 of the polynomials $P_\sigma^\eta(\lambda)$, with $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$ depending on whether we consider \mathcal{S}^\pm . While the A_P are constant, the roots λ_0 are non-trivial functions of (\bar{K}, ε) . Our discussion considers here the general case $r \neq 1$, but it is readily adapted to the particular case $r = 1$.

A. Location of the singularities in the plane (\bar{K}, ε)

A first source of singularity for the derivatives of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ is the non-differentiability of the roots with respect to (\bar{K}, ε) , which happens when the discriminant Δ_σ^η of one of the polynomials $P_\sigma^\eta(\lambda)$ vanishes, so that the quantity $(\Delta_\sigma^\eta)^{1/2}$ in the expression of the roots is not anymore differentiable:

$$\Delta_\alpha^\eta = 0 \Leftrightarrow \varepsilon = \frac{(r + \eta\bar{K})^2}{r(1+r)} \quad \Delta_\beta^\eta = 0 \Leftrightarrow \varepsilon = \frac{(r + \eta\bar{K})^2}{r(1-r)} \quad (82)$$

$$\Delta_\gamma^\eta = 0 \Leftrightarrow \varepsilon = \frac{\bar{K}^2}{r} \quad \Delta_\delta^\eta = 0 \Leftrightarrow \varepsilon = \frac{(r - \eta\bar{K})^2}{r(1+r)} \quad (83)$$

Although there are eight distinct polynomials into play, the corresponding locus of points in the half-plane $(\bar{K} > 0, \varepsilon)$ is composed of portions of five parabolas only, see figure 1, due to the duality relations (40) and $P_\gamma^-(\lambda) = P_\gamma^+(-\lambda)$. Note that (for $r < 1$ if $\sigma = \beta$) the polynomial $P_\sigma^\eta(\lambda)$ has real roots when (\bar{K}, ε) is below the parabola $\Delta_\sigma^\eta = 0$, it has a double root when (\bar{K}, ε) is on the parabola, and it has complex roots when (\bar{K}, ε) is above the parabola.

A second source of singularity for the derivatives of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ is the non-differentiability of $\bar{\Sigma}^{(2)}$ with respect to the roots λ_0 of the polynomials. As it appears on equations (54,60), taken for $\lambda = 2$, and on equation (77), this may be due to logarithmic singularities in the real part, coming from the logarithm itself or from the behavior of the function $\bar{\text{Li}}_2(x)$ in the neighborhood of $x = 1$ and $x = \pm\infty$, and from the discontinuity of the Heaviside function in the imaginary part. This can happen only if one of the roots λ_0 of the considered polynomial tends to zero or two¹⁰.

¹⁰ For any fixed λ , the quantities $Q_I^{[1]}(\lambda)$ and $Q_J^{[1]}(\lambda)$ are polynomials in the coefficients of $P(\lambda)$, thus here C^∞ functions in the roots $\lambda_{1,2}$

We find that the condition of existence of a zero root is the same for the eight polynomials P_σ^η , where $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$:

$$\forall \sigma \in \{\alpha, \beta, \gamma, \delta\}, \forall \eta = \pm : P_\sigma^\eta(0) = 0 \Leftrightarrow \varepsilon = 0 \quad (84)$$

which corresponds to a single line in the plane (\bar{K}, ε) . Asking if one of the roots is equal to two is useful only for the six polynomials P_σ^η , with $\sigma \in \{\beta, \gamma, \delta\}$ and $\eta = \pm$, since the index α in (80) appears only in the *partie finie* i_α^\pm and j_α^\pm ; the expressions (74,76) are indeed smooth functions of the roots, as well as (77) except in $\lambda_{1,2} = 0$. Then we find that the condition of existence of a root $\lambda_0 = 2$ depends only on the sign of η , it is the same for the three polynomials $P_\sigma^+(\lambda)$ from one hand, and for the three polynomials $P_\sigma^-(\lambda)$ from the other hand:

$$\forall \sigma \in \{\beta, \gamma, \delta\}, \forall \eta = \pm : P_\sigma^\eta(2) = 0 \Leftrightarrow r\varepsilon = -4(1 + \eta\bar{K}) \quad (85)$$

which corresponds to two lines only in the plane (\bar{K}, ε) , that are interchanged by reflection with respect to the vertical axis, where they cross.

There exist points of the plane (\bar{K}, ε) that are *doubly* singular, that combine the two sources of singularity for a given polynomial $P_\sigma^\eta(\lambda)$: The polynomial there has a double root equal to zero or two. As shown in figure 1, these are not only intersection points of the parabola $\Delta_\sigma^\eta = 0$ and the line $\varepsilon = 0$ or $r\varepsilon = -4(1 + \eta\bar{K})$, but also tangent points, since $P_\sigma^\eta(\lambda)$, with real coefficients, cannot have both a real root and a complex root. In this subsection, contrarily to the subsection VI C for $r = 1$, we do not discuss the case of these doubly singular points, nor the case of the points of intersection between singularity curves associated to different polynomials, and what follows will be valid only for the other points, that is for the generic points, of the singularity curves.

We have not found any clear physical interpretation of the singularity curves, which must be linked to the existence of a Fermi surface which imposes sharp boundaries $k = q = k_F$ in the domain of variation of \mathbf{k} and \mathbf{q} in equation (16). At the Fermi surface, $\lambda = 0$ and $\lambda = 2$ correspond to a particle and a hole having equal and equal-and-opposite momenta, respectively. Then, by using the expectation of reference [36] that highly singular points should be obtained when both $F_{\mathbf{k},\mathbf{q}}(\mathbf{K}, \omega)$ and its first order differential with respect to \mathbf{k} and \mathbf{q} vanish at some point of the Fermi surface, we obtain the multiply-singular point $(\bar{K} = r, \varepsilon = 0)$, for $\lambda = 0$.

B. On the parabolas: The effect of a double root

Let us first study the singularities on the parabolas $\Delta_\sigma^\eta = 0$, $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$, in a point of the plane (\bar{K}, ε) where the polynomial $P_\sigma^\eta(\lambda)$ has a double root $\lambda_{0,0}^{(\eta\sigma)}$. To simplify, we will approach the parabola only from $\Delta_\sigma^\eta > 0$, where $P_\sigma^\eta(\lambda)$ has real roots, $\lambda_1^{(\eta\sigma)} < \lambda_2^{(\eta\sigma)}$, arbitrarily close to $\lambda_{0,0}^{(\eta\sigma)}$. As $\lambda_{0,0}^{(\eta\sigma)}$ is different from zero and from two, and given the footnote 10, only the second line in the equation (54) and its counterpart in the functional J can lead to singularities. Inspired by the footnote, we express the $Q_I^{[1]}(\lambda_{1,2}^{(\eta\sigma)})$ as linear combinations of their sum S_I and of their difference D_I ,

$$S_I = Q_I^{[1]}(\lambda_1^{(\eta\sigma)}) + Q_I^{[1]}(\lambda_2^{(\eta\sigma)}) \quad \text{and} \quad D_I = Q_I^{[1]}(\lambda_2^{(\eta\sigma)}) - Q_I^{[1]}(\lambda_1^{(\eta\sigma)}) \quad (86)$$

The contribution of S_I to the real part of $I_\sigma^\eta(2)$ contains as a factor the logarithm of expressions that, like S_I , are symmetric functions of the roots, that is their product or the product of their deviation from two; as the whole this is a smooth function of (\bar{K}, ε) . Remarkably, the contribution of D_I to the real part of $I_\sigma^\eta(2)$ is also a smooth function of (\bar{K}, ε) at the double root point, by virtue of the following property that we will apply, given the explicit value (74) of D_I , to the function $f(\lambda_1, \lambda_2) = (\lambda_2 - \lambda_1)^5 \ln\{\lambda_1(2 - \lambda_2)/[\lambda_2(2 - \lambda_1)]\}$:

Property 1: If $f(\lambda_1, \lambda_2)$ is a symmetric function of $(\lambda_1, \lambda_2) \in \mathbb{R}^2$ and a smooth function (C^∞) in a neighborhood of $(\lambda_{0,0}^{(\eta\sigma)}, \lambda_{0,0}^{(\eta\sigma)})$, then $f(\lambda_1^{(\eta\sigma)}, \lambda_2^{(\eta\sigma)})$ is a C^∞ function of (\bar{K}, ε) at the point where $P_\sigma^\eta(\lambda)$ has a double root $\lambda_{0,0}^{(\eta\sigma)}$.

To establish this property, let us remark that $\lambda_{1,2}^{(\eta\sigma)} - \lambda_{0,0}^{(\eta\sigma)} = \mp(\Delta_\sigma^\eta)^{1/2}/(2|A_\sigma^\eta|)$ up to a single additive C^∞ function of (\bar{K}, ε) , with A_σ^η being the leading coefficient of $P_\sigma^\eta(\lambda)$. As $f(\lambda_1, \lambda_2)$ is a symmetric function, the Taylor expansion

as well as in \bar{K} and ε . The quantity $Q_I^{[1]}(\lambda_0)$ is a polynomial in $\lambda_{1,2}$, thus is C^∞ in $\lambda_{1,2}$, but not necessarily C^∞ in \bar{K} and ε where the roots are not C^∞ functions of \bar{K} and ε . Also, the integral term in (54) and its counterpart in $J_1[P](\lambda)$ are polynomials in $\lambda_{1,2}$; but after summing over λ_0 , they become *symmetric* polynomials in $\lambda_{1,2}$, that is, according to a classical result, polynomials in $\lambda_1 + \lambda_2$ and $\lambda_1\lambda_2$, thus here C^∞ functions of \bar{K} and ε .

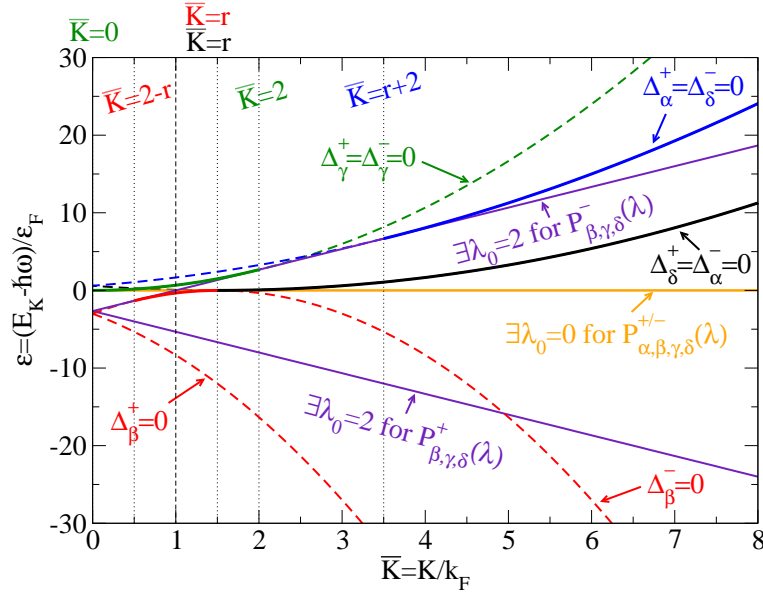


Figure 1: The singularity curves of the derivatives with respect to $(\bar{K}, \varepsilon) \in \mathbb{R}^+ \times \mathbb{R}$ of the dimensionless self-energy of order two $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$. (i) On the parabolas $\Delta_\sigma^\eta = 0$, where Δ_σ^η is the discriminant of the polynomial $P_\sigma^\eta(\lambda)$, $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta \in \{+, -\}$, the roots of the polynomials are non-differentiable functions of (\bar{K}, ε) ; this actually leads to a singularity of the derivatives of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ on the full line portions, not on the dashed line portions. (ii) $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ is not a smooth function of the roots on the horizontal half-line, where at least one (but also each) polynomial $P_\sigma^\pm(\lambda)$, $\sigma \in \{\alpha, \beta, \gamma, \delta\}$, has a root $\lambda_0 = 0$, and on the oblique half-line (downwards for $\eta = +$, upwards for $\eta = -$), where at least one (but also each) polynomial $P_\sigma^\eta(\lambda)$, $\sigma \in \{\beta, \gamma, \delta\}$, has one root $\lambda_0 = 2$. Vertical dotted lines mark the abscissa of the tangent points of the parabolas with the singularity lines; the values of the abscissas are given explicitly as functions of the impurity-to-fermion mass ratio $r = M/m$, in a color code and obliquity code identifying respectively the parabola and the line that are tangent. The vertical dashed line marks the abscissa $\bar{K} = 1$ of the crossing point of the horizontal and the oblique upwards singularity lines. In the figure, $r = 3/2$.

of $f(\lambda_1^{(\eta\sigma)}, \lambda_2^{(\eta\sigma)})$ in powers of $(\Delta_\sigma^\eta)^{1/2}$ produces only even powers, which are C^∞ functions of (\bar{K}, ε) , hence the result. \blacksquare

Likewise, we find that the real part of $J_\sigma^\eta(2)$ is a C^∞ function of (\bar{K}, ε) at the considered point. To study the piece J_1 , in the splitting (57), we introduce S_J and D_J [see equation (76)], by replacing in (86) the auxiliary polynomial Q_I with Q_J . In the case of the J_2 piece, which is multiplied by $[P(0)]^2/2$, a C^∞ function of (\bar{K}, ε) , we use the property 1 with $f(\lambda_1, \lambda_2) = \bar{\text{Li}}_2(2/\lambda_1) + \bar{\text{Li}}_2(2/\lambda_2)$, which is legitimate since $2/\lambda_{1,2}$ is here in the neighborhood of neither $\pm\infty$ nor the edge of the branch cut $\Re z \geq 1$ of the function $\text{Li}_2(z)$ in the complex plane.

Let us now consider the case of the imaginary part of $I_\sigma^\eta(2)$ and $J_\sigma^\eta(2)$. The Heaviside functions of the roots in the neighborhood of the considered point take the same value for $\lambda_{1,2}$, it is their value in the double root, which can be expressed in terms of a rectangular function, the indicator function of the interval $[0, 2]$, which vanishes everywhere except on this interval where it takes the value one:

$$\Pi_{[0,2]}(x) \equiv Y(2-x) - Y(-x) \quad (87)$$

As $P'(\lambda_{1,2})/|P'(\lambda_{1,2})|$ have opposite signs, only the function D_I and D_J contribute. Finally there appear antisymmetric functions of the roots, which do not obey property 1 and are not C^∞ in (\bar{K}, ε) at the considered point. In particular, we collect the pieces J_1 and J_2 so as to avoid stronger intermediate singularities, which amounts to considering the function $(\lambda_2 - \lambda_1)f(\lambda_1, \lambda_2)$ where $f(\lambda_1, \lambda_2) = \frac{\lambda_1 + \lambda_2}{24}[(\lambda_1 + \lambda_2)^2 - 10\lambda_1\lambda_2] + \frac{(\lambda_1\lambda_2)^2}{2} \ln(\lambda_2/\lambda_1)$ is C^∞ , symmetric, homogeneous of degree three and such that $f(1+\delta, 1-\delta) = \frac{4}{15}\delta^4 + O(\delta^5)$ when $\delta \rightarrow 0$. We obtain up to

an additive C^∞ function of (\bar{K}, ε) :

$$I_\sigma^\eta(2) \stackrel{\Delta_\sigma^\eta \rightarrow 0^+}{=} -\frac{i\pi \Pi_{[0,2]}(\lambda_{0,0}^{(\eta\sigma)})}{60(A_\sigma^\eta)^3} (\Delta_\sigma^\eta)^{5/2} + C^\infty \quad (88)$$

$$J_\sigma^\eta(2) \stackrel{\Delta_\sigma^\eta \rightarrow 0^+}{=} -\frac{i\pi \Pi_{[0,2]}(\lambda_{0,0}^{(\eta\sigma)})}{60\lambda_{0,0}^{(\eta\sigma)}(A_\sigma^\eta)^3} [(\Delta_\sigma^\eta)^{5/2} + O(\Delta_\sigma^\eta)^3] + C^\infty \quad (89)$$

As a consequence, the **third order** derivative of $\Im I_\sigma^\eta(2)$ and of $\Im J_\sigma^\eta(2)$ along the direction normal to the parabola $\Delta_\sigma^\eta = 0$ diverges as the inverse of the square root of the distance to the parabola, provided the double root of the polynomial $P_\sigma^\eta(\lambda)$ is in the interval $]0, 2[$, which happens on the portion of parabola between its tangent points with the lines $\exists \lambda_0^{(\eta\sigma)} = 0$ and $\exists \lambda_0^{(\eta\sigma)} = 2$ of equations (84) and (85).

In the case $\sigma = \alpha$, one must consider the symmetrized *partie finie* i_α^\pm and j_α^\pm . In reality, their singularities interfere with those of $I_\delta^\mp(2)$ and $J_\delta^\mp(2)$, as can be seen on the expression (79) of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$, since the parabolas $\Delta_\alpha^\pm = 0$ and $\Delta_\delta^\mp = 0$ coincide. One thus has to collect them to obtain

$$i_\alpha^\eta - I_\delta^{-\eta}(2) \stackrel{\Delta_\alpha^\eta \rightarrow 0^+}{=} -\frac{i\pi(\Delta_\alpha^\eta)^{5/2}}{60(A_\alpha^\eta)^3} \left\{ 1 - \Pi_{[0,2]}(-\lambda_{0,0}^{(\eta\alpha)}) \right\} + C^\infty \quad (90)$$

$$j_\alpha^\eta + J_\delta^{-\eta}(2) \stackrel{\Delta_\alpha^\eta \rightarrow 0^+}{=} -\frac{i\pi[(\Delta_\alpha^\eta)^{5/2} + O(\Delta_\alpha^\eta)^3]}{60\lambda_{0,0}^{(\eta\alpha)}(A_\alpha^\eta)^3} \left\{ 1 - \Pi_{[0,2]}(-\lambda_{0,0}^{(\eta\alpha)}) \right\} + C^\infty \quad (91)$$

where the duality (40) implies $-\lambda_{0,0}^{(\eta\alpha)} = \lambda_{0,0}^{(-\eta\delta)}$.

It remains to add all contributions to $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ according to the compact writing (79), for each of the five possible distinct parabolas, at least to verify the absence of cancellations of the contributions of the functionals $I[P]$ and $J[P]$:

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \stackrel{\Delta_\beta^\eta \rightarrow 0^+}{=} \frac{3i\pi \Pi_{[0,2]}(\frac{\eta\bar{K}+r}{r-1})}{640r(1-r)^2\bar{K}(\bar{K}+\eta r)} [(\Delta_\beta^\eta)^{5/2} + O(\Delta_\beta^\eta)^3] + C^\infty \quad (92)$$

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \stackrel{\Delta_\gamma^+ = \Delta_\gamma^- \rightarrow 0^+}{=} \frac{3i\pi[\Pi_{[0,2]}(-\bar{K}) - \Pi_{[0,2]}(\bar{K})]}{640r\bar{K}} (\Delta_\gamma^+)^{5/2} + C^\infty \quad (93)$$

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \stackrel{\Delta_\alpha^\eta = \Delta_\delta^{-\eta} \rightarrow 0^+}{=} \frac{-3i\pi[1 - \Pi_{[0,2]}(\frac{\eta\bar{K}+r}{1+r})]}{640r(1+r)^2\bar{K}(\bar{K}+\eta r)} [(\Delta_\alpha^\eta)^{5/2} + O(\Delta_\alpha^\eta)^3] + C^\infty \quad (94)$$

Note, in these expressions, the occurrence of a prefactor that diverges at the tangent point of the considered parabola $\Delta_\sigma^\eta = 0$ ($\sigma \in \{\beta, \gamma, \alpha\}$) with the horizontal axis $\varepsilon = 0$, as well as at the intersection point, of abscissa $\bar{K} = 0$, of the parabolas of the same class $\sigma \in \{\alpha, \beta\}$ but of opposite η . The portions of parabola where a divergence of the **third order** derivative of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ in the normal direction actually occurs are represented in bold lines on figure 1; the other portions are in dashed lines.

C. On the horizontal line: The effect of a zero root

Let us study now the singularities on the horizontal line $\varepsilon = 0$, in a point of the plane (\bar{K}, ε) where one (and in practice each) of the polynomials $P_\sigma^\eta(\lambda)$, with $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$, has a zero root, the other root being different from zero and two. In the neighborhood of this point, $P_\sigma^\eta(\lambda)$ has a real root $\lambda_0^{(\eta\sigma)}$ that linearly vanish in ε , therefore changing sign, as

$$\lambda_0^{(\eta\sigma)} \stackrel{\varepsilon \rightarrow 0}{=} -\frac{r\varepsilon}{P_\sigma^{\eta'}(0)} - \frac{A_\sigma^\eta}{[P_\sigma^{\eta'}(0)]^3} (r\varepsilon)^2 + O(\varepsilon^3), \quad (95)$$

the other root $\lambda_0^{(\eta\sigma)} = r\varepsilon/(A_\sigma^\eta \lambda_0^{(\eta\sigma)})$ having a finite limit.

Let us first look at the *partie finie* contributions i_α^η and j_α^η to the self-energy of order two, see equation (80). As the roots of the polynomials are C^∞ functions of (\bar{K}, ε) in the neighborhood of the considered point, the quantity i_α^η , as well as the contribution of the functional J_1 to j_α^η , are also C^∞ , by virtue of equations (74) and (76). On the other hand, after multiplication of the contribution of the functional J_2 by $[P_\alpha^\eta(0)]^2/2$, see (77), we find that the *second order* derivative of j_α^η with respect to ε has a logarithmically divergent imaginary part in $\varepsilon = 0$, and a discontinuous real part.

Can the contributions $I_\sigma^\eta(2)$ and $J_\sigma^\eta(2)$ lead to stronger singularities? In the expression (54) taken for $\lambda = 2$, the only *a priori* non C^∞ piece is in $Q_I^{[1]}(\lambda_0)[\ln|\lambda_0| \pm i\pi Y(-\lambda_0)]$, with the indices σ and η being omitted for simplicity. But here $Q_I^{[1]}(\lambda_0)$ vanishes *cubically* in λ_0 , as can be seen by the simple change of variable $t = x\lambda_0$ in the integral defining $Q_I^{[1]}$:

$$Q_I^{[1]}(\lambda_0) \equiv \int_0^{\lambda_0} dt \frac{[P(t)]^2}{2} = \frac{A_P^2}{2} \lambda_0^3 \int_0^1 dx (x-1)^2 (\lambda_0 x - \lambda_0')^2 \quad (96)$$

With the help of the relation $sY(-s\varepsilon) = Y(s) - Y(\varepsilon)$, true for any $s = \pm 1$ but in practice used with $s = P'(0)/|P'(0)|$, we obtain, by reintroducing the indices:

$$I_\sigma^\eta(2) \xrightarrow{\varepsilon \rightarrow 0} -\frac{(r\varepsilon)^3 [1 + O(\varepsilon)]}{6P_\sigma^{\eta'}(0)} [\ln|\varepsilon| + i\pi Y(\varepsilon)] + C^\infty \quad (97)$$

so that one must take the *third* order derivative of $I_\sigma^\eta(2)$ with respect to ε to have a logarithmic divergence in its real part, and a discontinuity in its imaginary part. In the case of $J_1[P](2)$, we make the same reasoning by replacing Q_I with Q_J :

$$Q_J^{[1]}(\lambda_0) \equiv \int_0^{\lambda_0} dt \frac{[P(t)]^2 - [P(0)]^2}{2t} = \frac{A_P^2}{2} \lambda_0^2 \int_0^1 \frac{dx}{x} [(x-1)^2 (\lambda_0 x - \lambda_0')^2 - \lambda_0'^2] \quad (98)$$

This vanishes *quadratically* in λ_0 , and by taking the derivative of $J_1[P](2)$ just *twice* with respect to ε one obtains a logarithmic divergence in the real part and a discontinuity in the imaginary part. However, the singularity coming from the functional J_2 is even more severe, even after multiplication by $[P(0)]^2/2$, see (60) and footnote 8 on the asymptotic behavior of the function $\bar{\text{Li}}_2(x)$: As a result, the second order derivative of $J_\sigma^\eta(2)$ with respect to ε diverges as the *square* of the logarithm of ε for the real part, and, on the $\lambda_0 > 0$ side, as the logarithm of ε for the imaginary part.

Collecting all the contributions to $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$, we find however that the expected singularity in $\varepsilon = 0$ in the second order derivative do not appear, due to a perfect cancellation of the contributions of j_α^η , $J_\delta^{-\eta}(2)$ and $J_\beta^\eta(2)$. As in equation (91), there is thus a clever combination to consider,

$$j_\alpha^\eta + J_\delta^{-\eta}(2) - J_\beta^\eta(2) = \mathcal{J}_\alpha^\eta - \mathcal{J}_\beta^\eta + C^\infty \quad (99)$$

for which we find after rather long calculations:

$$\begin{aligned} \mathcal{J}_\sigma^\eta &\equiv Q_{J_\sigma^\eta}^{[1]}(\lambda_0^{(\eta\sigma)}) [\ln|\lambda_0^{(\eta\sigma)}| + i\pi Y(\varepsilon)] \\ &+ \frac{(r\varepsilon)^2}{2} \left[-\bar{\text{Li}}_2(2/\lambda_0^{(\eta\sigma)}) + i\pi Y(\varepsilon) \ln|\lambda_0^{(\eta\sigma)}| \right] \end{aligned} \quad (100)$$

We used, inter alia, the duality relation (40), which implies $\lambda_0^{(-\eta\delta)} = -\lambda_0^{(\eta\alpha)}$, $P_\delta^{-\eta'}(0) = -P_\alpha^{\eta'}(0)$ and $Q_{J_\delta^{-\eta}}^{[1]}(\lambda_0^{(-\eta\delta)}) = Q_{J_\alpha^\eta}^{[1]}(\lambda_0^{(\eta\alpha)})$, the already encountered relation $sY(-s\varepsilon) = Y(s) - Y(\varepsilon)$, here with $s_\eta = P_\alpha^{\eta'}(0)/|P_\alpha^{\eta'}(0)|$, the relation $\ln[|\lambda_2^{(\eta\alpha)}|/|\lambda_1^{(\eta\alpha)}|] = s_\eta \ln|\lambda_0^{(\eta\alpha)}| + C^\infty$. And also the fact that $\ln[|\lambda_0^{(\eta\alpha)}|/\lambda_0^{(\eta\beta)}]$ is a C^∞ function of ε in $\varepsilon = 0$, and that the expression $\bar{\text{Li}}_2(1/x) - \bar{\text{Li}}_2(-1/x) - (\pi^2/2) \text{sgn}(x)$, because it is $\int_0^x (dt/t) \ln[|t-1|/|t+1|]$ according to (61), is a C^∞ function of $x \in]-1, 1[$. We mainly used the fact that the polynomials $P_\alpha^\eta(\lambda)$ and $P_\beta^\eta(\lambda)$ have the same first order derivative in $\lambda = 0$, which implies that the roots $\lambda_0^{(\eta\alpha)}$ and $\lambda_0^{(\eta\beta)}$ differ only to **second** order in ε , see (95), which explains why the clever combination (99) is a C^2 function of ε in $\varepsilon = 0$, while the terms \mathcal{J}_α and \mathcal{J}_β they are not C^2 .

By expanding the terms (100), and the combination (99), up to order three in ε , thanks in particular to (98), then including the contribution (97) of the $I_\sigma^\eta(2)$, we finally find that the **third** order derivative of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ has a real part that logarithmically diverges and an imaginary part that is discontinuous on the horizontal axis:

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \xrightarrow{\varepsilon \rightarrow 0} \frac{3r^4(\bar{K}^2 + r^2)}{64\bar{K}^2(\bar{K}^2 - r^2)^2} [\varepsilon^3 + O(\varepsilon^4)] [\ln|\varepsilon| + i\pi Y(\varepsilon)] + C^\infty \quad (101)$$

Here the prefactor diverges in the tangent point of the parabolas $\Delta_\sigma^\eta = 0$ with the horizontal axis, for $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$, which may be expected.

D. On the oblique lines : The effect of a root equal to two

To be complete let us study the singularities on the oblique line corresponding to $\eta = +$ or $\eta = -$ in equation (85), in a point of the plane (\bar{K}, ε) where one (and in practice each) of the polynomials $P_\sigma^\eta(\lambda)$, with fixed $\sigma \in \{\beta, \gamma, \delta\}$ and η , has a root equal to two, the other root being different from zero and two. In the neighborhood of such a point, the two roots of $P_\sigma^\eta(\lambda)$ are of course real; we shall note $\lambda_0^{(\eta\sigma)}$ the one that is arbitrarily close to two,

$$\lambda_0^{(\eta\sigma)} - 2 \stackrel{d_\eta \rightarrow 0}{\equiv} -\frac{d_\eta}{P_\sigma^{\eta'}(2)} + O(d_\eta^2) \quad (102)$$

where the numerator, equal to $P_\sigma^\eta(2)$, is an algebraic distance to the singularity line:

$$d_\eta \equiv r\varepsilon + 4\eta\bar{K} + 4 = P_\sigma^\eta(2), \quad \forall \sigma \in \{\beta, \gamma, \delta\} \quad (103)$$

The other root $\lambda_0'^{(\eta\sigma)}$ remains outside a neighborhood of zero and two.

As seen in the previous subsection V A, singularities can originate here only from the terms $I_\sigma^\eta(2)$ and $J_\sigma^\eta(2)$. For each term, we find at the considered point that the third order derivative in the direction normal to the oblique line has a real part that diverges logarithmically and an imaginary part that is discontinuous.

We first determine the part with singular derivatives of the functional $I[P]$, by omitting the indices $\sigma \in \{\beta, \gamma, \delta\}$ and η for simplicity. In equation (54) written for $\lambda = 2$, one has to keep the first term, as well as the third term for the root λ_0 close to two. To isolate the contribution of this root to $u[P(2)]$, let us use the factorization (48) and the relation $Y(sx) = Y(-s) + sY(x)$, where $s = \pm 1$ and x is any real, taken here to be the linear approximation (102) of $\lambda_0 - 2$. As $P'(\lambda_0)$, $P'(2)$ and $A_P(2 - \lambda_0')$ have the same sign when λ_0 is sufficiently close to two, and as $\ln|\lambda_0/d|$ is locally a C^∞ function of d , we finally obtain in the neighborhood of $d = 0$:

$$I[P](2) = [Q_I^{[1]}(2) - Q_I^{[1]}(\lambda_0)][\ln|d| + i\pi Y(d)] + C^\infty \quad (104)$$

The prefactor vanishes indeed cubically in d , as can be seen thanks to (48) and to the change of variable $x = t - \lambda_0$ in the integral over t that defines Q_I :

$$Q_I^{[1]}(2) - Q_I^{[1]}(\lambda_0) = \frac{A_P^2}{2} \int_0^{2-\lambda_0} dx x^2 (x + \lambda_0 - \lambda_0')^2 \stackrel{d \rightarrow 0}{\equiv} \frac{d^3}{6P'(2)} + O(d^4) \quad (105)$$

We perform the same analysis for the functional $J[P]$ which, let us recall it, was split in two contributions according to (57). The result for $J_1[P]$ can be deduced directly from (104) by substituting the polynomial Q_I with the polynomial Q_J . Contrarily to (104), the prefactor

$$\begin{aligned} Q_J^{[1]}(2) - Q_J^{[1]}(\lambda_0) &= \frac{A_P^2}{2} \int_{\lambda_0}^2 \frac{dt}{t} [(t - \lambda_0)^2 (t - \lambda_0')^2 - \lambda_0^2 \lambda_0'^2] \\ &= \frac{A_P^2 \lambda_0'^2}{2} \left[-4u + 6u^2 + \frac{16(1 - \lambda_0')}{3\lambda_0'^2} u^3 - \frac{4u^4}{3\lambda_0'^2} \right], \end{aligned} \quad (106)$$

where $u \equiv 1 - \lambda_0/2$, vanishes only linearly in d , which leads to a singularity in the first order derivative. However, there is a partial cancellation with the contribution of $J_2[P]$: By transforming in (60) the first term and the third term written for the root λ_0 which is nearest to two, with the techniques having led to (104), and by using the fact that $\bar{\text{Li}}_2(2/\lambda_0)$ is a smooth function of λ_0 except in $2/\lambda_0 = 1$, where we have the expansion

$$\bar{\text{Li}}_2(2/\lambda_0) = \bar{\text{Li}}_2(1/(1-u)) \stackrel{u \rightarrow 0}{\equiv} -\left[u + \frac{1}{2}u^2 + \frac{1}{3}u^3 + O(u^4) \right] \ln|u| + C^\infty, \quad (107)$$

we find with a rather long calculation that

$$J_\sigma^\eta(2) \stackrel{d_\eta \rightarrow 0}{\equiv} \frac{d_\eta^3}{12P_\sigma^{\eta'}(2)} [1 + O(d_\eta)][\ln|d_\eta| + i\pi Y(d_\eta)], \quad \forall \sigma \in \{\beta, \gamma, \delta\} \quad (108)$$

where we have restored the indices. This equivalent is precisely half of the one obtained for $I_\sigma^\eta(2)$, for which we give the following simple interpretation: In the integral (44) defining $J[P](\lambda)$, here with $\lambda = 2$, only the contribution of a neighborhood of the upper bound $t = 2$ can lead to singularities, since it is from there that the root λ_0 which is closest to two enters (or exits) the interval of integration when the distance from the singularity line is varied. Also the term

$[P(0)]^2 u[P(0)]/t$ in the integrand of (44) can be ignored, and t can be approximated by two in the denominator of $[P(t)]^2 u[P(t)]/t$. Then one indeed recovers exactly half of the integrand of $I[P](2)$.

By collecting all the contributions thanks to the compact notation (79), we do not find any particular cancellation between them, so that the **third** order derivative of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ in the direction normal to the oblique singularity lines has a logarithmically divergent real part and a discontinuous imaginary part:

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \stackrel{d_\eta \rightarrow 0}{=} \frac{3\eta r[d_\eta^3 + O(d_\eta^4)][\ln|d_\eta| + i\pi Y(d_\eta)]}{128\bar{K}(2 + \eta\bar{K})[(2 + \eta\bar{K})^2 - r^2]} + C^\infty \quad (109)$$

where d_η , an algebraic distance from these lines, is given by (103). Note that the denominator of the prefactor in (109) vanishes, as expected, at the points where the considered oblique line is tangent to the parabolas $\Delta_\sigma^\eta = 0$ of same index η , for $\sigma = \beta, \gamma$ and δ . In turn, the fact that the denominator vanishes in $\bar{K} = 0$ corresponds to the crossing points of the two oblique lines, where the distances d_\pm coincide and the contributions of index $\eta = \pm$ interfere; summing them up leads to a finite prefactor.

VI. SOME PHYSICAL APPLICATIONS

A. Some results on the complex energy recovered

The analytic properties of the resolvent of the Hamiltonian $\hat{G}(z)$, more precisely of its matrix elements, forbid the resolvent to have a pole in the complex plane, out of those on the real axis associated to the discrete spectrum of \hat{H} . Nevertheless, in the thermodynamic limit, $\hat{G}(z)$ has a branch cut at the location of the continuous spectrum of \hat{H} , so that the analytic continuation of $\hat{G}(z)$ from the upper half-plane $\Im z > 0$ to the lower half-plane $\Im z < 0$, indicated by the exponent p.a. in what follows, can have complex poles [38].

This discussion extends to the Green's function $\omega \mapsto \mathcal{G}(\mathbf{K}, \omega)$, which is a matrix element of the resolvent in the state $|\psi_{\mathbf{K}}^0\rangle$ of the impurity of momentum $\hbar\mathbf{K}$ in the presence of the unperturbed Fermi sea, see equation (5). If $\mathbf{K} = \mathbf{0}$, we expect that the Green's function has one (and only one) pole on the real axis, in $\omega_0(\mathbf{0})$, which corresponds to the only discrete eigenstate of \hat{H} , its ground state, since we have supposed here that the monomeric branch is the minimal energy branch, see the introduction. If $\mathbf{K} \neq \mathbf{0}$, $\omega \mapsto \mathcal{G}(\mathbf{K}, \omega)$ should not have anymore a real pole, since no energy argument prevents the impurity from emitting pairs of particle-hole excitations in the fermionic gas, see the introduction; on the other hand, its analytic continuation $\mathcal{G}^{\text{p.a.}}(\mathbf{K}, \omega)$ to the lower complex half-plane $\Im \omega < 0$ should have a pole in $\omega = \omega_0(\mathbf{K})$ that continuously emerges from the real pole $\omega_0(\mathbf{0})$ and that, by virtue of (3), is a solution of the implicit equation

$$\Delta E(\mathbf{K}) \equiv \hbar\omega_0(\mathbf{K}) = E_{\mathbf{K}} + \Sigma^{\text{p.a.}}(\mathbf{K}, \omega_0(\mathbf{K})) \quad (110)$$

where $\Delta E(\mathbf{K})$ is called complex energy of the impurity [36] and $\Sigma^{\text{p.a.}}(\mathbf{K}, \omega)$ is the analytic continuation of the self-energy. Whether \mathbf{K} is zero or not, only the existence of a pole at the (real or not) angular frequency $\omega_0(\mathbf{K})$ allows us to state that the impurity, through the coupling with the Fermi sea, gives birth to a well defined quasi-particle, here a monomeron. This indeed seems to be the case even in the strongly interacting regime [21] provided that the mass of the impurity remains finite [39]. The imaginary part of the pole,

$$\Im \omega_0(\mathbf{K}) \equiv -\frac{\Gamma_0(\mathbf{K})}{2} < 0 \text{ if } \mathbf{K} \neq \mathbf{0}, \quad (111)$$

gives the rate Γ_0 at which the system leaves exponentially with time its initial state $|\psi_{\mathbf{K}}^0\rangle$: It is here a rate of emission of particle-hole pairs. Let us recall that the probability amplitude in $|\psi_{\mathbf{K}}^0\rangle$ also contains, in general, a power law decreasing term, which is of little practical importance in the weak coupling regime $g \rightarrow 0^-$ [38].

The results of the previous sections allow us to calculate explicitly the complex energy of the impurity up to second order in the coupling constant g . One has just to replace in (14) the self-energy with its approximation of order at most two, evaluated in the non-perturbed angular frequency $\omega_0^{(0)}(\mathbf{K}) = E_{\mathbf{K}}$ since $\Sigma^{(1)}$ does not depend on the angular frequency:

$$\Delta E(\mathbf{K}) = E_{\mathbf{K}} + \rho g + \frac{(\rho g)^2}{\epsilon_F} \bar{\Sigma}^{(2)}(\bar{K}, \varepsilon = 0) + O(g^3) \quad (112)$$

given the rescalings (20) and (21). We then take the limit $\varepsilon \rightarrow 0$ in each term of the expression (80). Each polynomial $P_\sigma^\pm(\lambda)$ has a root that tends to zero and brings, see subsection VC, a zero contribution to the functionals $I[P]$

and $J_1[P]$, contrarily to the other root. In addition, the contribution of the piece $J_2[P]$ vanishes due to the factor $[P(0)]^2 \propto \varepsilon^2$ in (57). From the relations $\text{sgn}(y)[Y(2 + \frac{y}{x}) - Y(\frac{y}{x})] = Y(y) - Y(2x + y)$ and $|y| = y[Y(y) - Y(-y)]$, that hold for all pairs of non-zero real numbers x and y and that are used here for the coefficients of the quadratic terms and the linear terms of the polynomial $P_\delta^\eta(\lambda)$, we finally obtain

$$\bar{\Sigma}^{(2)}(\bar{K}, 0) = C(\bar{K}) + \sum_{s=0,1,r} D_s(\bar{K})u(s - \bar{K}) + D_s(-\bar{K})u(s + \bar{K}), \quad (113)$$

Due to an unexpected cancellation of the contributions of the *partie finie* i_α^\pm and j_α^\pm , the result does not involve as contributing points $s \pm \bar{K}$ the (half-)coefficients $-r \pm \bar{K}$ of the linear terms of the polynomials $P_\delta^\pm(\lambda)$. The function $u(X)$ is here the one of equation (32), and we have introduced the auxiliary functions

$$\begin{aligned} C(\bar{K}) &= \frac{3r(11 + \bar{K}^2)}{20(1 - r^2)}, \quad D_0(\bar{K}) = \frac{3\bar{K}^4}{20r}, \quad D_r(\bar{K}) = -\frac{3(\bar{K} - r)^4(\bar{K} + 4r)}{20r\bar{K}(1 - r^2)^2} \\ \text{and } D_1(\bar{K}) &= -\frac{3r(\bar{K} - 1)^3}{20\bar{K}(1 - r^2)^2}[(r^2 - 2)\bar{K}(\bar{K} + 3) + 6r^2 - 2] \end{aligned} \quad (114)$$

As a whole this reproduces, in a concise form, the results of reference [36]. It agrees with those of [5] which were limited (for $\mathbf{K} \neq \mathbf{0}$) to the imaginary part of the energy and to $r = 1$. In particular, $\Re \bar{\Sigma}^{(2)}(\bar{K}, 0)$ vanishes indeed for large \bar{K} as in [36], which implies a sum rule implicitly used in reference [36],

$$\sum_{s=0,r,1} D_s(\bar{K}) + D_s(-\bar{K}) = 0 \quad \forall \bar{K} \quad (115)$$

As a consequence, for $0 < \bar{K} < \min(1, r)$, the imaginary part of the sum over s in equation (113) reduces to $-\pi D_0(\mathbf{K})$ and the rate of emission of particle-hole pairs simplifies to

$$\Gamma_0^{(2)}(\mathbf{K}) = \frac{(\rho g)^2}{\hbar \epsilon_F} \frac{3\pi \bar{K}^4}{10r} \quad (116)$$

to order g^2 . According to figure 1, $\bar{\Sigma}^{(2)}(\bar{K}, 0)$ is a C^∞ function of \bar{K} over \mathbb{R}^+ except in $\bar{K} = 1$, in $\bar{K} = r$ and, unfortunate oversight of reference [36], in $\bar{K} = 0$.

B. Quasi-particle residue and Anderson orthogonality catastrophe

The monomeron is a well defined quasi-particle if it has a non-zero quasi-particle residue Z . This can be extracted from the propagator $\mathcal{G}(\mathbf{K}, \omega)$ defined in equation (3) by isolating a quasi-particle propagator from a regular part

$$\mathcal{G}^{\text{p.a.}}(\mathbf{K}, \omega) = \frac{Z}{\hbar\omega - \hbar\omega_0} + \mathcal{G}^{\text{reg}}(\mathbf{K}, \omega) \quad (117)$$

where the pole ω_0 is solution of the equation

$$\hbar\omega_0 - E_{\mathbf{K}} - \Sigma^{\text{p.a.}}(\mathbf{K}, \omega_0) = 0 \quad (118)$$

Then Z is simply the residue of $\mathcal{G}(\mathbf{K}, \omega)$:

$$Z = \lim_{\omega \rightarrow \omega_0} \hbar(\omega - \omega_0) \mathcal{G}^{\text{p.a.}}(\mathbf{K}, \omega) = \frac{1}{1 - \partial_{\hbar\omega} \Sigma^{\text{p.a.}}(\mathbf{K}, \omega_0)} \quad (119)$$

and in the weakly attractive limit one gets the following perturbative expansion up to second order

$$Z \stackrel{g \rightarrow 0^-}{=} 1 + \partial_{\hbar\omega} \Sigma^{(2)}(\mathbf{K}, E_{\mathbf{K}}/\hbar) + O(g^3) \quad (120)$$

or using ε instead of $\hbar\omega$ and taking into account equation (118) we get

$$Z \stackrel{g \rightarrow 0^-}{=} 1 + \left(\frac{\rho g}{\epsilon_F} \right)^2 \partial_\varepsilon \bar{\Sigma}^{(2)}(\bar{K}, 0) + O(g^3) \quad (121)$$

Here we calculate the derivative $\partial_\varepsilon \bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ for an infinite impurity-to-fermion mass ratio $r = M/m$. In this limit it is not difficult to see that the trinomials (36,37,38,39) to leading order in r drop off the dependence on $\eta = \pm 1$, and one obtains the limit

$$p_\sigma(\lambda) = \lim_{r \rightarrow +\infty} \frac{P_\sigma^\eta(\lambda)}{r} \quad \forall \sigma \in \{\alpha, \beta, \gamma, \delta\} \quad (122)$$

Therefore also the functionals $I_\sigma^\eta(\lambda)$ and $J_\sigma^\eta(\lambda)$, as well as their corresponding *partie finie* in equation (80), drop off the dependence on η to leading order in r , and equation (79) becomes

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \xrightarrow{r \rightarrow +\infty} \frac{9}{16r^2} [j_\alpha^+ - J_\beta^+(2) + J_\delta^+(2)] + O(1) \quad (123)$$

Using result (122), we find that the functionals $J_\sigma^\eta(\lambda)$ show a logarithmic divergence

$$J_\sigma^\eta(\lambda) \xrightarrow{r \rightarrow +\infty} r^2 \ln r \int_0^\lambda dt \frac{p_\sigma^2(t) - p_\sigma^2(0)}{2t} + O(r^2) \quad (124)$$

while their corresponding *partie finie* contribute only to subleading order, i.e. $\text{Pf}[J_\sigma^\eta](+\infty) \xrightarrow{r \rightarrow +\infty} O(r^2)$. This leads to the following result

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \xrightarrow{r \rightarrow +\infty} \ln r \frac{9}{16} \int_0^2 dt \frac{p_\delta^2(t) - p_\delta^2(0) - [p_\beta^2(t) - p_\beta^2(0)]}{2t} + O(1) \quad (125)$$

which, after the straightforward integration in t , becomes

$$\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \xrightarrow{r \rightarrow +\infty} -\frac{9}{4} \varepsilon \ln r + O(1) \quad (126)$$

Then the quasi-particle residue (121) presents a logarithmic divergence

$$\lim_{g \rightarrow 0^-} \frac{Z - 1}{(\rho g / \epsilon_F)^2} \xrightarrow{r \rightarrow +\infty} -\frac{9}{4} \ln r + O(1) \quad (127)$$

in agreement with the result of reference [36]. As discussed in [36] this logarithmic divergence is a signature of the Anderson orthogonality catastrophe stating that in the limit of $r \rightarrow +\infty$ the monomeron is not a well defined quasi-particle.

C. A non-perturbative regularisation of the divergence of the second order derivative of $\Delta E^{(2)}(\mathbf{K})$ at the Fermi surface for $M = m$ ($r = 1$)

Overall, the fact of being able to analytically calculate the self-energy up to second order in g has as the most striking consequence the prediction of singularities in the third order derivative of $\Sigma^{(2)}(\mathbf{K}, \omega)$. In order to make more accessible an experimental signature, it is convenient to try to reduce the order of the derivatives in which these singularities appear, by identifying the singular point with highest multiplicity in the plane (\bar{K}, ε) . The discussion of section V identified in this plane singularity lines (84) and (85), on which the polynomials $P_\sigma^\eta(\lambda)$ have roots equal to zero or two, and singularity parabolas (82,83) on which these polynomials have double roots. In the half-plane $\bar{K} > 0$, the singularity lines cross at $(\bar{K}, \varepsilon) = (1, 0)$. This point is also on one of the parabolas only when the impurity has the same mass of a fermion, from which the magic point considered in this section:

$$(\bar{K}, \varepsilon) \rightarrow (1, 0) \quad \text{for } r = 1 \quad (128)$$

In particular, the associated singularities are exactly at the Fermi surface and, as suggested in reference [36] and as we shall see, they appear in the derivatives of order **two** only.

Here the most accessible observable in a cold atom experiment seems to be the complex energy $\Delta E(\mathbf{K})$ of the quasi-particle, simply by radio frequency spectroscopy between an internal state of the impurity not coupled to the fermions, and a coupled internal state. The shift and the broadening of the line due to the presence of the fermions gives access to the real part and the imaginary part of $\Delta E(\mathbf{K})$, with an uncertainty which has already reached respectively $5 \cdot 10^{-3} \epsilon_F$ and $10^{-4} \epsilon_F$ [9]. We assume that $\Delta E(\mathbf{K})$ can be measured with a sufficiently good precision in the neighborhood of $K = k_F$, such that it is possible to numerically take the second order derivative with respect to

K . Perturbation theory, whose results have been already published in [36] and recovered in subsection VI A, leads, for a weakly interacting limit taken at fixed \bar{K} different from one, to

$$\lim_{g \rightarrow 0^-} \frac{d^2}{d\bar{K}^2} \frac{\Delta E(\mathbf{K}) - E_{\mathbf{K}}}{(\rho g)^2 / \epsilon_F} \stackrel{\bar{K} \rightarrow 1}{=} -\frac{9}{4} \ln |\bar{K} - 1| - \frac{27}{20} (2 + \ln 2) + \frac{9i\pi}{4} \left[Y(\bar{K} - 1) - \frac{4}{5} \right] + o(1) \quad (129)$$

of real part that diverges logarithmically and discontinuous imaginary part. Perturbation theory is however much more vague when we take the limit at $\bar{K} = 1$,

$$\lim_{g \rightarrow 0^-} \left[\frac{d^2}{d\bar{K}^2} \frac{\Delta E(\mathbf{K}) - E_{\mathbf{K}}}{(\rho g)^2 / \epsilon_F} \right]_{\bar{K}=1} = +\infty \quad (130)$$

since it does not specify how the divergence is produced.

1. A self-consistent heuristic approach

How can we go beyond result (130) by using the ingredients already available in the present work? We must perform a non-perturbative treatment, as e.g. a self-consistent approximation. The simplest thing consists in replacing the self-energy $\Sigma(\mathbf{K}, \omega)$, which appears in the implicit equation (110) on the complex energy, with its expansion up to order two included in g , $\rho g + \Sigma^{(2)}(\mathbf{K}, \omega)$. A simple improvement of this minimalist prescription is to include the last contribution to $\Sigma^{(3)}(\mathbf{K}, \omega)$ in equation (19) coming from a mean-field shift on ω , given that at fixed wave vector and angular frequency,

$$\Sigma^{(2)}(\mathbf{K}, \omega - \rho g / \hbar) \stackrel{g \rightarrow 0^-}{=} \Sigma^{(2)}(\mathbf{K}, \omega) - \frac{\rho g}{\hbar} \partial_{\omega} \Sigma^{(2)}(\mathbf{K}, \omega) + O(g^2) \quad (131)$$

Physically, this global shift takes into account the fact that the mean-field shift ρg experienced by the impurity is exactly the same in all subspaces at zero, one, two, \dots pairs of particle-hole excitations, once the limit of zero-range interaction has been taken. We shall stick then to the (non-perturbative) self-consistent heuristic approximation

$$\Delta E(\mathbf{K}) \stackrel{\text{heuris.}}{=} E_{\mathbf{K}} + \rho g + \Sigma^{(2)\text{p.a.}}(\mathbf{K}, \frac{\Delta E(\mathbf{K}) - \rho g}{\hbar}) \quad (132)$$

which can be written, in terms of a reduced unknown ε_e , complex effective value of the variable ε (hence the index e), in the dimensionless compact form

$$-\varepsilon_e(\bar{K}) \stackrel{\text{heuris.}}{=} \left(\frac{\rho g}{\epsilon_F} \right)^2 \bar{\Sigma}^{(2)\text{p.a.}}(\bar{K}, \varepsilon_e(\bar{K})) \quad \text{where} \quad \varepsilon_e(\bar{K}) \equiv \frac{E_{\mathbf{K}} + \rho g - \Delta E(\mathbf{K})}{\epsilon_F} \quad (133)$$

which we differentiate twice with respect to \bar{K} to identify the useful derivatives of $\bar{\Sigma}^{(2)}$:

$$-\frac{d^2 \varepsilon_e}{d\bar{K}^2} \stackrel{\text{heuris.}}{=} \left(\frac{\rho g}{\epsilon_F} \right)^2 \left[\partial_{\bar{K}}^2 + 2 \frac{d\varepsilon_e}{d\bar{K}} \partial_{\bar{K}} \partial_{\varepsilon} + \left(\frac{d\varepsilon_e}{d\bar{K}} \right)^2 \partial_{\varepsilon}^2 + \frac{d^2 \varepsilon_e}{d\bar{K}^2} \partial_{\varepsilon} \right] \bar{\Sigma}^{(2)\text{p.a.}} \quad (134)$$

taken here at the point $(\bar{K}, \varepsilon = \varepsilon_e(\bar{K}))$. Let us recall that the exponent p.a. means *analytic continuation* to the complex values of ω from the upper half-plane to the lower half-plane.

2. Singularities of the second order derivatives of $\bar{\Sigma}^{(2)}$ and scaling law prediction

In order to see how the second order derivative of $\varepsilon_e(\bar{K})$ behaves in the neighborhood of $\bar{K} = 1$ in the limit $g \rightarrow 0^-$, it is sufficient to initially determine the singularities of the second order derivatives of $\bar{\Sigma}^{(2)}(\mathbf{K}, \varepsilon)$ for ε real. By transposing to the case $(\bar{K}, \varepsilon) \rightarrow (1, 0)$ the techniques developed in section V, we note that some magic cancellations,

as the quasi-identity of certain roots $\lambda_0^{(\eta\alpha)}$ and $\lambda_0^{(\eta\beta)}$ of the polynomials P_α^η and P_β^η , which made the second order derivatives regular, do not happen anymore, and we laboriously end up with the following results:

$$\partial_{\bar{K}}^2 \bar{\Sigma}^{(2)}(\bar{K} = 1, \varepsilon) \stackrel{\varepsilon \rightarrow 0}{=} -\frac{9}{4} \ln |\varepsilon| + O(1) \quad (135)$$

$$\partial_\varepsilon^2 \bar{\Sigma}^{(2)}(\bar{K} = 1, \varepsilon) \stackrel{\varepsilon \rightarrow 0}{=} \frac{9}{128} (\ln |\varepsilon|)^2 + O(\ln |\varepsilon|) \quad (136)$$

$$\partial_\varepsilon \partial_{\bar{K}} \bar{\Sigma}^{(2)}(\bar{K} = 1, \varepsilon) \stackrel{\varepsilon \rightarrow 0}{=} \frac{9}{8} \ln |\varepsilon| + O(1) \quad (137)$$

The unknown $\varepsilon_e(\bar{K})$ is of second order in g , as well as its first order derivative, thus the derivatives (136) and (137), that diverge only logarithmically in g are suppressed in equation (134) by the factors $d\varepsilon_e/d\bar{K} = O(g^2)$ and $(d\varepsilon_e/d\bar{K})^2 = O(g^4)$. As for the first order derivative with respect to ε in (134), which does not diverge, it is suppressed by the factor $(\rho g/\epsilon_F)^2$, as can be seen after collecting with the term of the first member in this same equation. Hence the drastic simplification in the limit $g \rightarrow 0^-$, even in the neighborhood of $\bar{K} = 1$:

$$-\partial_{\bar{K}}^2 \varepsilon_e(\bar{K}) \stackrel{\text{approx.}}{=} \left(\frac{\rho g}{\epsilon_F} \right)^2 \partial_{\bar{K}}^2 \bar{\Sigma}^{(2)\text{p.a.}}(\bar{K}, \varepsilon_e(\bar{K})) + O\left[\left(\frac{\rho g}{\epsilon_F}\right)^4 \ln \left|\frac{\rho g}{\epsilon_F}\right|\right] \quad (138)$$

Our heuristic self-consistent approach thus predicts that the first member of the equation (130), evaluated in $\bar{K} = 1$, diverges logarithmically when $g \rightarrow 0^-$:

$$\left[\frac{d^2}{d\bar{K}^2} \frac{\Delta E(\mathbf{K}) - E_{\mathbf{K}}}{(\rho g)^2/\epsilon_F} \right]_{\bar{K}=1} \stackrel{\text{heuris.}}{=} -\frac{9}{4} \ln \left[\left(\frac{\rho g}{\epsilon_F} \right)^2 \right] + O(1) \quad (139)$$

It is actually possible to find this result, to make it more precise and to extend it to $\bar{K} \neq 1$, by performing a clever calculation of the second order derivative of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ with respect to \bar{K} . Let us start from the identities (29) and (45), and obtain the second order derivatives of the integral quantities $I_\sigma^\eta(\lambda)$, with $\lambda = 2$ or Λ , $\eta = \pm$ and $\sigma \in \{\alpha, \beta, \gamma, \delta\}$, by taking the derivative of their defining expressions (43) and (44) with respect to \bar{K} under the integral sign [the same trick is valid for the derivative with respect to ε and leads directly to (136) and (137)]. As can be verified on the equations (36,37,38,39), $\partial_{\bar{K}} P_\sigma^\eta(t) = 2\eta t$ with ε and t fixed, thus

$$\partial_{\bar{K}}^2 I_\sigma^\eta(\lambda) = \int_0^\lambda dt 4t^2 u[P_\sigma^\eta(t)] \quad \text{and} \quad \partial_{\bar{K}}^2 J_\sigma^\eta(\lambda) = \int_0^\lambda dt 4t u[P_\sigma^\eta(t)] \quad (140)$$

where the function u is the one of equation (32) and $u^{[2]}$ in (43,44) one of the primitives of order two. To see which one of these terms have a finite limit when $(\bar{K}, \varepsilon) \rightarrow (1, 0)$, and can only contribute to $\partial_{\bar{K}}^2 \bar{\Sigma}^{(2)}$ as a slowly varying background, it is sufficient to replace the trinomials P_σ^η with their value for $\bar{K} = 1$ and $\varepsilon = 0$, see table I.

σ	$\eta = +$	$\eta = -$
α	$2t^2 + 4t$	$2t^2$
β	$4t$	0
γ	$t^2 + 2t$	$t^2 - 2t$
δ	$2t^2$	$2t^2 - 4t$

Table I: The trinomials $P_\sigma^\eta(t)$ for the multi critical point $(\bar{K}, \varepsilon) = (1, 0)$.

We than see that only the polynomial $P_\beta^-(t)$ leads to a divergence. As $r = 1$, it manifests itself only via the functional $J[P]$, which is particularly neat on equation (80), so that

$$\partial_{\bar{K}}^2 \bar{\Sigma}^{(2)}(\bar{K}, \varepsilon) \stackrel{(\bar{K}, \varepsilon) \rightarrow (1, 0)}{=} -\frac{9}{32} \partial_{\bar{K}}^2 J_\beta^-(2) + \frac{9}{40} (-17 + 14 \ln 2 + 2i\pi) + o(1) \quad (141)$$

where the additive constant was obtained by specializing to $\varepsilon = 0$ and by comparing with (129). To calculate the integral giving $\partial_{\bar{K}}^2 J_\beta^-(2)$ in (140), it remains to use equation (54) with $Q_I(t) = 4t$ and to simplify the imaginary part with the help of the relation $-\text{sgn}(x)[Y(2 + \frac{y}{x}) - Y(\frac{y}{x})] = Y(y) - Y(2x + y)$ valid for any real number x and y :

$$\frac{1}{8} \partial_{\bar{K}}^2 J_\beta^-(2) = u(\varepsilon) + [1 - (\frac{\varepsilon/4}{\bar{K} - 1})^2] \{u[\varepsilon - 4(\bar{K} - 1)] - u(\varepsilon)\} - \frac{1}{2} - \frac{\varepsilon/4}{\bar{K} - 1} \quad (142)$$

To continue and to draw the consequences in (138), we must extend this result to the case $\Im(-\varepsilon) > 0$ then analytic continue it to the case $\Im(-\varepsilon) < 0$, which is what we are going to do. Let us first note a remarkable property: The terms of the second member of (142) are positively homogeneous functions of $(\bar{K} - 1, \varepsilon)$ of degree zero [invariant by global multiplication of $\bar{K} - 1$ and ε by any real number $\tau > 0$], **except** the first term. This first term thus fixes the global value of (142); as ε has to be taken here of order $|\varepsilon_e(\bar{K} = 1)| \approx (\rho g / \epsilon_F)^2$, it immediately leads to the logarithmic behavior (139). The other terms of (142) give the dependence in $\bar{K} - 1$, not described by (139), which is produced on a characteristic scale $|\varepsilon| \approx (\rho g / \epsilon_F)^2$. We obtain thus, within our self-consistent heuristic approach (132), the following scaling law for the second order derivative of the complex energy of the impurity in the neighborhood of the Fermi surface ($\bar{K} \rightarrow 1$) in the weakly interacting limit ($g \rightarrow 0^-$):

$$\frac{d^2}{d\bar{K}^2} \frac{\Delta E(\mathbf{K}) - E_{\mathbf{K}}}{(\rho g)^2 / \epsilon_F} \stackrel{\text{heuris.}}{=} -\frac{9}{4} \ln \left[\left(\frac{\rho g}{\epsilon_F} \right)^2 \right] + F \left(\frac{4(\bar{K} - 1)}{(\rho g / \epsilon_F)^2} \right) + o(1) \quad (143)$$

where the scaling function $F(x)$ remains to be specified. A simple but remarkable consequence of this scaling law is that the **third** order derivative of the complex energy of the impurity does not tend uniformly to zero in the limit of weak interaction:

$$\frac{d^3}{d\bar{K}^3} \frac{\Delta E(\mathbf{K})}{\epsilon_F} \stackrel{g \rightarrow 0^-}{\not\rightarrow} 0 \quad \text{in a neighborhood of } \bar{K} = 1 \quad (144)$$

3. Analytic continuation to a complex energy variable and numerical emergence of the scaling law

In order to see the scaling law (143) emerge when the strength of the interaction is reduced, we have implemented the self-consistent heuristic program of equation (133). This led us to overcome a practical obstacle, that is to determine the analytic continuation of $\bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)$ to complex values of ε . Let us give the main steps that we followed to realize it. (i) Results of section IV can be generalized directly to the case $\Im(-\varepsilon) > 0$, since equation (16) has the energy $\hbar\omega + i0^+$ in the denominator. This corresponds to the complex upper half-plane for the energy variable z of the resolvent of the Hamiltonian $\hat{G}(z)$, so that one can extend $\hbar\omega$ to a positive imaginary part in equation (20), and correspondingly ε to a negative imaginary part, without crossing the branch cut of the resolvent, thus without the need for any analytic continuation. (ii) In this favorable case $\Im(-\varepsilon) > 0$, the roots of the polynomials $P_\sigma^\eta(\lambda)$ are all complex, so we must use the form (62) of the functional $J_2[P_\sigma^\eta]$, and the form (55) of the functional $I[P_\sigma^\eta](\lambda)$, in which we must care to replace $u[P_\sigma^\eta(\lambda)]$ with $\ln[-P_\sigma^\eta(\lambda)]$. This follows from the remark below equation (33) and from the fact that $-P_\sigma^\eta(\lambda)$ tends to the real axis from the upper complex half-plane when $\Im(-\varepsilon) \rightarrow 0^+$. Alternatively this follows from the result of the integration of (23) for ϵ positive non-infinitesimal, which leads formally to $u(x \pm y - i\epsilon) = \ln(-x \mp y + i\epsilon)$ thus to $u(z) = \ln(-z)$. In the aforementioned expressions, let us recall it, \ln and Li_2 are the usual branch of the complex logarithm and dilogarithm function, of branch cut \mathbb{R}^- and $[1, +\infty[$. (iii) To verify the two previous assertions (i) and (ii), we can take the limit $\Im(-\varepsilon) \rightarrow 0^+$ in those generalizations of (55) and (62), in the case where the roots λ_0^c of the polynomial $P_\sigma^\eta(\lambda)$ have real limits λ_0^r . We then have to recover exactly expressions (54) and (60). We have scrupulously verified that this is indeed the case, by using the relation $\Pi_{[0, \lambda]}(y) - \Pi_{[0, \lambda]}(x) = Y[(\lambda - x)(\lambda - y)] - Y[xy]$ satisfied for the rectangular function $\Pi_{[0, \lambda]}$ for any real $x < y$, as well as the property

$$\frac{d}{d\Im(-\varepsilon)} [P_\sigma^\eta(\lambda_0^c)] = 0 \implies \frac{d\lambda_0^c}{d\Im(-\varepsilon)} \stackrel{\Im(-\varepsilon) \rightarrow 0^+}{\rightarrow} \frac{1}{P'(\lambda_0^r)} \quad (145)$$

which allows us to know if the roots λ_0^c , thus the arguments of \ln and of Li_2 , reach the real axis from the upper or lower complex half-plane. This leads to:

$$\ln(\lambda - \lambda_0^c) \stackrel{\Im(-\varepsilon) \rightarrow 0^+}{\rightarrow} \ln|\lambda - \lambda_0^r| - i\pi \frac{P'(\lambda_0^r)}{|P'(\lambda_0^r)|} Y(\lambda_0 - \lambda) \quad (146)$$

$$\text{Li}_2\left(\frac{\lambda}{\lambda_0^c}\right) \stackrel{\Im(-\varepsilon) \rightarrow 0^+}{\rightarrow} \text{Li}_2\left(\frac{\lambda}{\lambda_0^r}\right) + i\pi \frac{P'(\lambda_0^r)}{|P'(\lambda_0^r)|} \ln \left| \frac{\lambda_0^r}{\lambda} \right| [Y(\lambda - \lambda_0^r) - Y(-\lambda_0^r)] \quad (147)$$

knowing that $\text{sgn}(\lambda)Y(\lambda/\lambda_0^r - 1) = Y(\lambda - \lambda_0^r) - Y(-\lambda_0^r)$ and $\text{Li}_2(x \pm i0^+) = \pm i\pi(\ln|x|)Y(x - 1)$ for any real x . In these expressions, λ is any real number and the polynomial P is the limit of the polynomial P_σ^η for ε real. (iv) To finally analytically continue the functionals $I[P]$ and $J[P]$, thus the self-energy $\bar{\Sigma}^{(2)}(\mathbf{K}, \varepsilon)$ from the half-plane $\Im(-\varepsilon) > 0$ to the half-plane $\Im(-\varepsilon) < 0$, it is sufficient to know if the argument Z of each function \ln and Li_2 moves from the upper half-plane to the lower half-plane or vice versa. In the first case, we move the branch cut of \ln from the real negative

half-axis to the purely imaginary negative half-axis, and the one of Li_2 from $[1, +\infty[$ to $1 + i\mathbb{R}^-$, that is we rotate them by $\pi/2$ and $-\pi/2$ respectively:

$$\ln^{\text{p.a.}\downarrow} Z = \ln_{3\pi/2} Z \text{ and } \text{Li}_2^{\text{p.a.}\downarrow}(Z) = \text{Li}_2(Z) + \ln_\pi Z [\ln_\pi(1-Z) - \ln_{\pi/2}(1-Z)] \quad (148)$$

where the arrow \downarrow recalls the movement of Z in the complex plane, and

$$\ln_\theta Z \equiv \ln |Z| + i \arg_\theta Z \quad (149)$$

is defined with the branch $\theta - 2\pi < \arg_\theta Z \leq \theta$ of the argument of the complex number Z . In the opposite case where Z moves from the lower half-plane to the upper half-plane, we rotate the branch cut of \ln by an angle $-\pi/2$, so as to displace it to the purely imaginary positive half-axis, and we rotate the one of Li_2 by an angle $\pi/2$, so as to displace it to $1 + i\mathbb{R}^+$:

$$\ln^{\text{p.a.}\uparrow} Z = \ln_{\pi/2} Z \text{ and } \text{Li}_2^{\text{p.a.}\uparrow}(Z) = \text{Li}_2(Z) + \ln_\pi Z [\ln_\pi(1-Z) - \ln_{3\pi/2}(1-Z)] \quad (150)$$

We have numerically implemented this procedure of analytic continuation, by iteratively solving the self-consistent equation (133) and by calculating the second order derivative of $\varepsilon_e(\bar{K})$ using the middle-point method. We show the result on figure 2, for three values of $\rho g/\epsilon_F$ corresponding to subsequently weaker interactions. The choice of the origin and the units on the axis presuppose a scaling law of the form (143), towards which the numerics seem indeed to converge. Let us remark however, that even in this self-consistent approach, the second order derivative of $\varepsilon_e(\bar{K})$ presents, as a function of \bar{K} , discontinuities which affect the real part as well as the imaginary part, and that do not disappear when $\rho g/\epsilon_F \rightarrow 0^-$. Unfortunately, we shall see that the position and the number of these discontinuities do not have any physical meaning since they depend on the form under which we write the different functions before analytically continue them.

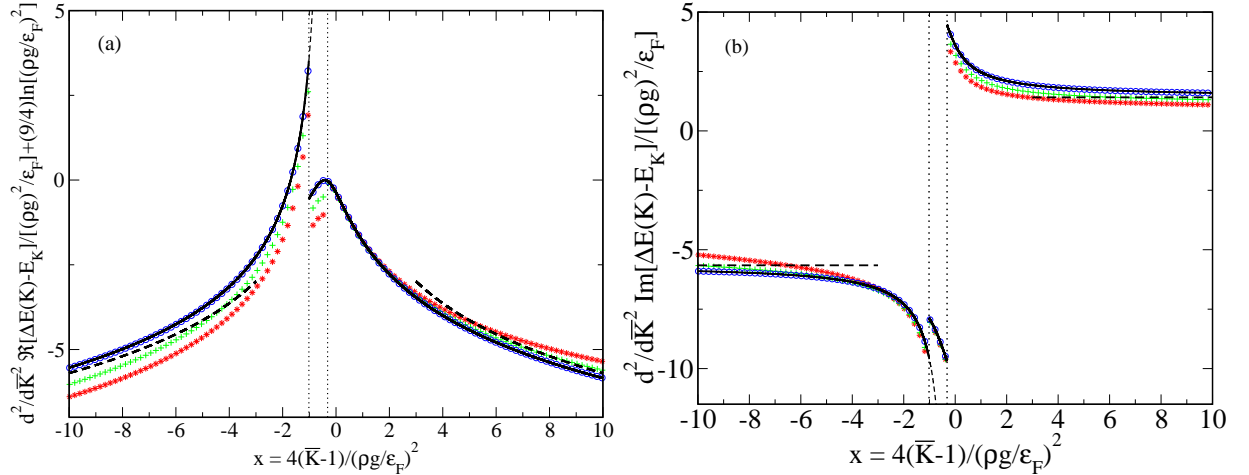


Figure 2: Second order derivative of the complex energy of the impurity [(a): real part shifted by $(9/4) \ln[(\rho g/\epsilon_F)^2]$, (b): imaginary part] obtained by numerical resolution of the self-consistent equation (133), for a mass ratio $r = M/m = 1$ and for values of $\rho g/\epsilon_F$ equal to -0.15 (red stars), -0.1 (green plus signs) and -0.01 (blue circles), the last value having practically reached the limit $g \rightarrow 0^-$. In the chosen units system, we can see emerge a scaling law of the form (143). Black solid line: Analytic prediction in the limit $g \rightarrow 0^-$; the location of the corresponding discontinuities are identified by the vertical dotted lines of abscissas x'_{jump} and x_{jump} from left to right, see equation (155). Black thin dashed line: Analytic prediction corresponding to another possible writing of the function $\partial_{\bar{K}}^2 J_{\beta}^-(2)$ before its analytic continuation; it differs from the black solid line only in between the two vertical dotted lines. Black thick dashed line: Perturbation theory (129) deduced from reference [36], limited to its validity domain, that is the tails.

To finish, let us show how to analytically obtain the limits of the results of figure 2 when $g \rightarrow 0^-$, that is how to obtain an explicit expression of the corresponding scaling function $F(x)$, where $x = 4(\bar{K} - 1)/(\rho g/\epsilon_F)^2$. We take as the starting point equations (141) and (142), which is legitimate to directly extend (without analytic continuation) to the complex values of ε with $\Im(-\varepsilon) > 0$, by formally consider that $u(z) = \ln(-z)$ on \mathbb{C} , where \ln is the principal branch of the complex logarithm, to obtain

$$\partial_{\bar{K}}^2 \bar{\Sigma}^{(2)}(\bar{K}, \varepsilon)|_{\Im(-\varepsilon) > 0} \stackrel{(\bar{K}, \varepsilon) \rightarrow (1, 0)}{=} -\frac{9}{4} \left\{ \ln\left[\left(\frac{\rho g}{\epsilon_F}\right)^2\right] + f_x(-\bar{\varepsilon}) \right\} + C_{\text{bg}} + o(1) \quad (151)$$

with $\bar{\varepsilon} \equiv \varepsilon/(\rho g/\epsilon_F)^2$, $C_{bg} = (9/20)(7 \ln 2 - 6 + i\pi)$ and

$$f_x(-\bar{\varepsilon})|_{\Im(-\bar{\varepsilon})>0} = \ln(x - \bar{\varepsilon}) - \frac{\bar{\varepsilon}^2}{x^2} \ln(1 - x/\bar{\varepsilon}) - \frac{\bar{\varepsilon}}{x} \quad (152)$$

where we used the fact that the function $x \mapsto \ln(x - \bar{\varepsilon}) - \ln(-\bar{\varepsilon}) - \ln(1 - x/\bar{\varepsilon})$, which is C^∞ on \mathbb{R} since the arguments of the complex logarithm cannot cross its branch cut \mathbb{R}^- , is zero in $x = 0$ and of derivative zero everywhere, therefore it is identically zero. Then, one has to analytically continue the function $f_x(-\bar{\varepsilon})$ from $\Im(-\bar{\varepsilon}) > 0$ to $\Im(-\bar{\varepsilon}) < 0$, at $\bar{K} - 1$ thus x fixed, by following the procedure exposed around equations (148) and (150). The argument $x - \bar{\varepsilon}$ of the first logarithm crosses the real axis downwards; the argument $1 - x/\bar{\varepsilon}$ of the second logarithm crosses the real axis upwards if $x > 0$, and downwards if $x < 0$. We finally obtain

$$f_x^{\text{p.a.}\downarrow}(-\bar{\varepsilon}) = \ln_{3\pi/2}(x - \bar{\varepsilon}) - \frac{\bar{\varepsilon}^2}{x^2} \ln_{\pi Y(-x)+\pi/2}(1 - x/\bar{\varepsilon}) - \frac{\bar{\varepsilon}}{x} \quad (153)$$

The scaling function is then given by

$$F(x) = -\frac{9}{4} f_x^{\text{p.a.}\downarrow}(-\bar{\varepsilon}_e^{(2)}(\bar{K} = 1)) + C_{bg} \quad (154)$$

where $-\bar{\varepsilon}_e^{(2)}(\bar{K}) = (\Delta E^{(2)}(\bar{K}) - E_{\mathbf{K}} - \rho g)/[(\rho g)^2/\epsilon_F] = \bar{\Sigma}^{(2)}(\bar{K}, 0)$ is the value of $-\bar{\varepsilon}_e(\bar{K})$ to second order in perturbation theory, which can be deduced from equation (113) or from reference [36].

Notice on figure 2 that the numerical self-consistent results indeed converge towards this scaling function $F(x)$ when $\rho g/\epsilon_F \rightarrow 0^-$. The observed discontinuities as functions of x take place when the arguments of the logarithms in equation (153) become purely imaginary and thus cross their branch cut:

$$x_{\text{jump}} = \Re[\bar{\varepsilon}_e^{(2)}(\bar{K} = 1)] \quad \text{and} \quad x'_{\text{jump}} = \frac{1}{\Re[1/\bar{\varepsilon}_e^{(2)}(\bar{K} = 1)]} \quad (155)$$

which bring in $F(x)$ a purely imaginary jump at $x = x_{\text{jump}}$ (the first logarithm has a real prefactor) and a complex jump at $x = x'_{\text{jump}}$ (the second logarithm has a complex prefactor). The values of the abscissas (155) are actually in decreasing order, and are identified by vertical dotted lines on figure 2.

The positions and the numbers of these predicted discontinuities, therefore also the values of the scaling function $F(x)$, are actually arbitrary. To see it, it is sufficient to choose for the function $f_x(-\bar{\varepsilon})$ a different but equivalent form *before* the analytic continuation. The property set after equation (152) allows us to write

$$f_x(-\bar{\varepsilon})|_{\Im(-\bar{\varepsilon})>0} = \left(1 - \frac{\bar{\varepsilon}^2}{x^2}\right) [\ln(x - \bar{\varepsilon}) - \ln(-\bar{\varepsilon})] + \ln(-\bar{\varepsilon}) - \frac{\bar{\varepsilon}}{x} \quad (156)$$

whose analytic continuation to negative values of $\Im(-\bar{\varepsilon})$ following *the same* prescriptions (148) and (150) leads to

$$f_x^{\text{p.a.}\downarrow}(-\bar{\varepsilon}) \stackrel{\text{bis}}{=} \left(1 - \frac{\bar{\varepsilon}^2}{x^2}\right) [\ln_{3\pi/2}(x - \bar{\varepsilon}) - \ln_{3\pi/2}(-\bar{\varepsilon})] + \ln_{3\pi/2}(-\bar{\varepsilon}) - \frac{\bar{\varepsilon}}{x} \quad (157)$$

The corresponding scaling function $F_{\text{bis}}(x)$, represented as a thin dashed line on figure 2, differs from the one deduced from (153) only between the two vertical dotted lines ($x'_{\text{jump}} < x < x_{\text{jump}}$); it features a complex discontinuity (instead of purely imaginary) in $x = x_{\text{jump}}$, and has no longer a discontinuity in $x = x'_{\text{jump}}$.

Is it possible to make the remaining discontinuity disappear, at least on the real part of $F(x)$? Coming from $x = -\infty$, we start in the left Riemann sheet of the function (157), that can be followed continuously up to $x = +\infty$ by turning the angle of the branch cut from $3\pi/2$ to 2π . Similarly, starting at $x = +\infty$, the right Riemann sheet of the same function (157) can be followed up to $x = -\infty$, by rotating the branch cut from $3\pi/2$ to π . As $\ln_{2\pi}(x - \bar{\varepsilon}) = 2i\pi + \ln_{\pi}(x - \bar{\varepsilon})$ for any $x \in \mathbb{R}$ and any complex $-\bar{\varepsilon}$ of negative imaginary part, the branches of $f_x^{\text{p.a.}\downarrow}(-\bar{\varepsilon})$ in the two Riemann sheets differ by the quantity $2i\pi[1 - (\bar{\varepsilon}/x)^2]$ which, neither zero nor purely imaginary, makes a discontinuity inevitable.

Ultimately, we do not know how to determine the true physical value of the scaling function $F(x)$, even in the apparently innocent framework of the self-consistent approximation (132), at least for $|x| \lesssim 1$, that is for $4|\bar{K} - 1| \lesssim (\rho g/\epsilon_F)^2$.

D. Smoothness of the complex energy $\Delta E^{(2)}(\mathbf{K})$ at finite temperature

Since the singularities in the derivatives of the impurity complex energy $\Delta E^{(2)}(\mathbf{K})$ are a consequence of the existence of a Fermi surface it is natural to ask what happens when the temperature of the system is non zero. In this case, one obtains

$$\Delta E_T^{(2)}(\mathbf{K}) = g^2 \int_{\mathbb{R}^3} \frac{d^3 q}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d^3 k}{(2\pi)^3} \left[\frac{2\mu}{\hbar^2 k^2} - \frac{1 - \bar{n}(\mathbf{k})}{F_{\mathbf{k},\mathbf{q}}(\mathbf{K}, E_{\mathbf{K}}/\hbar)} \right] \bar{n}(\mathbf{q}) \quad (158)$$

The difference with the zero-temperature result is that the Heaviside functions have been replaced by the Fermi functions

$$\bar{n}(\mathbf{k}) = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu_F)} + 1} \quad (159)$$

with μ_F being the chemical potential of the Fermi gas and $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / (2m)$ the kinetic energy of a fermion with wave vector \mathbf{k} . In the strongly degenerate regime $k_B T \ll \mu_F$, the chemical potential is close to the Fermi energy and the Fermi function has a width

$$\delta k_{\text{typ}} = \frac{T}{T_F} k_F \quad (160)$$

as can be seen by linearizing the dispersion relation $\epsilon_{\mathbf{k}}$ around $k = k_F$. We thus expect that the divergence of the second order derivative of $\Delta E^{(2)}(\mathbf{K})$, for equal masses $m = M$, is interrupted in $\Delta E_T^{(2)}(\mathbf{K})$ at a distance $|\bar{K} - 1| \approx T/T_F$. To confirm this prediction in the experimentally relevant range we integrate numerically¹¹ equation (158) for decreasing values of T/T_F , see the resulting second order derivatives in figure 3.

At zero temperature, in subsection VI C 2 we have seen the emergence of a scaling law for the second order derivatives of $\Delta E^{(2)}(\mathbf{K})$ of typical K -width given by $(\rho g / \epsilon_F)^2 k_F$. We thus predict that one can observe the zero temperature effects studied in this work even at a non-zero temperature provided that

$$\frac{T}{T_F} \ll \left(\frac{\rho g}{\epsilon_F} \right)^2 \quad (161)$$

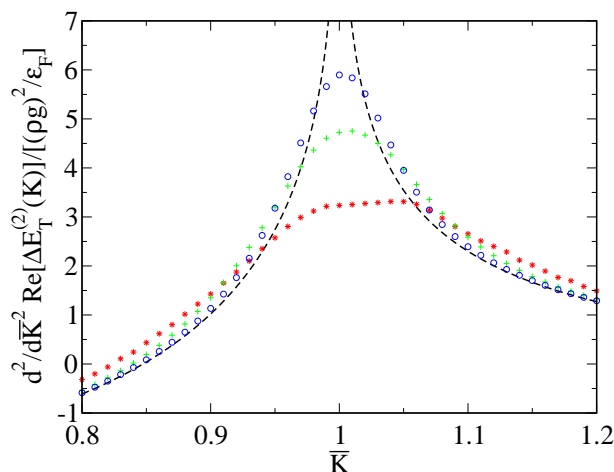


Figure 3: Second order derivative of the non-zero temperature complex energy of the impurity of order two obtained by numerical integration of equation (158), for a mass ratio $r = M/m = 1$ and for values of T/T_F equal to 0.1 (red stars), 0.05 (green plus signs), 0.025 (blue circles). Black thick dashed line: Zero temperature result [36]. At $0 < T \ll T_F$, the typical scale on which the divergence of the zero temperature result is interrupted is given by the difference of the abscissas of the crossing points between the non-zero (symbols) and zero temperature (dashed line) results. It scales linearly in T/T_F .

¹¹ For a given temperature $T \neq 0$, the chemical potential μ_F is adjusted such as to reproduce the fermionic density at zero temperature, i.e. $\rho = \int_{\mathbb{R}^3} \frac{d^3 k}{(2\pi)^3} \bar{n}(\mathbf{k})$.

E. Moments of the momentum of the particle-hole pair emitted by the impurity, according to Fermi's golden rule. Application to the damping rate and to the diffusion coefficient of the impurity momentum

In this part we suppose that the impurity is prepared at time $t = 0$ in the state of well defined wave vector \mathbf{K} , in the presence of the unperturbed Fermi sea. This initial state of the system is directly coupled, by the interaction potential \hat{V} between the impurity and the fermions, to the excited fermionic states of one particle-hole pair, while the impurity recoils, absorbing the corresponding momentum change. We wish to describe the evolution of the system at short times, in the weakly interacting regime.

In the thermodynamic limit, the initial state is a discrete state $|i\rangle$, and the final states $|f\rangle$ with one particle-hole pair belong to a continuum. Fermi's golden rule then gives the rate of emission of one particle-hole pair by the impurity, to second order included in the coupling constant g . Here, the elementary transition rate of $|i\rangle$ towards $|f\rangle$ simply reads $\delta\Gamma_{if} = (2\pi g^2/\hbar)\delta(E_f - E_i)$, where $E_{i/f}$ is the total kinetic energy of the impurity and the fermions, in the initial or final state.

With the calculus techniques developed in this article, we have easily access to all moments of the wave vector $\mathbf{k} - \mathbf{q}$ of the emitted particle-hole pair, as predicted by Fermi's golden rule, that is to zeroth order in g :

$$\langle(\mathbf{k} - \mathbf{q})^n\rangle^{(0)} = \frac{2\pi g^2}{\hbar\Gamma_0^{(2)}(\mathbf{K})} \int_{q < k_F} \frac{d^3 q d^3 k}{(2\pi)^6} (\mathbf{k} - \mathbf{q})^n \delta(E_{\mathbf{K}-\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}} - E_{\mathbf{K}}) \quad (162)$$

where the integer power \mathbf{k}^n of a vector \mathbf{k} is the vector $\mathbf{k}||\mathbf{k}|^{n-1}$ for odd n , and the scalar $||\mathbf{k}|^n$ for even n :

$$\mathbf{k}^n \equiv \mathbf{k}||\mathbf{k}|^{n-1} \text{ (} n \text{ odd)}, \quad \mathbf{k}^n \equiv ||\mathbf{k}|^n \text{ (} n \text{ even)} \quad (163)$$

The total departure rate $\Gamma_0(\mathbf{K})$, here written to order two in g , is simply the total rate of emission of a pair at this order, and it is already given by (112)-(113). By conservation of the total momentum, this also gives access to the moments of the momentum change $\delta\mathbf{K} = \mathbf{K}_{\text{fin}} - \mathbf{K}$ experienced by the impurity, to order zero in g , that we shall use physically in the subsection VIE 3:

$$\langle(\delta\mathbf{K})^n\rangle^{(0)} = (-1)^n \langle(\mathbf{k} - \mathbf{q})^n\rangle^{(0)} \quad (164)$$

Before proceeding to the calculation of these moments, let us give a **warning** in the limit of a zero-range interaction. We have indeed taken such a limit in equation (162), $b \rightarrow 0$ in the lattice model. The momentum distribution of the impurity interacting with the fermions, however, has an asymptotic tail C/\mathcal{K}^4 at large wave numbers \mathcal{K} , where C is called the “contact”, so that its average kinetic energy must diverge [48, 50–53], as well as the moments of $\delta\mathbf{K}$ and of $\mathbf{k} - \mathbf{q}$ of order $n > 1$. Physically this is due to non-resonant transition processes neglected by the Fermi's golden rule that may be easily taken into account by calculating the evolution operator to first order in g . Also the expression (162), that may be considered as mathematically interesting in itself and that will appear in the kinetic equation models as the one of reference [47], has for a zero-range interaction a clear physical meaning only for $n = 0$ and $n = 1$.

However, expression (162) is **legitimate** in the framework of our perturbative treatment of the lattice model interaction, where the coupling constant g tend to zero with a fixed interaction range (lattice spacing) b : Contrarily to the usual experimental regime for cold atoms, the impurity-to-fermion scattering at zero energy is supposed to be strongly non-resonant, with a scattering length a much smaller than b in the absolute value, see equations (8) and (13). The constant C (the contact) is proportional to the derivative of the total energy with respect to $1/a$, both for a zero-range interaction [50, 51] and for the lattice model [48, 53] once $k_F b \ll 1$ and $Kb \ll 1$, and the leading correction to the energy of the ideal gas is here the mean-field one ρg , so that $C = O(\rho a^2)$ and the contribution of the term in C/\mathcal{K}^4 to the moments of order $n \geq 2$ of the impurity wave vector is $O(\rho a^2/b^{n-1})$, given that wave vectors are restricted to the first Brillouin zone. This contribution, even though divergent if $b \rightarrow 0$ for a fixed, is actually of second order in g : It is negligible in the expressions (162) and (164) that are of order zero in g .

1. Moments of even order n

We can directly reuse the calculations of subsection IIIB, with the notable simplification that $\hbar\omega = E_{\mathbf{K}}$ in equation (17), and $\varepsilon = 0$ in equation (20). Moreover, only the imaginary part of the result matters, $\Im[1/F_{\mathbf{k},\mathbf{q}}(\mathbf{K}, E_{\mathbf{K}})]$ giving π times the Dirac delta distribution that ensures conservation of kinetic energy in Fermi's golden rule, so that

$$\langle(\mathbf{k} - \mathbf{q})^n\rangle^{(0)} \stackrel{n \text{ even}}{=} \frac{k_F^n (\rho g)^2}{\epsilon_F \hbar \Gamma_0^{(2)}(\mathbf{K})} \frac{9r}{4K} \int_0^{+\infty} d\lambda \lambda^n \Im[\psi^+(\lambda) - \psi^-(\lambda)] \quad (165)$$

where \bar{K} is the initial wave number of the impurity in units of k_F , and $\psi^\pm(\lambda)$ is given by (34) or (35) if λ is smaller or larger than 2. As in subsection IV A, we write the integral over $[2, +\infty[$ as the difference of the integrals over $[0, +\infty[$ and $[0, 2]$ of the same integrand. Since all polynomials $P_\sigma^\eta(\lambda)$ now vanish in zero, it is convenient to introduce the reduced polynomials $p_\sigma^\eta(\lambda) \equiv P_\sigma^\eta(\lambda)/\lambda$:

$$p_\alpha^\eta(\lambda) = (1+r)\lambda + 2(r + \eta\bar{K}), \quad p_\beta^\eta(\lambda) = (1-r)\lambda + 2(r + \eta\bar{K}) \quad (166)$$

$$p_\gamma^\eta(\lambda) = \lambda + 2\eta\bar{K}, \quad p_\delta^\eta(\lambda) = (1+r)\lambda + 2(-r + \eta\bar{K}) \quad (167)$$

all of degree one, with real root $\lambda_0^{(\eta\sigma)}$, for $\sigma \in \{\alpha, \beta, \gamma, \delta\}$ and $\eta = \pm$. The expressions (34) and (35) lead to the functions $\Im u^{[s]}(X) = \pi Y(X) X^s/s!$, $s = 2$ or $s = 3$, to be taken in the values of the polynomials $P_\sigma^\eta(\lambda)$. Since $\lambda > 0$, we can replace $Y[P_\sigma^\eta(\lambda)]$ with $Y[p_\sigma^\eta(\lambda)]$. From the powers of $P_\sigma^\eta(\lambda)$ one can pull out factors λ^s . This directly leads, without integrating by parts, to a functional of the type $\int_0^\lambda dt \mathcal{Q}(t) Y[p(t)]$, where $\mathcal{Q}(t)$ is any polynomial and $p(t)$ is a polynomial of degree one with real coefficients. Writing $p(t) = at + b$, of root $\lambda_0 = -b/a$, we can simplify the imaginary part of relation (54) as

$$\int_0^\lambda dt \mathcal{Q}(t) Y(at + b) = [\mathcal{Q}^{[1]}(\lambda) - \mathcal{Q}^{[1]}(-\frac{b}{a})] Y(a\lambda + b) + \mathcal{Q}^{[1]}(-\frac{b}{a}) Y(b) \quad (168)$$

In practice, $p(t)$ is one of the reduced polynomials $p_\sigma^\eta(\lambda)$, and $\mathcal{Q}(t)$ is the corresponding auxiliary polynomial, given by

$$\begin{aligned} \mathcal{Q}_\sigma^\eta(\lambda) &= \frac{\lambda^{n+1}}{48r^3} [p_\sigma^\eta(\lambda)]^2 [p_\sigma^\eta(\lambda) - 6r] \quad \forall \sigma \in \{\alpha, \beta\}, \\ \mathcal{Q}_\gamma^\eta(\lambda) &= \frac{\lambda^{n+2}}{8r^2} [p_\gamma^\eta(\lambda)]^2, \quad \mathcal{Q}_\delta^\eta(\lambda) = -\mathcal{Q}_\alpha^{-\eta}(-\lambda) \end{aligned} \quad (169)$$

The last identity results from the duality property $p_\delta^\eta(\lambda) = -p_\alpha^{-\eta}(-\lambda)$; by simple integration over λ , it leads to the relation $\mathcal{Q}_\delta^{\eta[1]}(\lambda) = \mathcal{Q}_\alpha^{-\eta[1]}(-\lambda)$, which allows us, later in the calculation, to eliminate the contributions in $Y(-r \pm \bar{K})$ thanks to the relation $Y(-r \pm \bar{K}) = 1 - Y(r \mp \bar{K})$ without any remainder. The final result thus has the same structure as the imaginary part of equation (113): It is a pure combination of Heaviside functions without remainders since the quantity $C(\mathbf{K})$ in (113) is real:

$$\langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} \stackrel{n \text{ even}}{=} \frac{k_F^n (\rho g)^2}{\epsilon_F \hbar \Gamma_0^{(2)}(\mathbf{K})} \frac{9\pi r}{4\bar{K}} \sum_{s=0,r,1} \sum_{\eta=\pm} Y(s + \eta\bar{K}) \mathcal{D}_s^\eta(\bar{K}) \quad (170)$$

The prefactors $\mathcal{D}_s^\eta(\bar{K})$ of the Heaviside functions are given by

$$\begin{aligned} \mathcal{D}_0^\eta(\bar{K}) &= \eta \mathcal{Q}_\gamma^{\eta[1]}(\lambda_0^{(\eta\gamma)}), \quad \mathcal{D}_1^\eta(\bar{K}) = \sum_{\sigma=\beta,\gamma,\delta} \eta [\mathcal{Q}_\sigma^{\eta[1]}(2) - \mathcal{Q}_\sigma^{\eta[1]}(\lambda_0^{(\eta\sigma)})], \\ \mathcal{D}_r^\eta(\bar{K}) &= \eta [\mathcal{Q}_\beta^{\eta[1]}(\lambda_0^{(\eta\beta)}) - \mathcal{Q}_\delta^{-\eta[1]}(\lambda_0^{(-\eta\delta)})] \end{aligned} \quad (171)$$

The primitives $\mathcal{Q}_\sigma^{\eta[1]}(\lambda)$ of the polynomials $\mathcal{Q}_\sigma^\eta(\lambda)$ that vanish in $\lambda = 0$ may be calculated, we shall however give an explicit result only for the $s = 0$ contribution: It is extremely simple, and it fully determines the result for small values of \bar{K} , see hereafter. One has the relation

$$\mathcal{D}_s^-(\bar{K}) = -\mathcal{D}_s^+(-\bar{K}) \quad \forall \bar{K}, \quad (172)$$

due to the fact that $\psi^-(\lambda)$ can be deduced from $\psi^+(\lambda)$ in equation (165) by changing \bar{K} to $-\bar{K}$. Also, the prefactors obey a sum rule similar to equation (115), as a direct consequence of the sum rule on the auxiliary polynomials:

$$\sum_{\eta=\pm} \sum_{\sigma=\beta,\gamma,\delta} \eta \mathcal{Q}_\sigma^\eta(\lambda) = 0 \quad \forall \lambda \quad \text{thus} \quad \sum_{s=0,r,1} \sum_{\eta=\pm} \mathcal{D}_s^\eta(\bar{K}) = 0 \quad \forall \bar{K} \quad (173)$$

This causes the sum over η and s into equation (170) to reduce to $-\mathcal{D}_s^-(\bar{K})$ for $0 < \bar{K} < \min(1, r)$, in which case, given the equations (112), (113), (114):

$$\langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} \stackrel{n \text{ even}}{=} \frac{60(2\bar{K})^n}{(n+3)(n+4)(n+5)} \quad (174)$$

2. Moments of odd order n

Odd order moments are vectors. They are invariant by rotation around the axis $\hat{\mathbf{K}} \equiv \mathbf{K}/K$, that is the direction of \mathbf{K} , so that they are parallel to that direction. The trick of averaging over $\hat{\mathbf{K}}$ has now to be applied to the scalar quantity $\hat{\mathbf{K}} \cdot \langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)}$, which amounts to adding a factor w in the integrand of equation (23) and a factor x/y in the imaginary part of (24), the variables x and y being those of (25). This leads finally to the single integral

$$\langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} \stackrel{n \text{ odd}}{=} \hat{\mathbf{K}} \frac{k_F^n (\rho g)^2}{\epsilon_F \hbar \Gamma_0^{(2)}(\mathbf{K})} \frac{9\pi r}{8\bar{K}^2} \int_0^{+\infty} d\lambda \lambda^{n-1} [\tilde{\psi}^+(\lambda) - \tilde{\psi}^-(\lambda)] \quad (175)$$

with, for $\eta = \pm$,

$$\tilde{\psi}^\eta(\lambda) \equiv \int_{\max(1-\lambda, 0)}^1 \bar{q} d\bar{q} \int_{\max(\lambda-\bar{q}, 1)}^{\lambda+\bar{q}} \bar{k} d\bar{k} x Y(x + 2\eta \bar{K} \lambda) \quad (176)$$

This double integral is of the same form as (30) with $\varepsilon = 0$, except that the function $u(X)$ of (32) must be replaced with $\tilde{u}_\lambda^\eta(X) = (X - 2\eta \bar{K} \lambda) Y(X)$ which parametrically depends on λ and on η . Fortunately the calculation procedure exposed below (33) applies to a generic function $u(X)$. The explicit value of $\tilde{\psi}^\eta(\lambda)$ can then be deduced directly from expressions (34) and (35) by replacing u with \tilde{u} , and the resulting primitives of order s are simply

$$\tilde{u}_\lambda^{\eta[s]}(X) = Y^{[s+1]}(X) - 2\eta \bar{K} \lambda Y^{[s]}(X), \quad \text{with } Y^{[s]}(X) = \frac{X^s}{s!} Y(X) \quad (177)$$

The rest follows, as in the case of even order moments, with the same reduced polynomials (166,167), with different expressions for the auxiliary polynomials:

$$\begin{aligned} \mathcal{Q}_\sigma^\eta(\lambda) &= \frac{\lambda^{n+1}}{192r^3} [p_\sigma^\eta(\lambda)]^2 \{ [p_\sigma^\eta(\lambda)]^2 - 4p_\sigma^\eta(0)p_\sigma^\eta(\lambda) + 48\eta r \bar{K} \} \quad \forall \sigma \in \{\alpha, \beta\}, \\ \mathcal{Q}_\gamma^\eta(\lambda) &= \frac{\lambda^{n+2}}{24r^2} [p_\gamma^\eta(\lambda)]^2 [p_\gamma^\eta(\lambda) - 6\eta \bar{K}], \quad \mathcal{Q}_\delta^\eta(\lambda) = -\mathcal{Q}_\alpha^{-\eta}(-\lambda) \end{aligned} \quad (178)$$

but with the same duality relations, in particular $\mathcal{Q}_\delta^{\eta[1]}(\lambda) = \mathcal{Q}_\alpha^{-\eta[1]}(-\lambda)$. This leads to a result of the same form as (170) up to the vectorial factor $\hat{\mathbf{K}}/(2\bar{K})$:

$$\langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} \stackrel{n \text{ odd}}{=} \hat{\mathbf{K}} \frac{k_F^n (\rho g)^2}{\epsilon_F \hbar \Gamma_0^{(2)}(\mathbf{K})} \frac{9\pi r}{8\bar{K}^2} \sum_{s=0, r, 1} \sum_{\eta=\pm} Y(s + \eta \bar{K}) \mathcal{D}_s^\eta(\bar{K}) \quad (179)$$

Here the prefactors $\mathcal{D}_s^\eta(\bar{K})$ of the Heaviside functions are still given by the expressions (171), now written for the auxiliary polynomials (178). As for even n , we have the relation (172), since $\tilde{\psi}^-(\lambda)$ can be deduced from $\tilde{\psi}^+(\lambda)$ in equation (175) by changing \bar{K} to $-\bar{K}$, and we also have the chain of sum rules (173), as shown by an explicit calculation on the auxiliary polynomials (178). For $0 < \bar{K} < \min(1, r)$, we thus have the equivalent of the result (174), with a different factor in the denominator:

$$\langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} \stackrel{n \text{ odd}}{=} \frac{60(2K)^n \hat{\mathbf{K}}}{(n+3)(n+4)(n+6)} \quad (180)$$

3. Damping rate and diffusion coefficient of the impurity momentum

By conservation of the total momentum, see equation (164), and by applying Fermi's golden rule, we can deduce from the moments (162) of the momentum of the emitted particle-hole pair, the initial rate of variation of the moments of the impurity momentum \mathbf{P} away from its initial value $\hbar \mathbf{K}$:

$$\frac{d}{dt} \langle (\mathbf{P} - \hbar \mathbf{K})^n \rangle(t=0) \stackrel{g \rightarrow 0^-}{=} (-\hbar)^n \Gamma_0^{(2)}(\mathbf{K}) \langle (\mathbf{k} - \mathbf{q})^n \rangle^{(0)} + O(g^3) \quad (181)$$

where the integer power of a vector is taken in the sense of (163). Two values of n deserve further developments. The case $n = 1$ corresponds to the initial damping rate of the average momentum of the impurity,

$$\frac{d}{dt} \langle \mathbf{P} \rangle(t=0) \equiv -\Gamma_P(\mathbf{K}) \langle \mathbf{P} \rangle(t=0) \quad (182)$$

It has been studied in reference [35] with the Fermi liquid theory, which is exact for any coupling constant g but only holds for an arbitrary weak \bar{K} . Here, we obtain a complementary prediction, which is exact for any \bar{K} but holds for an arbitrary weak coupling constant: To order two in g ,

$$\Gamma_P^{(2)}(\mathbf{K}) = \Gamma_0^{(2)}(\mathbf{K}) \hat{\mathbf{K}} \cdot \langle (\mathbf{k} - \mathbf{q}) \rangle^{(0)} / K \quad (183)$$

where we recall that $\hat{\mathbf{K}} \equiv \mathbf{K}/K$. As its explicit expression is of a reasonable length, we give in the usual reduced form $\bar{\Gamma}_P^{(2)}(\bar{K}) \equiv \hbar \Gamma_P^{(2)}(\mathbf{K}) \epsilon_F / (\rho g)^2$ and with the presentation adopted in reference [36]: We distinguish (i) the region of small wave numbers $0 < \bar{K} < \min(1, r)$, where

$$\bar{\Gamma}_P^{(2)}(\bar{K}) = \frac{9\pi \bar{K}^4}{35r}, \quad (184)$$

(ii) the region of intermediate wave numbers for an impurity lighter than a fermion, $r < \bar{K} < 1$, where

$$\begin{aligned} \bar{\Gamma}_P^{(2)}(\bar{K}) = & \frac{3\pi r}{35(r^2 - 1)^3} [(3r^4 - 9r^2 + 10)\bar{K}^4 - 14(r^2 + 3)\bar{K}^2 \\ & + 35r(r^2 + 3)\bar{K} - 35r^2(r^2 + 3) + 14r^3(r^2 + 3)\bar{K}^{-1} - r^5(r^2 + 3)\bar{K}^{-3}], \end{aligned} \quad (185)$$

(iii) the intermediate region for an impurity on the contrary heavier than a fermion, $1 < \bar{K} < r$, where

$$\begin{aligned} \bar{\Gamma}_P^{(2)}(\bar{K}) = & \frac{3\pi r}{35(r^2 - 1)^3} [-(1 + 3r^{-2})\bar{K}^4 + 14(3 + r^2)\bar{K}^2 - 35(1 + 3r^2)\bar{K} \\ & + 35r^2(3 + r^2) - 14r^2(1 + 3r^2)\bar{K}^{-1} + (3 - 9r^2 + 10r^4)\bar{K}^{-3}] \end{aligned} \quad (186)$$

and (iv) the region of large wave numbers, $\max(1, r) < \bar{K}$, where

$$\bar{\Gamma}_P^{(2)}(\bar{K}) = \frac{3\pi r}{35(1 + r)^3} [35\bar{K} + 14r^2\bar{K}^{-1} - (r^4 + 3r^3 + 9r^2 + 9r + 3)\bar{K}^{-3}] \quad (187)$$

The prediction of reference [35] for $\Gamma_P(\mathbf{K})$, based on the Fermi liquid theory, is indeed an equivalent of our result at $\bar{K} \rightarrow 0$ when we specialize it to the limit of weak interaction, which amounts to replacing the effective mass m_\downarrow^* of the impurity with its bare mass M and the effective coupling constant of the monomeron with its value to order one in g , $\gamma^{(1)} = mk_{\text{Fa}}/(\pi\mu)$.

The case $n = 2$ corresponds to the initial momentum diffusion coefficient of the impurity, that is to the derivative of the variance of its momentum:

$$\frac{d}{dt} [\langle \mathbf{P}^2 \rangle - \langle \mathbf{P} \rangle^2] (t = 0) \equiv 2D_P(\mathbf{K}) \quad (188)$$

We obtain here its value to leading order, that is to second order in g :

$$2D_P^{(2)}(\mathbf{K}) = \hbar^2 \Gamma_0^{(2)}(\mathbf{K}) \langle (\mathbf{k} - \mathbf{q})^2 \rangle^{(0)} \quad (189)$$

For conciseness, we give the explicit value only for $0 < \bar{K} < \min(1, r)$, readily deduced from equations (116) and (174):

$$2D_P^{(2)}(\mathbf{K}) = \frac{(\rho g)^2}{\hbar \epsilon_F} (\hbar k_F)^2 \frac{12\pi \bar{K}^6}{35r} \quad (190)$$

This diffusion coefficient is actually the trace of the momentum diffusion tensor, which is anisotropic for $\mathbf{K} \neq \mathbf{0}$ and can be calculated to order g^2 with the techniques of this article. From Γ_P and D_P we can deduce the damping rate of the impurity kinetic energy. It is worth recalling the warning that follows equation (162): Contrarily to $\Gamma_P(\mathbf{K})$, the meaning of the coefficient $D_P(\mathbf{K})$ remains to be clarified for a zero-range interaction, if we describe the evolution of the impurity coupled to the fermions beyond the kinetic equation model of reference [47].

VII. CONCLUSION

The problem considered here of one impurity interacting with an ideal Fermi gas of spin-polarized fermions (at zero temperature) belongs to the general class of polaronic problems. It shows with beauty and simplicity the very general

fact that a particle, through the effect of a coupling to a system of continuous spectrum (in the thermodynamic limit), gives birth to a quasi-particle, with an energy at rest, a mass, a dispersion relation, etc, different from those of the bare particle. The problem shows a renewed interest thanks to cold atoms experiments, which involve a mixture of two species or two spin-states of the same fermionic species.

This problem was mainly studied at zero total momentum, that is for an immobile impurity before coupling to the Fermi sea. The main physical motivation was indeed to determine the energy at rest and the effective mass of the quasi-particle, which allows one to estimate the equation of state of the Fermi “liquid” consisting of a non-zero density of impurities, and thus the critical ratio of chemical potential between the impurities and the fermions below which this Fermi liquid is more favorable than the paired superfluid phase [10, 11]. In this case, the variational approach of references [10, 31, 33] remains quantitatively correct in the strongly interacting regime, which allows one to go beyond the perturbative study of reference [5].

The case of a moving impurity is more subtle. The quasi-particle acquires a finite lifetime in its considered momentum subspace since it can slow down by emitting particle-hole pairs in the Fermi sea [4, 35], which is not reproduced by the variational approach in a neighborhood of zero momentum [36]. So we turned to the weakly interacting regime in a perturbative calculation up to second order included in the coupling constant g . Going against some stereotypes, we think that this regime is rather interesting: Non-systematic predictions may lead to very different scaling laws, see for example [53], while the strongly interacting regime (the unitary limit) is often subject to rather technical debates on the pure numbers that are the values of the observables, and whose ultimate determination needs the heavy machinery of quantum Monte Carlo simulations.

Let us now review some salient results of this long article.

Perhaps unexpectedly, the self-energy function $\Sigma(\mathbf{K}, \omega)$ of the impurity, when limited to second order included in g , can be expressed in a fully explicit way, that is the sextuple integral over the momenta of the virtually created particle-hole pair defining the second order contribution $\Sigma^{(2)}(\mathbf{K}, \omega)$ is exactly solvable, see equations (79) and (80). This allows us to show that $\Sigma^{(2)}(\mathbf{K}, \omega)$ is not a smooth function of \mathbf{K} and ω , which is a consequence of the discontinuity of the wave vectors distribution of the fermions $n(\mathbf{k})$ at the Fermi surface $k = k_F$. We find in general that the first singularities appear in the third order derivatives of $\Sigma^{(2)}(\mathbf{K}, \omega)$, and that the region of these singularities in the plane $(K, \varepsilon = (E_{\mathbf{K}} - \hbar\omega)/\epsilon_F)$ has a well defined mathematical origin, see figure 1: Either the polynomials appearing in the explicit expression (79,80) have a double root, in which case the singularities are located on some parabolas and are given by equations (92), (93), (94); or these polynomials have a root equal to zero or two, in which case the singularities are located on some straight lines and are given by equation (101) or by equation (109). However, it is possible to have already some singularities in the second order derivatives of $\Sigma^{(2)}(\mathbf{K}, \omega)$, in particular in $K = k_F$ for an impurity and fermions of the same mass m , see equations (135), (136), (137).

Then we concentrated on a physical quantity directly accessible to cold atom experiments, *via* radio-frequency spectroscopy: This is the complex energy $\Delta E(\mathbf{K})$ of the impurity with wave vector \mathbf{K} . In principle, it can be obtained from the self-energy $\Sigma(\mathbf{K}, \omega)$ after analytic continuation to ω in the lower complex half-plane, by solution of the implicit equation (110). To second order in g , the singularities in the derivatives of the self-energy directly result into singularities of the derivatives of the complex energy with respect to K , which were already present in reference [36]; at this order, one finds for equal masses that $\partial_K^2 \Delta E^{(2)}(\mathbf{K})$ tends logarithmically to $+\infty$ in $K = k_F$, which is a limitation of the perturbative approach. In order to determine the real behavior of $\partial_K^2 \Delta E(\mathbf{K})$ in the neighborhood of $K = k_F$, for g close to zero but finite, in a way taking advantage of our analytical expression for $\Sigma^{(2)}(\mathbf{K}, \omega)$, we have performed a self-consistent approximation of the implicit equation for $\Delta E(\mathbf{K})$: We have included the mean-field shift to all order in g but we have replaced the self-energy by its expansion up to order g^2 only, see the equations (132) and (133) for equal masses. The $g \rightarrow 0^-$ resulting scaling law (143) leads to $\partial_K^2 [\Delta E(\mathbf{K}) - \hbar^2 K^2/(2m)] \propto -g^2 \ln g^2$ in $K = k_F$, simply because the $-\ln|K - k_F|$ divergence of $\partial_K^2 \Delta E^{(2)}(\mathbf{K})$ in the perturbative theory is interrupted in the self-consistent theory at a distance from $K = k_F$ proportional to g^2 . Another interesting prediction (144) of the scaling law (143) is that the third-order derivative $\partial_K^3 \Delta E(\mathbf{K})$ around k_F does not tend to zero uniformly with K , when $g \rightarrow 0^-$. Also, we plotted in figure 2 the function $F(x)$ that appears in the scaling law (143), although it is not fully determined by our self-consistent approximation, due to an ambiguity in the analytic continuation of $\Sigma^{(2)}(\mathbf{K}, \omega)$ to values of ω with a negative imaginary part, see the end of subsection VIC 3. Our pioneering study is thus not final. To be complete, we give in (161) a condition for the non-zero temperature effects to be negligible in an experiment.

We concluded by a physical application a bit out of the mainstream of this paper: Taking advantage of the techniques of integral calculus that we developed to obtain (80), we could calculate all the moments (174) and (180) of the momentum of the particle-hole pair emitted by the moving impurity in the Fermi sea, according to Fermi’s golden rule, that is to zeroth order in g . This gives access to the damping rate of the mean momentum of the impurity, for an arbitrary initial momentum but to second order in g , see equations (184,185,186,187). This is complementary to the Fermi liquid theory, which is non perturbative in g but restricted to arbitrarily low momenta [35]. This also gives access to the momentum diffusion coefficient of the impurity to second order in g , see its fully explicit expression at low momenta on equation (190). These moments may of course be observed experimentally with cold atoms, provided that

one is able to prepare a quasi-monochromatic impurity wave packet, e.g. by accelerating a Bose-Einstein condensate; it remains then to put this wave packet in contact with a polarized Fermi gas and to measure its momentum distribution by time-of-flight [54, 55]. Finally, we note that the second moment, not to mention the higher order ones, raises a paradox, that we solve in the beginning of subsection VIE in the weakly interacting regime (but not in the regime of arbitrary interactions of reference [47]): The impurity interacts with the fermions, so that its wave vector distribution should have an asymptotic $1/K^4$ tail [48, 50–53], the variance of \mathbf{K} should diverge and the notion of momentum diffusion should be meaningless.

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- [1] E.M. Lifshitz, L.P. Pitaevskii, *Statistical Physics Part 2* (Pergamon Press, 1980).
 - [2] A.L. Fetter, J.D. Walecka, *Quantum Theory of Many-Particle Systems* (Dover, Mineola, 2003).
 - [3] J.D. Walecka, *Nuovo Cimento* **16**, 342 (1960).
 - [4] R.F. Bishop, *Nucl. Phys. B* **17**, 573 (1970).
 - [5] R.F. Bishop, *Ann. Phys.* **78**, 391 (1973).
 - [6] G.B. Partridge, W. Li, R.I. Kamar, Y. Liao, R.G. Hulet, *Science* **311**, 503 (2006).
 - [7] M.W. Zwierlein, C.H. Schunck, A. Schirotzek, W. Ketterle, *Nature (London)* **442**, 54 (2006); Y. Shin, M.W. Zwierlein, C.H. Schunck, A. Schirotzek, W. Ketterle, *Phys. Rev. Lett.* **97**, 030401 (2006).
 - [8] M. Koschorreck, D. Pertot, E. Vogt, B. Fröhlich, M. Feld, M. Köhl, *Nature* **485**, 619 (2012).
 - [9] C. Kohstall, M. Zaccanti, M. Jag, A. Trenkwalder, P. Massignan, G. M. Bruun, F. Schreck, R. Grimm, *Nature* **485**, 615 (2012).
 - [10] F. Chevy, *Phys. Rev. A* **74**, 063628 (2006).
 - [11] C. Lobo, A. Recati, S. Giorgini, S. Stringari, *Phys. Rev. Lett.* **97**, 200403 (2006).
 - [12] S. Nascimbène, N. Navon, K. Jiang, F. Chevy, C. Salomon, *Nature (London)* **463**, 1057 (2010).
 - [13] N. Navon, S. Nascimbène, F. Chevy, C. Salomon, *Science* **328**, 729 (2010).
 - [14] C. Chin, R. Grimm, P. Julienne, E. Tiesinga, *Rev. Mod. Phys.* **82**, 1225 (2010).
 - [15] V. Efimov, *Sov. J. Nucl. Phys.* **12**, 589 (1971); V. Efimov, *Nucl. Phys. A* **210**, 157 (1973); A. Bulgac, V. Efimov, *Sov. J. Nucl. Phys.* **22**, 296 (1975).
 - [16] D.S. Petrov, *Phys. Rev. A* **67**, 010703 (2003).
 - [17] E. Braaten, H.-W. Hammer, *Phys. Rep.* **428**, 259 (2006).
 - [18] Y. Castin, C. Mora, L. Pricoupenko, *Phys. Rev. Lett.* **105**, 223201 (2010).
 - [19] L.H. Thomas, *Phys. Rev.* **47**, 903 (1935).
 - [20] M. Correggi, G. Dell’Antonio, D. Finco, A. Michelangeli, A. Teta, *Rev. Math. Phys.* **24**, 1250017 (2012).
 - [21] N. Prokof’ev, B. Svistunov, *Phys. Rev. B* **77**, 020408(R) (2008); *ibid.*, *Phys. Rev. B* **77**, 125101 (2008).
 - [22] M. Punk, P.T. Dumitrescu, W. Zwerger, *Phys. Rev. A* **80**, 053605 (2009).
 - [23] C. Mora, F. Chevy, *Phys. Rev. A* **80**, 033607 (2009).
 - [24] R. Combescot, S. Giraud, X. Leyronas, *Europhys. Lett.* **88**, 60007 (2009).
 - [25] C.J.M. Mathy, Meera M. Parish, D.A. Huse, *Phys. Rev. Lett.* **106**, 166404 (2011).
 - [26] C. Trefzger, Y. Castin, *Phys. Rev. A* **85**, 053612 (2012).
 - [27] Zhihao Lan and C. Lobo, *Journal of the Indian Institute of Science* **94**, 179 (2014); P. Massignan, M. Zaccanti, G.M. Bruun, *Rep. Prog. Phys.* **77**, 034401 (2014).
 - [28] P. Massignan, *Europhys. Lett.* **98**, 10012 (2012).
 - [29] Ran Qi, Hui Zhai, *Phys. Rev. A* **85**, 041603(R) (2012).
 - [30] G.M. Bruun, P. Massignan, *Phys. Rev. Lett.* **105**, 020403 (2010).
 - [31] R. Combescot, A. Recati, C. Lobo, F. Chevy, *Phys. Rev. Lett.* **98**, 180402 (2007).
 - [32] S. Giraud, PhD thesis, University Pierre et Marie Curie (2010), “*Contribution à la théorie des gaz de fermions ultrafroids fortement polarisés*”, tel.archives-ouvertes.fr/tel-00492339
 - [33] R. Combescot, S. Giraud, *Phys. Rev. Lett.* **101**, 050404 (2008).
 - [34] Y. Nishida, *Phys. Rev. A* **85**, 053643 (2012).
 - [35] G.M. Bruun, A. Recati, C.J. Pethick, H. Smith, S. Stringari, *Phys. Rev. Lett.* **100**, 240406 (2008).
 - [36] C. Trefzger, Y. Castin, *Europhys. Lett.* **104**, 50005 (2013).
 - [37] Meera M. Parish, J. Levinsen, *Phys. Rev. A* **87**, 033616 (2013).

- [38] C. Cohen-Tannoudji, J. Dupont-Roc, G. Grynberg, *Processus d'interaction entre photons et atomes* (InterEditions et Editions du CNRS, 1988).
- [39] C. Trefzger, Y. Castin, Europhys. Lett. **101**, 30006 (2012).
- [40] A. Sinatra, C. Lobo, Y. Castin, J. Phys. B **35**, 3599 (2002).
- [41] C. Mora, Y. Castin, Phys. Rev. A **67**, 053615 (2003).
- [42] L. Pricoupenko, Y. Castin, J. Phys. A **40**, 12863 (2007).
- [43] E. Burovski, N. Prokof'ev, B. Svistunov, M. Troyer, New J. Phys. **8**, 153 (2006).
- [44] O. Juillet, New J. Phys. **9**, 163 (2007).
- [45] Xiaoling Cui, Hui Zhai, Phys. Rev. A **81**, 041602(R) (2010).
- [46] P. Massignan, G. M. Bruun, Eur. Phys. J. D **65**, 83 (2011).
- [47] Hyungwon Kim, D.A. Huse, Phys. Rev. A **85**, 043603 (2012).
- [48] F. Werner, Y. Castin, Phys. Rev. A **86**, 013626 (2012).
- [49] Y. Castin, J. Phys. IV (France) **116**, 89 (2004).
- [50] S. Tan, Ann. Phys. **323**, 2952 (2008) ; S. Tan, Ann. Phys. **323**, 2971 (2008).
- [51] E. Braaten, L. Platter, Phys. Rev. Lett. **100**, 205301 (2008) ; E. Braaten, D. Kang, L. Platter, Phys. Rev. A **78**, 053606 (2008).
- [52] S. Zhang, A.J. Leggett, Phys. Rev. A **79**, 023601 (2009).
- [53] F. Werner, L. Tarruell, Y. Castin, Eur. Phys. J. B **68**, 401 (2009).
- [54] F. Ferlaino, R.J. Brecha, P. Hannaford, F. Riboli, G. Roati, G. Modugno, M. Inguscio, Journal of Optics B: Quantum and Semiclassical Optics, **5**(2):S3 (2003).
- [55] I. Ferrier-Barbut, M. Delehaye, S. Laurent, A.T. Grier, M. Pierce, B.S. Rem, F. Chevy, Ch. Salomon, Science **345**, 1035 (2014).