On the (anisotropic) uniform metallic ground states of fermions interacting through arbitrary two-body potentials in $d$ dimensions

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(Received 16 April 2003 and accepted 28 July 2003)

We demonstrate that the skeleton of the Fermi surface $S_{f,\sigma}$ pertaining to a uniform metallic ground state (corresponding to fermions with spin index $\sigma$) is determined by the Hartree-Fock contribution $\Sigma_{HF}^{\sigma}(k)$ to the dynamic self-energy $\Sigma_{\sigma}(k;\varepsilon)$. That is to say, in order for $k \in S_{f,\sigma}$, it is necessary (but for anisotropic ground states in general not sufficient) that the following equation be satisfied:

$$\varepsilon_k + \hbar \Sigma_{HF}^{\sigma}(k) = \varepsilon_f,$$

where $\varepsilon_k$ stands for the underlying non-interacting energy dispersion and $\varepsilon_f$ for the exact interacting Fermi energy. The Fermi surface $S_{f,\sigma}$ consists of the set of $k$ points which in addition to satisfying the above equation fulfill

$$S_{\sigma}(k) = 0,$$

where

$$S_{\sigma}(k) := \frac{1}{\pi} \int_0^\infty \frac{d\varepsilon}{\varepsilon} \text{Im}[\Sigma_{\sigma}(k;\varepsilon_f + \varepsilon) + \Sigma_{\sigma}(k;\varepsilon_f - \varepsilon)].$$

The set of $k$ points which satisfy the first of the above two equations but fail to satisfy the second constitute the pseudogap region of the putative Fermi surface of the interacting system. We consider the behaviour of the ground-state momentum-distribution function $n_{\sigma}(k)$ for $k$ in the vicinity of $S_{f,\sigma}$ and show that, whereas for the uniform metallic ground states of the conventional single-band Hubbard Hamiltonian, described in terms of an on-site interaction, $n_{\sigma}(k_{f,\sigma}^{-}) \geq \frac{1}{2}$ and $n_{\sigma}(k_{f,\sigma}^{+}) \leq \frac{1}{2}$ (here $k_{f,\sigma}^{-}$ and $k_{f,\sigma}^{+}$ denote vectors infinitesimally close to $S_{f,\sigma}$, located respectively inside and outside the underlying Fermi sea), for interactions of non-zero range these inequalities can be violated (without thereby contravening the stability condition $n_{\sigma}(k_{f,\sigma}^{-}) \geq n_{\sigma}(k_{f,\sigma}^{+})$). This aspect is borne out by the $n_{\sigma}(k)$ pertaining to the normal states of for instance liquid $^3$He (corresponding to a range of applied pressure) as determined by means of quantum Monte Carlo calculations. We further demonstrate that for Fermi-liquid metallic states of fermions interacting through interaction potentials of non-zero range (e.g. the Coulomb potential), the zero-temperature limit of $n_{\sigma}(k)$ does not need to be equal to $\frac{1}{2}$ for $k \in S_{f,\sigma}$; this in strict contrast with the uniform Fermi-liquid metallic states of the single-band Hubbard Hamiltonian (if such states at all exist). This aspect should be taken into account while analyzing the $n_{\sigma}(k)$ deduced from the angle-resolved photoemission data concerning real materials. We discuss, in the light of the findings of the present work, the growing experimental evidence with regard to the ‘frustration’ of the kinetic energy of the charge carriers in the normal states of the copper-oxide-based high-temperature superconducting compounds.
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   6.1. The case when \( 0 < \gamma < 1, \ 0 < \tau < 1 \)  

   6.1.1. \( 0 < \gamma < \tau < 1 \)  

   6.1.2. \( 0 < \tau < \gamma < 1 \)  

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Acknowledgements  

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References  

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### § 1. INTRODUCTION

Theoretical investigation of anisotropic interacting metallic systems is specifically demanding through the possibility, even for isotropic interaction potentials, of the deformation of the Fermi surface in these systems with respect to the underlying non-interacting Fermi surface [1–3]. For recent approaches to this problem we refer the reader to [4,5] and the references herein.

Building on recent work [6] concerning the uniform metallic ground states (GSs) of the conventional single-band Hubbard Hamiltonian [7–10] for arbitrary spatial dimensions \( d \), in this work we consider similar states for arbitrary two-body interaction potentials (provided only that these possess Fourier transform) corresponding to systems of fermions whose non-interacting energy dispersion \( \varepsilon_k \) can be both bounded (as is the case for the single-band Hubbard Hamiltonian) and unbounded from above (as in the case of the free-fermion model where \( \varepsilon_k = \hbar^2|k|^2/[2m] \), in which \( m \) stands for the fermion bare mass). Our results, of which a number we have presented in the abstract, make explicit some of the fundamental differences between systems in which the interaction potential \( v(r - r') \) is of contact type, of strictly bounded and of unbounded range. Following the general considerations leading to the equations defining \( S_{\tau,\sigma} \), presented above, in this paper we deduce the most general expression for \( n_\sigma(k) \) in the close vicinity of \( S_{\tau,\sigma} \) and for specific cases deal with this expression in considerable detail. Amongst others, we show that, in contrast with the case of the conventional single-band Hubbard Hamiltonian, \( n_\sigma(k) \) can become smaller (greater) than \( \frac{1}{2} \) for \( k \) inside (outside) the Fermi sea and infinitesimally close to \( S_{\tau,\sigma} \), without infringing on the condition \( n_\sigma(k_{\tau,\sigma}) - n_\sigma(k^\tau_{\tau,\sigma}) \geq 0 \) implied by the assumption of the stability of the GS of the system under consideration. This aspect is significant in that in cases where \( n_\sigma(k_{\tau,\sigma}) < \frac{1}{2} \), by continuity \( n_\sigma(k) \) is expected to be more suppressed for \( k \) inside the Fermi sea (at least in the vicinity of \( S_{\tau,\sigma} \)) in comparison with cases where \( n_\sigma(k_{\tau,\sigma}) \geq \frac{1}{2} \), implying thus an increase in the contribution of the correlated kinetic energy \( \sum k,\sigma \epsilon_k n_\sigma(k) \) to the GS total energy of the system under consideration (see later). In this connection, note that \( \sum k,\sigma n_\sigma(k) \) is equal to the total number \( N \) of particles in the GS and therefore independent of the magnitude of the coupling constant of interaction.

For a number of reasons of contemporary interest, a reliable description of \( n_\sigma(k) \) seems timely and desirable. Foremost amongst these are investigations regarding the determination of the mechanism of superconductivity in the copper-oxide-based high-temperature superconducting materials (hereafter referred to as cuprates or cuprate compounds); for recent reviews see [11–13]. Both the earlier angle-resolved photoemission results [14] (see in particular Fig. 3(F) herein) and the recent in-plane optical-conductivity data concerning \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8+\delta \) [15,16] (see also [17]) reveal decrease in the in-plane kinetic energy of the system upon entering into the superconducting state, by an amount commensurate with the expected superconducting condensation energy.\(^1\) A similar trend has been observed in the measured out-of-plane (i.e. the \( c \)-axis) optical conductivities of \( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}, \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), and \( \text{YBa}_2\text{Cu}_3\text{O}_{6+\delta} \) [18].\(^2\) Assuming the sufficiency of the BCS variational wavefunction to de-
scribe the superconducting states of the cuprate compounds (an assumption that has been widely anticipated), one readily observes that \( n_\sigma(k_{F,\sigma}) < \frac{1}{2} \), with \( k_{F,\sigma} \in S_{\tau,\sigma} \), in combination with the assumption of continuity of \( n_\sigma(k) \) for \( k \) inside the Fermi sea and in the vicinity of \( S_{\tau,\sigma} \), is tantamount to an excess kinetic energy in the normal GS of the underlying system in comparison with the kinetic energy in the paired state (see the previous paragraph).

The above-indicated experimental results on the one hand and the feasibility of \( n_\sigma(k_{F,\sigma}) < \frac{1}{2} \) for the metallic states of fermions interacting through potentials of at least finite range on the other clearly signify the likelihood of the existence of a crucial relationship between the latter potentials and the unconventional properties of the metallic states of the cuprate compounds (see also [37,38]). In this connection it is relevant to mention in the conventional single-band Hubbard Hamiltonian does not support d_{x^2-y^2} long-range pairing order at non-zero temperatures, an aspect strongly anticipated by earlier Monte Carlo results (which incidentally also do not support extended s-wave pairing) on finite systems [44–48]. Further, the view is increasingly gaining prominence that the long range of the Coulomb potential, such as obtained within the framework of the so-called 'cluster dynamical mean-field' approximation [40,41] (see also [42,43]), plays a crucial role in stabilizing one from amongst a number of competing orders in the cuprate compounds over some relevant range of parameters. Of these, one concerns the periodic (but incommensurate with respect to the underlying lattice) ordering of spin and charge (also referred to as spin-charge stripes; for general reviews see [66,67] and the references herein), which appears to compete against macroscopic phase separation [68]. This statement requires some qualification. Macroscopic phase separation is believed not to concern the Hubbard Hamiltonian [69,70], but solely the t-J Hamiltonian. However, even for the t-J Hamiltonian the actual situation is not firmly established; on the one hand, Green-function Monte Carlo results (concerning finite systems) have been interpreted as implying phase separation at hole dopings and interaction strengths appropriate to the cuprate superconductors [71], while, on the other hand, subsequent numerical calculations [70] based on ‘density-matrix renormalization group’ (DMRG) method performed on larger systems have upheld the viewpoint that the 'stripes' state would have a lower energy than the phase-separated state. In spite of these opposing observations, it is generally believed that the sensitivity of the results corresponding to the t-J Hamiltonian on such details as, for instance, the shape and size of the clusters on which computations are carried out does not warrant an a priori neglect of the long range of the Coulomb interaction [61,63,64] (see also [72]). Later in this paper we shall discuss and document the significance of a non-contact-type interaction in accurately describing the normal liquid state of \(^3\text{He}\).

Using the experimental angle-resolved photoemission data it is possible to determine \( n_\sigma(k) \) for \( k \) in the vicinity of \( S_{\tau,\sigma} \), as has been reported in [73] for Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (Bi2212) and Bi\(_2\)Sr\(_2\)Cu\(_1\)O\(_{6+\delta}\) (Bi2201), in both the overdoped and the underdoped regime. In [73] the Fermi surface has been asserted as being the locus of the \( k \) points at which, firstly, the (experimental) single-particle spectral function \( A_\sigma(k,\varepsilon) \) is peaked for \( \varepsilon = \varepsilon_F \) and, secondly, \( n_\sigma(k) \) takes the value \( \frac{1}{2} \) (see [74]); in [73] the absolute value of \( n_\sigma(k) \) is determined by equating with unity the maximum value achieved by the experimental \( n_\sigma(k), \forall k \), a procedure which evidently adds uncertainty to the experimentally determined \( n_\sigma(k) \). As demonstrated in [6], and in view of the findings in the present work, the

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3 According to this assumption, the zero-temperature BCS occupation fraction \( v_0^2 \equiv 1 - n_0^2 \) (see [35], Chapter 3 and in particular Fig. 3.1) plays the same role as \( n_\sigma(k) \) does in relation to the underlying normal GS. For completeness, within the framework of the conventional BCS theory, and at zero temperature, the \( n_\sigma(k) \) pertaining to the normal GS coincides with the unit-step function, equal to unity for \( k \) inside the Fermi sea and to zero for \( k \) outside. Consequently, at zero temperature the BCS state accommodates a higher kinetic energy than the underlying uncorrelated normal GS (for a quantitative consideration see § 3.4 in [35]). Note in passing that Chester’s [36] findings do not apply to a pairing, or reduced, Hamiltonian such as the one employed in the conventional BCS theory.

4 The superconducting order parameter in the cuprate compounds is generally considered to have the d_{x^2-y^2} symmetry [11–13]. Note in passing that in practice the inter-planar coupling of the electronic degrees of freedom is capable of stabilizing a d-wave superconducting state at finite temperatures, such as obtained within the framework of the so-called ‘cluster dynamical mean-field’ approximation [40,41] (see also [42,43]).

5 Explicitly, in [73] the authors introduced three criteria to be obeyed “at a true FS [Fermi surface] crossing”, of which the second reads: “(2) \( n(k) \ n_\sigma(k) \) should be near 50% of its maximal value, or equivalently the maximal gradient point”. Elsewhere these workers stated: “a FS [Fermi surface] crossing should occur when \( n(k) \) loses about half of its maximum value (excluding the background)”. As we indicate in the main text, these workers fixed the scale of the experimentally determined \( n_\sigma(k) \) by identifying with unity the maximum value of the latter function over all the \( k \) points probed experimentally.
requirement \( n_\sigma(k) = \frac{1}{2} \) for \( k \in S_{r,\sigma} \) is not justified in general; \(^6\) firstly, within the framework of the conventional single-band Hubbard model, the latter is solely a necessary (and not sufficient) condition for metallic states to be Fermi-liquid (FL) and, secondly, for metallic states of fermions interacting through potentials of non-zero range the condition \( n_\sigma(k) = \frac{1}{2} \) for \( k \in S_{r,\sigma} \) is not demanded even for FL metallic states. In the light of these and neglecting for the moment the above-mentioned uncertainty concerning the absolute values of the experimentally determined \( n_\sigma(k) \), the results depicted in Fig. 2 of [73] have far-reaching implications. For instance, these results clearly show that a contact-type interaction cannot be capable of reliably describing Bi2212 and Bi2201 in the over-doped and the underdoped regimes (at no peak position of \( A_\sigma(k;\varepsilon_f) \) does \( n_\sigma(k) \) acquire a value reasonably close to \( \frac{1}{2} \); a number of these results further show that the pertinent single-particle spectral functions \( A_\sigma(k;\varepsilon) \), corresponding to the systems considered, are most probably free from quasi-particle \( \delta \)-function contributions (establishing the breakdown of the FL state) at regions of \( S_{r,\sigma} \) neighbouring the \( \mathbb{M} \) points of the underlying Brillouin zones (compare for instance Figs. 2(g) and 2(f) in [73] with the results in Eq. (109) below).

The organization of this paper is as follows. In § 2 we introduce the Hamiltonian on which the considerations in this paper are based: this Hamiltonian, which is expressed in terms of a single spin-degenerate energy dispersion \( \varepsilon_k \), is defined on the continuum; however, through some minor adjustments, which we explicitly specify, this reduces to the conventional single-band Hubbard Hamiltonian, defined on a lattice. In § 3 we present the details underlying the equations from which \( S_{r,\sigma} \) pertaining to the uniform GSs of the Hamiltonian introduced in § 2 is determined. In § 4 we expose an intimate relationship between \( S_{r,\sigma} \) and \( \Sigma_{\sigma}^{up}(k) \) mediated through the single-particle density matrix \( \rho_\sigma(r,r') \) which for uniform GSs, where the latter function depends on \( r-r' \), coincides with the Fourier transform of the GS momentum distribution function \( n_\sigma(k) \); the information with regard to \( S_{r,\sigma} \), through the singular nature of \( n_\sigma(k) \) for \( k \in S_{r,\sigma} \), is shown to be already fully reflected in the leading term in the asymptotic series of \( \rho_\sigma(r,r') \) for \( \|r-r'\| \to \infty \). In § 5 we examine the equation for \( S_{r,\sigma} \) in terms of \( \Sigma_{\sigma}^{up}(k) \) by applying this equation to an isotropic metallic GS for which \( S_{r,\sigma} \) is rotationally invariant and is fully determined by the concentration of the fermions in the system. By doing so we deduce expressions for the exchange potential \( \mu_{\kappa,\sigma} \) and correlation potential \( \mu_{c,\sigma} \), as encountered within the framework of the GS density-functional theory [75–77]. Our expression for \( \mu_{\kappa,\sigma} \) identically reproduces the exact \( \mu_{\kappa,\sigma} \) corresponding to the Coulomb-interacting uniform-electron-gas system. Making use of \( n_\sigma^{up}(k) \), the random-phase approximation (RPA) to \( n_\sigma(k) \), which for systems of Coulomb-interacting fermions asymptotically approaches the exact \( n_\sigma(k) \) in the high-density regime, we calculate \( \mu_{c,\sigma} \) which in the latter regime up to an unimportant additive constant reproduces the \( \mu_{c,\sigma} \) deduced from quantum Monte-Carlo calculations. In § 6 we consider the behaviour of \( n_\sigma(k) \) for \( k \) in the vicinity of \( S_{r,\sigma} \), both inside and outside the Fermi sea. Rather than being exhaustive, in this Section we attempt to contrast the important consequences that the range of interaction can have on the behaviour of \( n_\sigma(k) \) in the mentioned region of the \( k \) space. In § 7 we present a summary of the main aspects of this paper. Here we also briefly relate our theoretical findings with some available results concerning correlated fermion systems, specifically liquid \(^3\)He in the normal state. Finally, in appendix A which follows the main body of this paper we present an analysis which exposes the nature of inaccuracy in \( \rho_\sigma(k) \) as calculated on the basis of a finite-order perturbation series for the self-energy operator. For reasons that will be clarified in appendix A, the defining expression for \( S_{r,\sigma} \) as introduced in this paper (i.e. Eq. (53) below) more reliably reproduces \( S_{r,\sigma} \) than the conventional defining expression (i.e. Eq. (45)).

\section{Preliminaries}

In a recent work [6] we have in some detail considered the uniform metallic GSs of the single-band Hubbard Hamiltonian. Here we extend our investigations by considering uniform metallic GSs of the following Hamiltonian

\[ \hat{H} = \hat{H}_0 + g \hat{H}_1, \]

where

\[ \hat{H}_0 = \sum_{k,\sigma} \varepsilon_k \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma}, \]

\[ \hat{H}_1 = \frac{1}{2\Omega} \sum_{\sigma,\sigma'} \sum_{k,p,q} \hat{w}(\|q\|) \hat{c}^\dagger_{k+q,\sigma} \hat{c}^\dagger_{p-q,\sigma'} \hat{c}_{p,\sigma'} \hat{c}_{k,\sigma}. \]

In Eq. (1), \( g \) (which has the dimension of energy) stands for the coupling-constant of interaction, \( \varepsilon_k \) for a spin-degenerate single-particle energy dispersion (which may be equated with \( h^2 k^2 / 2m \)), the energy dispersion of non-interacting free fermions with mass \( m \), \( \hat{c}^\dagger_{k,\sigma} \) and \( \hat{c}_{k,\sigma} \) for the canonical creation and annihilation operators respectively for fermions with spin index \( \sigma \), \( \hat{w}(\|q\|) \equiv \]

\(^6\) For cases in which \( n_\sigma(k) \) is discontinuous at \( k \in S_{r,\sigma} \), in the present context the value assigned to \( n_\sigma(k) \) for \( k \in S_{r,\sigma} \) is the arithmetic mean of \( n_\sigma(k') \) for \( k' \) approaching \( k \) from inside and outside the Fermi sea. This mean value coincides with the zero-temperature limit of \( n_\sigma(k) \) for \( k \in S_{r,\sigma} \) [6].
\(v(∥q∥)\) for the Fourier transform of the two-body interaction potential \(v(r - r')\) (assumed to be isotropic), and \(Ω = L^d\) for the volume of the (macroscopic) \(d\)-dimensional hyper-cubic box occupied by the system. The wave-vector sums in Eqs. (2) and (3) are over a regular lattice (the underlying lattice constant being equal to \(2π/L\)) covering in principle the entire reciprocal space. On the basis of similar arguments as presented in [6], it goes over into the conventional single-band Hubbard Hamiltonian \([7–10]\) \(H\) corresponding to the on-site interaction energy \(U\); in cases where \(k + q\) and \(p - q\) on the right-hand side (RHS) of Eq. (3) lie outside the 1BZ, these vectors are to be identified with the vectors inside the 1BZ obtained from \(k + q\) and \(p - q\) through Umklapp processes. On relaxing the replacements in Eq. (4), while maintaining the above-mentioned restrictions concerning the wave vectors, the Hamiltonian in Eq. (1) coincides with an ‘extended’ Hubbard Hamiltonian.

Along the lines considered in [6], it can be shown that for the Fermi surface \(S_{\bar{v}N,σ}\) pertaining to the uniform metallic GS of \(\hat{H}\), one has

\[
S_{\bar{v}N,σ} = \{k \parallel (ε_κ - ε_{κσ})(ε_κ - ε_{κσ}) = 0\},
\]

where \(ε_κ = ε_κ + 0^+\) and

\[
\hat{ε}_{κσ} = ε_κ + \frac{β_{κσ}}{ν_κ(k)}.
\]

On the basis of similar arguments as presented in [6], it can be shown that \((ε_κ - ε_{κσ}) = 0\) implies that \((ε_κ - ε_{κσ}) = 0\), and vice versa so that, for \(k \in S_{\bar{v}N,σ}\), \(ε_{κσ}\) and \(ε_{κσ}\) are up to an infinitesimal difference equal. In Eq. (6),

\[
ν_κ(k) := \begin{cases} n_σ(k), \\ 1 - n_σ(k), \end{cases}
\]

where \(n_σ(k)\) stands for the number of fermions with spin index \(σ\) per site in the uniform \(N\)-particle GS of the Hubbard Hamiltonian; thus \(n := N/N_κ\). In Eq. (13), \(\hat{N}\) denotes the spin index complementary to \(σ\), that is for \(σ\rightleftharpoons ↑, \hat{σ} = ↓\) and vice versa.

In cases where \(\hat{v}(∥q∥)\) is unbounded for \(∥q∥ = 0\) (such as is the case for the two-body Coulomb potential), the expression in Eq. (15) has to be regularized; this is achieved by formally taking into account the interaction of the fermions with a positively charged uniform background through supplementing the Hamiltonian in Eq. (1) with \(g\hat{H}'\), where

\[
\hat{H}' := -n_0 \hat{w}(κ)\hat{N}, \quad κ \downarrow 0,
\]

in which \(\hat{N}\) stands for the total number operator. Following this, one obtains

\[
\hat{v}_{κσ} = n_σ(k + p) - n_σ(k + p),
\]

where \(\hat{w}(∥q∥)\) stands for the \(N\)-particle GS of \(\hat{H}\),

\[
\hat{v}_{κσ} = -\frac{1}{Ω} \sum_{σ'} \sum_{p',q'} \hat{w}(∥q'∥) \nonumber
\]

|\(\hat{v}(∥q∥)\)| for the Fourier transform of the two-body interaction potential \(v(r - r')\) (assumed to be isotropic), and \(Ω = L^d\) for the volume of the \(d\)-dimensional hyper-cubic box occupied by the system. The wave-vector sums in Eqs. (2) and (3) are over a regular lattice (the underlying lattice constant being equal to \(2π/L\)) covering in principle the entire reciprocal space. On the basis of similar arguments as presented in [6], it goes over into the conventional single-band Hubbard Hamiltonian \([7–10]\) \(H\) corresponding to the on-site interaction energy \(U\); in cases where \(k + q\) and \(p - q\) on the right-hand side (RHS) of Eq. (3) lie outside the 1BZ, these vectors are to be identified with the vectors inside the 1BZ obtained from \(k + q\) and \(p - q\) through Umklapp processes. On relaxing the replacements in Eq. (4), while maintaining the above-mentioned restrictions concerning the wave vectors, the Hamiltonian in Eq. (1) coincides with an ‘extended’ Hubbard Hamiltonian.

Along the lines considered in [6], it can be shown that for the Fermi surface \(S_{\bar{v}N,σ}\) pertaining to the uniform metallic GS of \(\hat{H}\), one has

\[
S_{\bar{v}N,σ} = \{k \parallel (ε_κ - ε_{κσ})(ε_κ - ε_{κσ}) = 0\},
\]

where \(ε_κ = ε_κ + 0^+\) and

\[
\hat{ε}_{κσ} = ε_κ + \frac{β_{κσ}}{ν_κ(k)}.
\]

On the basis of similar arguments as presented in [6], it can be shown that \((ε_κ - ε_{κσ}) = 0\) implies that \((ε_κ - ε_{κσ}) = 0\), and vice versa so that, for \(k \in S_{\bar{v}N,σ}\), \(ε_{κσ}\) and \(ε_{κσ}\) are up to an infinitesimal difference equal. In Eq. (6),

\[
ν_κ(k) := \begin{cases} n_σ(k), \\ 1 - n_σ(k), \end{cases}
\]

where \(n_σ(k)\) stands for the number of fermions with spin index \(σ\) per site in the uniform \(N\)-particle GS of the Hubbard Hamiltonian; thus \(n := N/N_κ\). In Eq. (13), \(\hat{N}\) denotes the spin index complementary to \(σ\), that is for \(σ\rightleftharpoons ↑, \hat{σ} = ↓\) and vice versa.

In cases where \(\hat{v}(∥q∥)\) is unbounded for \(∥q∥ = 0\) (such as is the case for the two-body Coulomb potential), the expression in Eq. (15) has to be regularized; this is achieved by formally taking into account the interaction of the fermions with a positively charged uniform background through supplementing the Hamiltonian in Eq. (1) with \(g\hat{H}'\), where

\[
\hat{H}' := -n_0 \hat{w}(κ)\hat{N}, \quad κ \downarrow 0,
\]

in which \(\hat{N}\) stands for the total number operator. Following this, one obtains

\[
\hat{v}_{κσ} = n_σ(k + p) - n_σ(k + p),
\]

where \(\hat{w}(∥q∥)\) stands for the \(N\)-particle GS of \(\hat{H}\),

\[
\hat{v}_{κσ} = -\frac{1}{Ω} \sum_{σ'} \sum_{p',q'} \hat{w}(∥q'∥) \nonumber
\]
From this, Eq. (6) and the results in Eqs. (18) and (17), one readily deduces that (cf. Eq. (56) in [6])
\[
n_{\sigma}(k)\varepsilon_{k;\sigma}^\leq + (1 - n_{\sigma}(k))\varepsilon_{k;\sigma}^\geq = \varepsilon_k + \hbar \Sigma_{\sigma}(k).
\]
(18)

This result will prove useful in our later considerations in this paper.

By introducing the decomposition
\[
\beta_{k;\sigma} = n_{\sigma}(k)\xi_{k;\sigma},
\]
(19)
which implies no restriction so long as \(n_{\sigma}(k) \neq 0\), one can express \(\varepsilon_{k;\sigma}^\leq\), introduced in Eq. (6) above, as follows:
\[
\varepsilon_{k;\sigma}^\leq = \varepsilon_k + g \xi_{k;\sigma}.
\]
(20)

From this, Eq. (6) and the results in Eqs. (18) and (17), one similarly has
\[
\varepsilon_{k;\sigma}^\geq = \varepsilon_k + g \frac{\partial_{k;\sigma} - n_{\sigma}(k)\xi_{k;\sigma}}{1 - n_{\sigma}(k)}.
\]
(21)

From the expression in Eq. (5) above and the ensuing details (see the text subsequent to Eq. (6)) one infers the following relationships from the expressions in Eqs. (20) and (21) (for \(k;\sigma \in S_{\sigma}\))
\[
\xi_{k;\sigma} \sim \frac{1}{g}(\varepsilon_k - \varepsilon_{k;\sigma}), \quad k \rightarrow k_F;\sigma,
\]
(22)
\[
\partial_{k;\sigma} \sim \frac{1}{g}(\varepsilon_k - \varepsilon_{k;\sigma}), \quad k \rightarrow k_F;\sigma.
\]
(23)

In other words, to the leading order in \((k - k_F;\sigma)\), one has
\[
\xi_{k;\sigma} \sim \partial_{k;\sigma} \quad \text{for} \quad k \rightarrow S_{\sigma}.
\]
(24)

Note that here, as well as in Eqs. (22) and (23), \(S_{\sigma}\) is considered as given, so that the expressions in these equations reflect some properties of \(S_{\sigma}\) rather than necessarily fully defining it.

In analogy with the expression in Eq. (19) above, we introduce the auxiliary function \(\eta_{k;\sigma}\), satisfying
\[
n_{\sigma}(k)\eta_{k;\sigma} = \partial_{k;\sigma} - \frac{1}{g}(\varepsilon_k - \varepsilon_{k;\sigma}).
\]
(25)

This expression is general for all \(k\) for which \(n_{\sigma}(k) \neq 0\). In the light of Eq. (23), and since, for interacting GSs, \(n_{\sigma}(k) \neq 0\) in a neighbourhood of \(S_{\sigma}\) (see later), we must have
\[
\eta_{k;\sigma} \sim 0 \quad \text{for} \quad k \rightarrow S_{\sigma}.
\]
(26)

Defining \(\zeta_{k;\sigma}\) as follows
\[
\zeta_{k;\sigma} := \frac{1}{g}(\varepsilon_k - \varepsilon_{k;\sigma})
\]
(27)
on account of Eq. (22) we similarly have
\[
\zeta_{k;\sigma} \sim 0 \quad \text{for} \quad k \rightarrow S_{\sigma}.
\]
(28)

On the basis of the above expressions, from Eqs. (20) and (21) for \(k \rightarrow k_F;\sigma \in S_{\sigma}\) we deduce
\[
\varepsilon_{k;\sigma}^\geq \sim \mu + a(k_F;\sigma) \cdot (k - k_F;\sigma) + g \zeta_{k;\sigma},
\]
(29)
\[
\varepsilon_{k;\sigma}^\leq \sim \mu + a(k_F;\sigma) \cdot (k - k_F;\sigma) - g \Lambda_{\sigma}(k(\zeta_{k;\sigma} - \eta_{k;\sigma})),
\]
(30)
where
\[
a(k_F;\sigma) := \nabla_k \varepsilon_k \bigg|_{k = k_F;\sigma},
\]
(31)
\[
\Lambda_{\sigma}(k) := \frac{n_{\sigma}(k)}{1 - n_{\sigma}(k)}.
\]
(32)

In Eqs. (29) and (30), \(\mu\) stands for the ‘chemical potential’ which for metallic states is infinitesimally greater than the Fermi energy \(\varepsilon_F\) (for details see [6,78]).

Making use of the equation of motion for the operator \(\hat{c}_{k;\sigma}\) in the Heisenberg picture, that is
\[
\frac{i\hbar}{\partial t}\hat{c}_{k;\sigma}(t) = \left[\hat{c}_{k;\sigma}(t), \hat{H}\right],
\]
(33)
from the defining expression in Eq. (8), one obtains
\[
\beta_{k;\sigma}^\leq = \frac{1}{g}\left\{\frac{\partial}{\partial t}G_{\sigma}(k; t - t') \bigg|_{t' = t} - \varepsilon_k n_{\sigma}(k)\right\},
\]
(34)
where the single-particle Green function in the time domain is defined as follows:
\[
G_{\sigma}(k; t - t') := -i \langle \Psi_N;0 | T\{\hat{c}_{k;\sigma}(t)\hat{c}_{k;\sigma}^\dagger(t')\} | \Psi_N;0 \rangle,
\]
(35)
in which \(T\) stands for the fermion time-ordering operator. We have (below \(\eta \downarrow 0\))
\[
\frac{\hbar}{\partial t}G_{\sigma}(k; t - t') \bigg|_{t' = t} = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} \varepsilon e^{i\varepsilon/\hbar} G_{\sigma}(k; \varepsilon)
\]
(36)
\[
= \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} \varepsilon G_{\sigma}(k; \varepsilon),
\]
where \(A_{\sigma}(k; \varepsilon)\) stands for the single-particle spectral function, defined in terms of \(G_{\sigma}(k; z)\), the analytic continuation of \(G_{\sigma}(k; \varepsilon)\) is \(\lim_{\eta \downarrow 0} G_{\sigma}(k; \varepsilon \pm i\eta)\), \(\varepsilon \sim \mu\), as follows:
\[ A_\sigma(k; \varepsilon) := \frac{1}{2\pi i} \{ \bar{G}_\sigma(k; \varepsilon - i\eta) - \bar{G}_\sigma(k; \varepsilon + i\eta) \}, \quad \eta \downarrow 0. \quad (37) \]

With (see Eq. (10) above)
\[ n_\sigma(k) = \frac{1}{\hbar} \int_{-\infty}^{\mu} d\varepsilon A_\sigma(k; \varepsilon), \quad (38) \]
from Eqs. (19), (34), (36) and (38) we deduce that
\[ \xi_{k;\sigma} = \frac{\beta^{\langle}_{k;\sigma}}{\nu^{\langle}_{\sigma}(k)} = \frac{1}{\hbar} \left\{ \int_{-\infty}^{\mu} d\varepsilon A_\sigma(k; \varepsilon) \right\} - \varepsilon_k, \quad (39) \]
which in combination with Eq. (22) leads to
\[ \frac{\int_{-\infty}^{\mu} d\varepsilon A_\sigma(k; \varepsilon)}{\int_{-\infty}^{\mu} d\varepsilon A_\sigma(k; \varepsilon)} \sim \varepsilon_f \quad \text{for} \quad k \to k_{F;\sigma} \in S_{F;\sigma}. \quad (40) \]

With
\[ Z_{k_{F;\sigma}} := n_\sigma(k_{F;\sigma}^-) - n_\sigma(k_{F;\sigma}^+), \quad (41) \]
from Eqs. (38) and (40) we obtain
\[ Z_{k_{F;\sigma}} = \frac{1}{\hbar} \int_{-\infty}^{\mu} d\varepsilon \left[ A_\sigma(k_{F;\sigma}^-; \varepsilon) - A_\sigma(k_{F;\sigma}^+; \varepsilon) \right], \quad (42) \]
which is alternative to the standard expression
\[ Z_{k_{F;\sigma}} = \frac{1}{\hbar} \int_{-\infty}^{\mu} d\varepsilon \left[ A_\sigma(k_{F;\sigma}^-; \varepsilon) - A_\sigma(k_{F;\sigma}^+; \varepsilon) \right], \quad (43) \]
directly obtained from the spectral representation of \( n_\sigma(k) \) in Eq. (38) above. The expression in Eq. (42) has been explicitly derived in [6] for the uniform metallic GSs of the single-band Hubbard Hamiltonian. Here as in [6] the single-particle energies \( \varepsilon_{k;\sigma}^{\langle} \) (associated with some fictitious particles [6]) correspond to the single-particle spectral function \( A_\sigma(k; \varepsilon) \), for which we have [6]
\[ A_\sigma(k; \varepsilon) = \hbar \{ \nu^{\langle}_{\sigma}(k) \delta(\varepsilon - \varepsilon_{k;\sigma}^{\langle}) + \nu^{\rangle}_{\sigma}(k) \delta(\varepsilon - \varepsilon_{k;\sigma}^{\rangle}) \}. \quad (44) \]

It is readily verified that the exact \( Z_{k_{F;\sigma}} \) is obtained by replacing \( A_\sigma(k; \varepsilon) \) in Eqs. (42) and (43) by \( A_\sigma(k; \varepsilon) \). In this connection note that, for stable (uniform) GSs, \( \varepsilon_{k;\sigma}^{\langle} \geq \mu \), \( \forall k \) [6]. The GS total energy of the interacting system is similarly exactly reproduced by replacing \( A_\sigma(k; \varepsilon) \) in the pertinent expression (see Eq. (41) in [6]) by \( A_\sigma(k; \varepsilon) \).

\[ S_{F;\sigma} := \{ k \parallel \varepsilon_k + \hbar \Sigma_\sigma(k; \varepsilon) = \varepsilon_f \}. \quad (45) \]

where, on general grounds, \( \text{Im}[\Sigma_\sigma(k; \varepsilon)] \equiv 0 \), \( \forall k \) [81,67,8]. From Eqs. (17) and (23) we deduce
\[ \varepsilon_k + \hbar \Sigma^{\text{HF}}_\sigma(k) = \varepsilon_f \quad \text{for} \quad k \in S_{F;\sigma}. \quad (46) \]

Comparison of this expression with the defining expression for \( S_{F;\sigma} \) in Eq. (45) reveals that to the leading order in \( (k - k_{F;\sigma}) \) we must have
\[ \Sigma_\sigma(k; \varepsilon) \sim \Sigma^{\text{HF}}_\sigma(k) \quad \text{as} \quad k \to k_{F;\sigma} \in S_{F;\sigma}. \quad (47) \]

The significance of this expression becomes more apparent by considering the Kramers-Kröning relation for \( \text{Re}[\Sigma_\sigma(k; \varepsilon)] \) in terms of \( \text{Im}[\Sigma_\sigma(k; \varepsilon)] \); since \( [82,78] \)
\[ \Sigma_\sigma(k; \varepsilon) - \Sigma^{\text{HF}}_\sigma(k) = o(1) \quad \text{for} \quad |\varepsilon| \to \infty, \quad (48) \]
the above-mentioned Kramers-Kröning relation reads
\[ \text{Re}[\Sigma_\sigma(k; \varepsilon)] = \Sigma^{\text{HF}}_\sigma(k) \]
\[ -\frac{\hbar}{\pi} \int_{-\infty}^{\infty} \frac{d\varepsilon'}{\varepsilon'} \text{sgn}(\mu - \varepsilon') \text{Im}[\Sigma_\sigma(k; \varepsilon')] \]. \quad (49) \]

From the leading term in the asymptotic series of the integral on the RHS of Eq. (49) for \( \varepsilon \to \varepsilon_f \), making use of the fact that \( \text{Im}[\Sigma_\sigma(k; \varepsilon)] \sim 0 \) as \( \varepsilon \to \varepsilon_f \), we obtain \([82]\)
\[ \Sigma_\sigma(k; \varepsilon) = \Sigma^{\text{HF}}_\sigma(k) + S_\sigma(k), \quad (50) \]
where
\[ S_\sigma(k) := \frac{1}{\pi} \int_{0}^{\infty} \frac{d\varepsilon}{\varepsilon} \text{Im}[\Sigma_\sigma(k; \varepsilon_f + \varepsilon) + \Sigma_\sigma(k; \varepsilon_f - \varepsilon)]. \quad (51) \]

Comparison of Eq. (47) with Eq. (50) reveals the necessity of the condition
\[ S_\sigma(k) = 0 \quad (52) \]
in order for \( k \in S_{F;\sigma} \). In the light of the results in Eqs. (47) and (50), we thus arrive at the following alternative defining expression for \( S_{F;\sigma} \) (cf. Eq. (45) above):
\[ S_{F;\sigma} = \{ k \parallel \varepsilon_k + \hbar \Sigma^{\text{HF}}_\sigma(k) = \varepsilon_f \land S_\sigma(k) = 0 \}. \quad (53) \]

The necessity of the additional condition \( S_\sigma(k) = 0 \) in the defining expression for \( S_{F;\sigma} \) stems from the fact that the equation in Eq. (46) applies for all \( k \) on a pre-supposed \( S_{F;\sigma} \), so that, in general Eq. (46) cannot be sufficient fully to define \( S_{F;\sigma} \). The significance of this aspect can be easiest appreciated by specializing Eq. (46) to the uniform metallic GSs of the single-band Hubbard Hamiltonian, in which case \( \Sigma^{\text{HF}}_\sigma(k) \) is independent of \( k \) and equal to \( \frac{1}{\hbar} \cdot \frac{\Sigma^{\text{HF}}_\sigma(k)}{n_\sigma} \) (see Eqs. (12), (17) and (4) above). The sufficiency of \( \varepsilon_k + \hbar \Sigma^{\text{HF}}_\sigma(k) = \varepsilon_f \) to define \( S_{F;\sigma} \) would in the

§ 3. EQUATIONS DETERMINING THE FERMI SURFACES OF UNIFORM METALLIC GROUND STATES

The Fermi surface \( S_{F;\sigma} \) is conventionally defined as follows \([79,80,6]\)
present case incorrectly imply that all solutions of the latter equation, which constitute the entire $S^{(0)}_{\sigma}$ (the Fermi surface corresponding to $\varepsilon_{k}$ and the partial number $N_{\sigma}$ of fermions with spin index $\sigma$ in the exact interacting GS), were in general points located on $S_{\sigma}$; the unconditional equality $S_{\sigma} = S^{(0)}_{\sigma}$, rather than the relationship $S_{\sigma} \subseteq S^{(0)}_{\sigma}$ deduced in [6], would rule out the feasibility that the pseudogap phenomenon is described in the space spanned by the uniform metallic GSs of the single-band Hubbard Hamiltonian [6], contradicting the results in [83–87]. Note that for isotropic GSs the condition $S_{\sigma}(k) = 0$ is automatically satisfied at any $k$ for which Eq. (46) is satisfied, on account of the fact that the metallic nature of a GS implies that $S_{\sigma}(\pm k) = 0$ for at least one $k$ (and all points related to this by symmetry) on $S_{\sigma}$, which by isotropy must remain valid for all $k$ on $S_{\sigma}$.

We note that along the lines of reasoning as in [6] it can be shown that $n_{\sigma}(k)$ is continuous (see Eq. (67) in [6]) at all $k$ which satisfy Eq. (46) but fail to satisfy Eq. (52). We further note that, since for $k \in S_{\sigma}$ up to infinitesimal corrections [6] we have $\varepsilon_{k,\sigma} = \varepsilon_{k,\sigma} = \varepsilon_{\sigma}$, Eq. (18) is seen to conform with the result in Eq. (46) above.

It is interesting to rewrite the condition $S_{\sigma}(k) = 0$ for $k \in S_{\sigma}$ in the following appealing form:

$$
\int_{-\infty}^{\varepsilon_{\sigma}} d\varepsilon \frac{\mathrm{Im}[\Sigma_{\sigma}(k; \varepsilon)]}{\varepsilon_{\sigma} - \varepsilon} = \int_{\varepsilon_{\sigma}}^{\infty} d\varepsilon \frac{\mathrm{Im}[\Sigma_{\sigma}(k; \varepsilon)]}{\varepsilon_{\sigma} - \varepsilon}, \quad k \in S_{\sigma}.
$$

(54)

The integrands on both sides of this expression are non-negative over the pertinent ranges of integration. In the light of this and of the inherent symmetry of these integrands for both $|\varepsilon - \varepsilon_{\sigma}| \to 0$ and $|\varepsilon - \varepsilon_{\sigma}| \to \infty$ (to the leading orders in $(\varepsilon - \varepsilon_{\sigma})$ and $1/(\varepsilon - \varepsilon_{\sigma})$ respectively [78]), Eq. (54) can be viewed as implying some degree of similarity between $|\mathrm{Im}[\Sigma_{\sigma}(k; \varepsilon - \varepsilon_{\sigma})]|$ and $|\mathrm{Im}[\Sigma_{\sigma}(k; \varepsilon_{\sigma} + \varepsilon)]|$ at intermediate values of $\varepsilon$ (as measured with respect to $\varepsilon_{\sigma}$) when $k \in S_{\sigma}$; for $k \not\in S_{\sigma}$, this similarity should be, if not absent, less pronounced. We point out that since $S_{\sigma}(k) = 0$ applies for all $k \in S_{\sigma}$, in principle one has (see later)

$$
\nabla_{k'} S_{\sigma}(k') \big|_{k' = k} = \lambda_{\sigma}(k) \hat{n}(k) \quad \text{for} \quad k \in S_{\sigma},
$$

(55)

where $\hat{n}(k)$ stands for the (outward) unit vector normal to $S_{\sigma}$ at $k \in S_{\sigma}$; here $k^{-}$ and $k^{+}$ denote vectors infinitesimally close to $k$, with the former inside and the latter outside the Fermi sea, and $\lambda_{\sigma}(k)$ stands for a scalar function which cannot be identically vanishing. For conciseness, in this work we shall denote the Fermi sea corresponding to fermions with spin index $\sigma$ by $F_{\sigma}$ and its complementary part with respect to the entire available reciprocal space, by $F_{\sigma}$ [6].

In writing the expression in Eq. (55) we have taken account of the fact that $S_{\sigma}(k)$ may not be continuously differentiable in a neighbourhood of some or all points $k \in S_{\sigma}$ (whence $k^{-}$ and $k^{+}$); however, in Eq. (55) we have not taken account of the possibility that $S_{\sigma}(k)$ may not be differentiable in a neighbourhood of $k \in S_{\sigma}$. The latter possibility in fact arises when, for instance, fermions in $d$ spatial dimensions interact through the long-range Coulomb potential, in which case $\nabla_{k} S_{\sigma}(k)$ is logarithmically divergent for $k$ approaching any point $k_{\sigma}$ on $S_{\sigma}$ (both from inside and from outside the Fermi sea). It follows that, for metallic states of systems of Coulomb-interacting fermions for which quasiparticles are well-defined in the neighbourhood of $S_{\sigma}$, the above-mentioned singularity of $\nabla_{k} S_{\sigma}(k)$ must be fully cancelled by a singular contribution arising from $\nabla_{k} S_{\sigma}(k)$ (see Eq. (50) above), so that, for these metallic states, Eq. (55) cannot be meaningful.

§ 4. EXPOSING A FURTHER CLOSE RELATIONSHIP BETWEEN $\Sigma_{\sigma}(k; \varepsilon_{\sigma})$ AND $S_{\sigma}$

The fact that, for $k \to k_{\sigma}$ (see Eq. (47) above), $S_{\sigma}(k; \varepsilon_{\sigma}) \sim \Sigma_{\sigma}^{\text{up}}(k)$ to leading order in $(k - k_{\sigma})$ (see Eq. (47) above), deserves some closer inspection. From Eqs. (12), (16) and (17) it is evident that $\Sigma_{\sigma}^{\text{up}}(k)$ is fully determined by $n_{\sigma}(k)$. For uniform GSs this function is the Fourier transform of the single-particle density matrix $g_{\sigma}(r - r')$, or

$$
\frac{1}{(2\pi)^{d}} \int \frac{d^{d}k}{(2\pi)^{d}} e^{ik \cdot r} n_{\sigma}(k).
$$

(56)

The singular nature of $n_{\sigma}(k)$ for $k \in S_{\sigma}$ has far-reaching consequences for the behaviour of $g_{\sigma}(r)$ for $||r|| \to \infty$ [90,6] and consequently for that of $\Sigma_{\sigma}^{\text{up}}(k)$ for $k$ in a
neighbourhood of $\mathcal{S}_{\pi,\sigma}$. To illustrate this aspect, it is convenient to introduce
\[ \hat{\mathbf{e}}_r := \frac{\mathbf{r}}{r} \quad \text{where} \quad r := \| \mathbf{r} \|. \tag{57} \]

Without loss of generality, we explicitly consider the case when $d = 2$ and assume that the angle $\varphi$ in the cylindrical coordinates $(k, \varphi)$ of $\mathbf{k}$ is measured with respect to the direction specified by $\hat{\mathbf{e}}_r$. We thus re-write Eq. (56) as follows:
\[ \varrho_{\sigma}(r) = \frac{1}{(2\pi)^2} \int_0^\infty dk \, k \mathcal{I}_\sigma(k, r), \tag{58} \]

where
\[ \mathcal{I}_\sigma(k, r) := \int_0^{2\pi} d\varphi \, e^{ikr \cos(\varphi)} \tilde{n}_\sigma(k, \varphi), \tag{59} \]
in which $\tilde{n}_\sigma(k, \varphi) \equiv n_\sigma(k)$. Making use of the stationary-phase method [89], we readily obtain
\[ \mathcal{I}_\sigma(k, r) \sim 2 \sqrt{\frac{2\pi}{kr}} \tilde{n}_\sigma(k \hat{\mathbf{e}}_r) \cos(kr - \pi/4), \quad r \to \infty, \tag{60} \]

where we have made use of the fact that by the time-reversal symmetry of the GS,
\[ \tilde{n}_\sigma(k, \pi) = \tilde{n}_\sigma(k, 0) \equiv n_\sigma(k \hat{\mathbf{e}}_r). \tag{61} \]

Thus, from Eqs. (58) and (60) we have
\[ \varrho_{\sigma}(r \hat{\mathbf{e}}_r) \sim \frac{2}{(2\pi)^{3/2} r^{1/2}} \int_0^\infty dk \, k^{1/2} n_\sigma(k \hat{\mathbf{e}}_r) \times \cos(kr - \pi/4), \quad r \to \infty. \tag{62} \]

Let $k_{F,\sigma}$ point in the direction of $\mathbf{r}$, i.e. $k_{F,\sigma} = k_{F,\sigma} \hat{\mathbf{e}}_r$. The singular nature of $n_\sigma(k \hat{\mathbf{e}}_r)$ at $k = k_{F,\sigma}$ implies that for the further simplification of the expression on the RHS of Eq. (62) it is necessary [78] to express the $k$ integral over $[0, \infty)$ in terms of at least two $k$ integrals over the disjoint intervals $[0, k_{F,\sigma})$ and $(k_{F,\sigma}, \infty)$; this subdivision should be carried out for all $k$ points at which $n_\sigma(k \hat{\mathbf{e}}_r)$ is singular; however, to avoid any complication unnecessary to our present considerations, here we deal with the case where the most dominant singularity of $n_\sigma(k \hat{\mathbf{e}}_r)$ is located at $k = k_{F,\sigma}$. Assuming $n_\sigma(k \hat{\mathbf{e}}_r)$ to be discontinuous at $k = k_{F,\sigma}$ and continuous elsewhere, through integration by parts, from Eq. (62) we obtain [90,78]
\[ \varrho_{\sigma}(r \hat{\mathbf{e}}_r) \sim \frac{Z_{k_{F,\sigma} \hat{\mathbf{e}}_r} \nu_{1/2}}{2^{1/2} \pi^{3/2}} \frac{\sin(k_{F,\sigma} r - \pi/4)}{r^{3/2}} 
+ \frac{n_\sigma(k \hat{\mathbf{e}}_r) \nu_{1/2}}{2^{1/2} \pi^{3/2}} \frac{\sin(kr - \pi/4)}{r^{3/2}}, \quad r \to \infty, \tag{63} \]

where for systems defined on lattice $k \hat{\mathbf{e}}_r$ denotes the vector from the origin to the Brillouin zone boundary (note that for these systems our assumption with regard to the uniformity of the underlying GSs implies that we should only consider $r \in \{ R_j \mid j = 1, \ldots, N_i \}$ and for those defined on the continuum $k = \infty$ so that $n_\sigma(k \hat{\mathbf{e}}_r) = 0$; for the former systems and for a given $\hat{\mathbf{e}}_r$, $n_\sigma(k \hat{\mathbf{e}}_r)$ may or may not be vanishing. In what follows, for simplicity we set $n_\sigma(k \hat{\mathbf{e}}_r)$ equal to zero. One observes that the full information concerning the shape and dimensions of $\mathcal{S}_{\pi,\sigma}$ is already contained in the leading-order term in the large-$\|r\|$ asymptotic series of $\varrho_{\sigma}(r)$.

For the Fock part $\Sigma^F_{\sigma}$ of the self-energy in the coordinate representation and for arbitrary GSs and two-body interaction functions $v(\mathbf{r} - \mathbf{r}')$ we have [78]
\[ \Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}') = -\frac{1}{\hbar} v(\mathbf{r} - \mathbf{r}') \varrho_{\sigma}(\mathbf{r}', r), \tag{64} \]

where in the case of uniform GSs $\varrho_{\sigma}(\mathbf{r}', r)$ is to be replaced by $\varrho_{\sigma}^{\pi}(\mathbf{r} - \mathbf{r})$. It follows that the information concerning $\mathcal{S}_{\pi,\sigma}$ contained in $\varrho_{\sigma}(\mathbf{r}, \mathbf{r}')$ is similarly contained in $\Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}')$. In particular, for any two-body potential other than those for which $v(\mathbf{r} - \mathbf{r}') \equiv 0$ when $\|\mathbf{r} - \mathbf{r}'\| \geq R > 0$, the behaviour of $\varrho_{\sigma}(\mathbf{r}, \mathbf{r}')$ for $||\mathbf{r} - \mathbf{r}'|| \to \infty$ directly determines that of $\Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}')$ for $||\mathbf{r} - \mathbf{r}'|| \to \infty$. For instance, for the uniform GSs of systems of particles in two-dimensional space (i.e. for $d = 2$) interacting through the Coulomb potential and for which $n_\sigma(k \hat{\mathbf{e}}_r)$ is discontinuous at $k = k_{F,\sigma}$, from Eqs. (63) and (64) we have (following our above convention, for uniform GSs we use the notation $\Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}')$ for what in the general case is denoted by $\Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}')$)
\[ \Sigma^F_{\sigma}(\mathbf{r}, \mathbf{r}') \sim \frac{e^2}{\hbar} \frac{Z_{k_{F,\sigma} \hat{\mathbf{e}}_r} \nu_{1/2}}{(2\pi)^{3/2} \epsilon_0} \frac{\sin(k_{F,\sigma} r - \pi/4)}{r^{3/2}}, \quad r \to \infty, \tag{65} \]

where $e^2$ stands for the particle-charge squared and $\epsilon_0$ for the vacuum permittivity (note that for $-e$ the electron charge, $e^2/\hbar = 3.874 \ldots \times 10^{-5}$ S is the quantized Hall conductance). 10 The fact that the oscillatory be-
haviour of the leading term in the asymptotic series of \( \Sigma_\nu^\sigma (r\hat{e}_r) \) for \( r \to \infty \) is entirely determined by \( k_{\nu,\sigma} \) indicates that, similar to \( n_\sigma (k) \), \( \Sigma_\nu^\nu (k) \) must be singular for all \( k \) on \( S_{\nu,\sigma} \); in the present case, where \( \Sigma_\nu^\nu (r\hat{e}_r) \) decays with one power of \( 1/r \) faster than \( g_\sigma (r\hat{e}_r) \) for \( r \to \infty \), the assumed discontinuity of \( n_\sigma (k) \) at \( k = k_{\nu,\sigma} \) implies singularity (explicitly, a logarithmic divergence in the behaviour of \( \nabla_k \Sigma_\nu^\nu (k) \) at \( k = k_{\nu,\sigma} \). These facts expose a fundamental distinction between systems of fermions interacting through potentials of finite range and potentials of infinite range. Notably, whereas for the uniform metallic GSs of the single-band Hubbard Hamiltonian one has \( n_\sigma (k) \geq \frac{1}{2} \) for \( k \) inside the Fermi sea and infinitesimally close to \( S_{\nu,\sigma} \), as we show later in this paper (§ 5), this is not necessarily the case when the interaction potential is of longer range than the intra-atomic potential encountered in the Hubbard Hamiltonian. In this connection, recall that for the uniform metallic GSs of the conventional single-band Hubbard Hamiltonian, \( \Sigma_\nu^{\nu} (k) = \frac{1}{\hbar} Un_\sigma \), which is independent of \( k \) and thus regular for all \( k \in 1BZ \).

It is important to point out that \( n_\sigma (k) \) is singular (not necessarily discontinuous) at all \( k \) satisfying Eq. (46) above. However, since according to Eq. (53) the satisfaction of Eq. (46) at a given \( k \) is not sufficient for \( k \in S_{\nu,\sigma} \), it follows that the \( k \) that for a given direction \( \hat{e}_r \) determines the leading term in the large-\( r \) asymptotic series of \( g_\sigma (r\hat{e}_r) \) (and of \( \Sigma_\nu^\nu (r\hat{e}_r) \)) is not necessarily a point of \( S_{\nu,\sigma} \). Since such a \( k \) point satisfies Eq. (46) but fails to satisfy Eq. (52), it follows that at this point \( n_\sigma (k) \) is continuous (see the paragraph preceding that containing Eq. (54) above) whereby the leading term in the large-\( r \) asymptotic series of \( g_\sigma (r\hat{e}_r) \) (and of \( \Sigma_\nu^\nu (r\hat{e}_r) \)) acquires an anomalous exponent, leading to a stronger power-law decay in the mentioned asymptotic term in comparison with the case corresponding to \( Z_{k\nu,\sigma} \neq 0 \) for \( k\hat{e}_r \in S_{\nu,\sigma} \); with reference to the expressions in Eqs. (63) and (65) above (where \( k = k_{\nu,\sigma} \), the above-indicated anomalous exponent would read \( 3/2 + \gamma \) and \( 5/2 + \gamma \) respectively, with \( \gamma > 0 \).

\[ n_\sigma := \frac{N_\sigma}{\Omega}. \]

With \( n := n_\sigma + n_{\bar{\sigma}} \), the total concentration of the fermions in the \( N \)-particle uniform GS of the system, we define the spin magnetization fraction \( m \) as follows

\[ m := \frac{n_\sigma - n_{\bar{\sigma}}}{n}. \]

Denoting by \( E(N, M) \) the GS total energy of the system described by the \( \hat{H} \) in Eq. (1), corresponding to the total number of particles \( N = \Omega n \) and the total spin magnetization \( M = \Omega (n_\sigma - n_{\bar{\sigma}}) \), we define

\[ \mathcal{E} (n, m) := \frac{1}{N} E(N, M), \]

which we assume to be a sufficiently smooth function of \( n \) and \( m \) in the thermodynamic limit [91] (appendix B herein). In this limit, for a metallic GS we have

\[ \varepsilon_\nu = \frac{\partial}{\partial n} (n\mathcal{E}(n, m)). \]

From this we obtain

\[ \frac{d}{dn_\alpha} (n\mathcal{E}(n, m)) = \varepsilon_\nu - (m \mp 1) \frac{\partial \mathcal{E}(n, m)}{\partial m}, \quad \alpha = \{ \sigma, \bar{\sigma} \}. \]

We now decompose \( \mathcal{E}(n, m) \) as follows:

\[ \mathcal{E}(n, m) \equiv \mathcal{E}_k(n, m) + \mathcal{E}_{xc}(n, m), \]

where \( \mathcal{E}_k(n, m) \), the ‘kinetic energy’ contribution to \( \mathcal{E}(n, m) \), corresponds to the GS of \( \hat{H}_0 \) in Eq. (80) below whose associated \( n \) and \( m \) are constrained to be the same as those pertaining to the exact GS of \( \hat{H} \). Thus, Eq. (71) defines the exchange-correlation energy contribution \( \mathcal{E}_{xc}(n, m) \). By the assumption of the isotropy of the GSs under consideration and in consequence of a Luttinger theorem [92], according to which the number of \( k \) points enclosed by \( S_{\nu,\sigma} \) and \( S_{\nu,\bar{\sigma}} \) are equal, we have \( S_{\nu,\sigma} = S_{\nu,\bar{\sigma}} = S_{\nu,\sigma}^{(0)}, \forall \sigma \). From this and in analogy with the result in Eq. (70) we have

\[ \mathcal{E}(n, m) \equiv \mathcal{E}_k(n, m) + \mathcal{E}_{xc}(n, m), \]
\[
\frac{d}{dn_\alpha}(n\tilde{E}_k(n, m)) = \varepsilon_{k,\alpha} - (m + 1)\frac{\partial E_k(n, m)}{\partial m}, \quad \alpha = \{\sigma, \bar{\sigma}\}. \tag{72}
\]

Combining the expressions in Eqs. (70), (71) and (72), for the exchange-correlation potential \(\mu_{xc;\sigma}\), defined through
\[
\mu_{xc;\alpha} := \frac{d}{dn_\alpha}(n\tilde{E}_{xc}(n, m)), \quad \alpha \in \{\sigma, \bar{\sigma}\}, \tag{73}
\]
we deduce that
\[
\mu_{xc;\alpha} = \varepsilon_{\sigma} - \varepsilon_{k,\alpha} - (m + 1)\frac{\partial E_{xc}(n, m)}{\partial m}, \quad \alpha = \{\sigma, \bar{\sigma}\}. \tag{74}
\]

By subtracting \(\mu_{xc;\bar{\sigma}}\) from \(\mu_{xc;\sigma}\), employing the expression in Eq. (74), we obtain
\[
\frac{\partial E_{xc}(n, m)}{\partial m} = \frac{1}{2}(\varepsilon_{k,\sigma;\sigma} - \varepsilon_{k,\sigma;\bar{\sigma}}), \tag{75}
\]
where
\[
\varepsilon_{k,\alpha} := \varepsilon_k + \mu_{xc;\alpha}, \quad \alpha = \{\sigma, \bar{\sigma}\}. \tag{76}
\]

From Eq. (75) we infer that in a paramagnetic state, where \(\varepsilon_{k,\alpha} \equiv \varepsilon_{k,\bar{\sigma}}\), we must have
\[
\frac{\partial E_{xc}(n, m)}{\partial m} = 0 \quad \text{(for paramagnetic states)} \tag{77}
\]
From Eqs. (74) and (77), for paramagnetic states we thus obtain
\[
\varepsilon_{\sigma} = \varepsilon_{k,\sigma} + \mu_{xc;\sigma} \equiv \varepsilon_{\sigma}^{(0)} + \mu_{xc;\sigma}, \quad \forall \sigma \quad (k_{\sigma;\sigma} \in S_{\sigma;\sigma}), \tag{78}
\]
which is a well-known theorem due to Seitz [93].

A result which from the perspective of our present work is of special interest is
\[
\mu_{xc;\alpha} = \hbar \Sigma^{HF}_\alpha(k_{\sigma;\sigma}) - (m + 1)\frac{\partial E_{xc}(n, m)}{\partial m}, \quad \alpha = \{\sigma, \bar{\sigma}\}, \tag{79}
\]
which is deduced through comparing Eqs. (46) and (74). For completeness, the non-interacting Hamiltonian
\[
\hat{H}_0 := \sum_{k,\sigma} \varepsilon_{k,\sigma} \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma}, \tag{80}
\]
with \(\varepsilon_{k,\sigma}\) as defined in Eq. (76) above, is the so-called Kohn-Sham Hamiltonian [76] encountered within the framework of the GS density-functional theory due to Hohenberg and Kohn [75] (for a review see [77]).

By repeating the above considerations in terms of the GS energy per particle \(\tilde{E}(n)\) (an explicit function of solely the total concentration \(n\) and not of the spin magnetization fraction \(m\)), and thus by introducing, analogously as in Eq. (71) above, the energy functions \(\tilde{E}_k(n)\) and \(\tilde{E}_{xc}(n)\) satisfying \(\tilde{E}_k(n) + \tilde{E}_{xc}(n) \equiv \tilde{E}(n)\), we arrive at (cf. Eq. (78))
\[
\varepsilon_{\sigma} = \varepsilon_{\sigma}^{(0)} + \mu_{xc}, \tag{81}
\]
in which \(\varepsilon_{\sigma}^{(0)}\) stands for the Fermi energy of the underlying paramagnetic non-interacting \(N\)-particle GS, and (cf. Eq. (73))
\[
\mu_{xc} := \frac{d}{dn}(n\tilde{E}_{xc}(n)). \tag{82}
\]

It is observed that, for paramagnetic GSs, Eq. (81) coincides with Eq. (78). In the case at hand, the non-interacting Kohn-Sham Hamiltonian \(\hat{H}_0\) in Eq. (80) is defined in terms of the spin-degenerate energy dispersion (cf. Eq. (76) above)
\[
\varepsilon_{k} := \varepsilon_k + \mu_{xc}, \tag{83}
\]
where \(\mu_{xc}\) is defined in Eq. (82). In the light of Eq. (81), the result in Eq. (83) expresses the fact that the energy eigenvalue corresponding to the highest occupied single-particle Kohn-Sham state coincides with the exact chemical potential. Following Eq. (77), in the present case the counterpart of the expression in Eq. (79) is as follows:
\[
\mu_{xc} = \hbar \Sigma^{HF}_{\alpha}(k_{\sigma;\sigma}), \quad \forall \sigma \quad (k_{\sigma;\sigma} \in S_{\sigma;\sigma}). \tag{84}
\]

Note that, since \(\mu_{xc}\) (\(\mu_{xc;\sigma}\)) is a potential, it is determined up to an additive constant, explicitly independent of \(n\) \((n\) and \(m\)); the difference \(\mu_{xc;\sigma} - \mu_{xc;\bar{\sigma}}\) is, however, not arbitrary.

We have employed the expression in Eq. (84) specialized to the paramagnetic GS of the Coulomb-interacting uniform-electron-gas system for \(d = 3\), with \(\varepsilon_k = \hbar^2||\vec{k}||^2/(2m_e)\), where \(m_e\) stands for the bare electron mass. Decomposing \(\mu_{xc;\sigma}\) into exchange and correlation contributions, that is
\[\tag{14}\]
\[
\mu_{xc;\sigma} = \mu_{x;\sigma} + \mu_{c;\sigma}, \tag{85}
\]
in Hartree atomic units, where \(g\) is equal to unity, we have
\[
\mu_{x;\sigma} = \frac{\gamma_0}{\pi r_s} \int_0^\infty dx \ln \left| \frac{1 - x}{1 + x} \right| n^{(0)}_{\sigma}(k_{\sigma}x), \quad \forall \sigma, \tag{86}
\]
\[
\mu_{c;\sigma} = \frac{\gamma_0}{\pi r_s} \int_0^\infty dx \ln \left| \frac{1 - x}{1 + x} \right| \times \left[ n_{\sigma}(k_{\sigma}x) - n^{(0)}_{\sigma}(k_{\sigma}x) \right], \quad \forall \sigma; \tag{87}
\]

\[\text{Here and in the subsequent expressions we use the spin index } \sigma \text{ in order to avoid the confusion that often ensues on suppression of } \sigma; \text{ some workers use } n(k) \text{ to denote } n_{\sigma}(k) \text{ for paramagnetic GSs, while others employ } n(k) \text{ to denote } \sum_{\sigma} n_{\sigma}(k).\]
here the bars (such as in $\tilde{k}_F$) indicate that the respective quantities are in Hartree atomic units. In Eqs. (86) and (87), $n_\sigma^{(0)}(\tilde{k}_F x)$ stands for the momentum distribution function pertaining to the GS of the non-interacting electron-gas system (equal to 1 for $0 \leq x < 1$ and 0 for $x > 1$) and $r_s$ for the average inter-particle distance $r_0$ in units of the Bohr radius:

$$\gamma_0 := \left( \frac{9\pi}{4} \right)^{1/3} = 1.919 \ldots,$$

(88)

and $\tilde{k}_F \equiv ||\tilde{k}_{F,\sigma}||$ denotes the Fermi wave number in units of the inverse of the Bohr radius, i.e.

$$\tilde{k}_F = \frac{\gamma_0}{r_s}.$$  

(89)

Making use of the standard result

$$\int_0^1 dx \, x \ln \left| \frac{1 - x}{1 + x} \right| = -1,$$

(90)

from the expression in Eq. (86) we trivially obtain the well-known exact result

$$\bar{\mu}_{xc;\sigma} = -\gamma_0 / \pi \frac{-0.610887 \ldots}{r_s} \text{ (Hartree)}. \hspace{1cm} (91)$$

We note that for $d = 3$ (see Eq. (82) above)

$$\bar{\mu}_{xc;\sigma} = \bar{\varepsilon}_{xc} - r_s \frac{d}{3} \frac{d}{dr_s} \bar{\varepsilon}_{xc}.$$  

(92)

With $\bar{\varepsilon}_{xc} = \bar{\varepsilon}_x + \bar{\varepsilon}_c$ (cf. Eq. (85) above), in which [94]

$$\bar{\varepsilon}_x = -3\gamma_0 / 4\pi r_s,$$

(93)

from Eq. (92) we identically reproduce the result in Eq. (91).

In order to display the significance of the expression for $\bar{\mu}_{xc;\sigma}$ in Eq. (87), we employ the $n_\sigma(k)$ due to Daniel and Vosko [95] evaluated within the framework of the random-phase approximation (RPA). 15 Our numerical calculation of $\bar{\mu}_{c;\sigma}$ based on the expression in Eq. (87) and the latter GS momentum distribution function reproduces, to within the numerical accuracy of our calculation, the exact result [94]

$$\bar{\mu}_{c;\sigma} \sim \frac{1 - \ln 2}{\pi^2} \ln(r_s) \text{ (Hartree) for } r_s < 0 \hspace{1cm} (94)$$

(Figs. 1 and 2). This result implies that for $r_s \downarrow 0$ the integral on the RHS of Eq. (87) approaches zero like $r_s \ln(r_s)$. The fact that the latter integral should be vanishing for $r_s \downarrow 0$ can be understood by the observation that $r_s$ is proportional to the coupling constant of interaction so that, for $r_s \downarrow 0$, $n_\sigma(k) - n_\sigma^{(0)}(k)$ should indeed approach zero for all $k$. However, the above-mentioned behaviour of the integral on the RHS of Eq. (87) very crucially depends on the precise way in which $n_\sigma(k)$ approaches $n_\sigma^{(0)}(k)$ for $r_s \downarrow 0$; even the slightest deviation of $n_\sigma(k)$ from the exact $n_\sigma(k)$ for $r_s \downarrow 0$ can significantly alter the behaviour of the latter integral for $r_s \downarrow 0$ and consequently of $\bar{\mu}_{c;\sigma}$. We suggest therefore that any parametrized form of $n_\sigma(k)$ should be required to reproduce a pre-determined $\bar{\mu}_{c;\sigma}$ through the expression in Eq. (87). To illustrate the significance of this aspect, by employing the expression in Eq. (92) above we have determined $\bar{\mu}_{c;\sigma}$ through use of an interpolation expression for $\bar{\varepsilon}_{xc;\sigma}$ [97,98] based on quantum Monte Carlo calculations [99] for the Coulomb-interacting uniform-electron-gas system at a number of densities. Comparison of this $\bar{\mu}_{c;\sigma}$ with the $\bar{\mu}_{c;\sigma}$ obtained through Eq. (87) in conjunction with $n^{\text{RPA}}_{\alpha\sigma}(k)$, reveals that to the numerical accuracy of our calculations the two results up to an unimportant additive constant (independent of $r_s$) coincide for small values of $r_s$ where $n^{\text{RPA}}_{\alpha\sigma}(k) - n^{(0)}_{\alpha\sigma}(k)$ constitutes the leading asymptotic contribution to $n^{\text{RPA}}_{\alpha\sigma}(k) - n^{(0)}_{\alpha\sigma}(k)$ (see Fig. 1). We have also determined $\bar{\mu}_{c;\sigma}$ by employing a very recent parametrized expression for $n_{\alpha\sigma}(k)$, asserted by Gori-Giori and Ziesche [100] to be valid in the range $r_s \lesssim 12$, and observed no resemblance whatever between this $\mu_{c;\sigma}$ and the aforementioned quantum-Monte-Carlo-based $\mu_{c;\sigma}$ over the entire range $r_s \lesssim 12$ (see caption of Fig. 2). The reason for this lies in the fact that, even at $r_s = 1$, $\mu_{c;\sigma}$ is smaller by one order of magnitude than $\mu_{xc;\sigma}$, with the disparity between these two quantities further increasing for smaller values of $r_s$ (this as evidenced by the fact that $\mu_{c;\sigma}/\mu_{xc;\sigma} \to 0$ for $r_s \downarrow 0$); it follows that no parameterization of $n_{\sigma}(k)$ is likely to reproduce $\mu_{c;\sigma}$ through the expression in Eq. (87) unless this reproduction has explicitly been enforced in the determination of the parameters of $n_{\sigma}(k)$. 15 Our numerical calculations reveal that for $r_s \geq 6.09887 \ldots$ $n^{\text{RPA}}_{\alpha\sigma}(k_{F,\sigma}) \geq \frac{1}{2}$ (for $r_s = 6.09887 \ldots$, $n^{\text{RPA}}_{\alpha\sigma}(k_{F,\sigma}) = 0.31760 \ldots$ so that for this $r_s$ we have $Z^{\text{RPA}}_{F,\sigma} = 0.182397 \ldots$ and $[n^{\text{RPA}}_{\alpha\sigma}(k_{F,\sigma}) + n^{\text{RPA}}_{\sigma\sigma}(k_{F,\sigma})]/2 = 0.408801 \ldots$) and that for $r_s \geq 7.769269 \ldots$ $n^{\text{RPA}}_{\alpha\sigma}(k_{F,\sigma}) \leq n^{\text{RPA}}_{\alpha\sigma}(k_{F,\sigma})$. The latter of course implies that, according to the RPA, the paramagnetic GS of the uniform electron-gas system should be unstable for $r_s \geq 7.769269 \ldots$. For completeness, according to Bloch [96] (see [91], pp. 682-684), within the framework of the Hartree-Fock approximation the latter GS is unstable towards a uniform ferromagnetic state for $r_s \geq 5.4802186 \ldots$. This is suggestive of the possibility that the instability as predicted by the RPA (which is an artefact of this approximation) may also be one towards a ferromagnetic GS.
§ 6. BEHAVIOUR OF \( n_\sigma(k) \) FOR \( k \) INFINITESIMALLY CLOSE TO \( S_{F;\sigma} \)

We now proceed with the investigation of the behaviour of \( n_\sigma(k) \) for \( k \) approaching \( S_{F;\sigma} \). Along the lines presented in [6], for \( k \in S_{F;\sigma} \) we have

\[
\Lambda_\sigma(k) = \Gamma_\sigma(k),
\]

(95)

where \( \Lambda_\sigma(k) \) has been defined in Eq. (32) above and

\[
\Gamma_\sigma(k) := \frac{\mu - \xi_{k;\sigma}}{\varepsilon_{k;\sigma} - \mu}.
\]

(96)

Making use of the expressions in Eqs. (29) and (30) above, we deduce that

\[
\Gamma_\sigma(k) \sim \frac{-a(k_{F;\sigma}) \cdot (k - k_{F;\sigma}) - g \zeta_{k;\sigma}}{a(k_{F;\sigma}) \cdot (k - k_{F;\sigma}) - g \Lambda_\sigma(k)(\zeta_{k;\sigma} - \eta_{k;\sigma})},
\]

\( k \to S_{F;\sigma}, \)

(97)

where on account of the assumed stability of the GS of the system both the numerator and the denominator on the RHS must be non-negative. The fundamental difference between the expression on the RHS of Eq. (97) and its counterpart specific to the uniform metallic GSs of the conventional single-band Hubbard Hamiltonian (cf. Eq. (76) in [6]) arises from \( \eta_{k;\sigma} \) which for the latter GSs is identically vanishing. Since we have earlier considered the Hubbard Hamiltonian in some detail [6], in what follows, unless we explicitly indicate otherwise, \( \eta_{k;\sigma} \neq 0 \).

As we shall see below, an identically non-vanishing \( \eta_{k;\sigma} \) has far-reaching consequences for the behaviour of \( n_\sigma(k) \) for \( k \) approaching \( S_{F;\sigma} \).

With reference to the expressions in Eqs. (28) and (26) above, we consider the following behaviours for \( \zeta_{k;\sigma} \) and \( \eta_{k;\sigma} \) as \( k \to k_{F;\sigma} \in S_{F;\sigma} \):

\[
|\zeta_{k;\sigma}| \sim |B(k_{F;\sigma})| |k - k_{F;\sigma}|^\gamma, \quad (98)
\]

\[
|\zeta_{k;\sigma}| \sim |B(k_{F;\sigma})| \ln |k - k_{F;\sigma}| |k - k_{F;\sigma}|^\gamma, \quad (99)
\]

\[
|\eta_{k;\sigma}| \sim |C(k_{F;\sigma})| |k - k_{F;\sigma}|^\gamma, \quad (100)
\]

\[
|\eta_{k;\sigma}| \sim |C(k_{F;\sigma})| \ln |k - k_{F;\sigma}| |k - k_{F;\sigma}|^\gamma, \quad (101)
\]

where \( B(k_{F;\sigma}) \), \( C(k_{F;\sigma}) \) and \( \tau \) are parameters. Below we consider a variety of possibilities corresponding to various ranges of values for the parameters \( \gamma \) and \( \tau \).

In the present case, in addition to the intervals in which \( \gamma \) and \( \tau \) lie \((0 < \gamma < 1 \text{ or } \gamma \geq 1, \text{ for instance})\), the precise relationship between \( \gamma \) and \( \tau \) (i.e. \( \gamma < \tau, \gamma = \tau \) and \( \gamma > \tau \)) is significant, an exhaustive analysis of all possible cases will be too extensive to consider here. We shall therefore explicitly deal with a limited number of cases which are representative and further pave the way for future complementary considerations. Below we consider the following cases: \( 0 < \gamma < \tau < 1; \) \( 0 < \tau < \gamma < 1; \) \( 0 < \gamma = \tau < 1; \gamma = 1, \tau = 1. \) For obvious reasons, when for instance Eq. (98) applies, the cases corresponding to \( 0 < \gamma < 1 \) and \( \gamma = 1 \) should be considered separately whereas, when Eq. (99) applies, we need to deal with one case only, corresponding to \( 0 < \gamma \leq 1. \) Similarly for Eqs. (100) and (101) and \( 0 < \tau < 1, \tau = 1 \) and \( 0 < \tau \leq 1 \) respectively.

Note that in principle the values of \( B, C, \gamma \) and \( \tau \) can depend on whether \( k \) approaches \( S_{F;\sigma} \) from the inside (outside) of the Fermi sea, in which case \( B(k_{F;\sigma}), C(k_{F;\sigma}), \gamma \) and \( \tau \) in Eqs. (98) – (101) should be denoted by \( B(k^-_{F;\sigma}), C(k^-_{F;\sigma}), \gamma^- \) and \( \tau^- \) \((B(k^+_{F;\sigma}), C(k^+_{F;\sigma}), \gamma^+ \) and \( \tau^+ \)) respectively.

6.1. The case when \( 0 < \gamma < 1, 0 < \tau < 1 \)

In this case from Eq. (97) we obtain

\[
\Gamma_\sigma(k) \sim \frac{1}{\Lambda_\sigma(k)} \frac{\zeta_{k;\sigma}}{\zeta_{k;\sigma} - \eta_{k;\sigma}}, \quad k \to S_{F;\sigma}. \quad \text{(102)}
\]

In the present case, the assumption with regard to the stability of the GS of the system under consideration implies that

\[
\zeta_{k;\sigma} < 0 \quad \text{and} \quad \zeta_{k;\sigma} < \eta_{k;\sigma}, \quad k \to S_{F;\sigma}, \quad \text{(103)}
\]

must hold; violation of these conditions imply that for \( k \) sufficiently close to \( S_{F;\sigma}, \xi_{k;\sigma} \) would increase above \( \mu \) and \( \zeta_{k;\sigma} \) would decrease below \( \mu \) respectively.

To proceed, we need to consider three different cases, corresponding to \( \gamma < \tau, \gamma > \tau \) and to \( \gamma = \tau \). In the last case, it is relevant whether \( \zeta_{k;\sigma} \) satisfies Eq. (98) or Eq. (99) and similarly whether \( \eta_{k;\sigma} \) satisfies Eq. (100) or Eq. (101). The case corresponding to \( \gamma = \tau = 1, \) with \( \zeta_{k;\sigma} \) and \( \eta_{k;\sigma} \) satisfying Eqs. (99) and (101) respectively, concerns in particular (i.e. \( a \) priori not exclusively) systems of Coulomb-interacting fermions (see the paragraph subsequent to that containing Eq. (55) above).

6.1.1. \( 0 < \gamma < \tau < 1 \)

For \( \gamma < \tau \), from Eq. (102) we obtain

\[
\Gamma_\sigma(k) \sim \frac{1}{\Lambda_\sigma(k)}, \quad k \to S_{F;\sigma}, \quad \text{(104)}
\]

which in conjunction with Eqs. (32) and (95) yields

\[
n_\sigma(k^+_{F;\sigma}) = \frac{1}{2}. \quad \text{(105)}
\]

Note that in this case, where \( |\zeta_{k;\sigma}| > |\eta_{k;\sigma}| \) for \( k \) sufficiently close to \( S_{F;\sigma} \), satisfaction of the first requirement in Eq. (103) above implies satisfaction of the second requirement. With
from Eq. (105) we obtain (see Eq. (41) above)

\[ n_\sigma(k_{F,\sigma}) = \frac{1}{2}, \quad Z_{k_{F,\sigma}} = 0 \quad (\gamma < \tau). \quad (107) \]

It follows that in the case under consideration the single-particle spectral function \( A_\sigma(k_{F,\sigma}; \varepsilon) \) is free from a quasi-particle peak at \( \varepsilon = \varepsilon_F \) (breakdown of the FL picture).

6.1.2. \( 0 < \tau < \gamma < 1 \)

For \( \gamma > \tau \), from Eq. (102) we have

\[ \Gamma_\sigma(k) \sim \frac{-1}{\lambda_\sigma(k)} \frac{\zeta_{\kappa,\sigma}}{\eta_{k,\sigma}} \sim + \infty, \quad k \rightarrow S_{\gamma,\sigma}. \quad (108) \]

Since here \( |\eta_{k,\sigma}| > |\zeta_{\kappa,\sigma}| \) for \( k \) sufficiently close to \( S_{\gamma,\sigma} \), for such \( k \) the stability conditions in Eq. (103) imply that \( \eta_{k,\sigma} > 0 \); hence we have +\( \infty \) on the RHS of Eq. (108). The result in Eq. (108) leads to

\[ n_\sigma(k_{\gamma,\sigma}^\pm) = 1, \quad Z_{k_{\gamma,\sigma}} = 0 \quad (\gamma > \tau). \quad (109) \]

In the case when such behaviour for \( n_\sigma(k) \) is unlikely, one is left to conclude that \( 0 < \tau < \gamma < 1 \) is equally unlikely to be satisfied for a realistic model of interacting fermion systems. It is interesting, however, to note that (see our pertinent discussions in § 1) \( n_\sigma(k_{\gamma,\sigma}^\pm) = 1 \) is not dissimilar to that observed in the experimentally determined \( n_\sigma(k) \) corresponding to Bi2212 and Bi2201, at the Fermi-surface points adjacent to the \( M \) points of the Brillouin zone (see Figs. 2(g) and (i) in [73]).

6.1.3. \( 0 < \tau = \gamma \leq 1 \) (includes Fermi liquids)

Here we explicitly deal with the instances where the expressions in Eqs. (99) and (101) apply. As we have indicated earlier (see the paragraph following that including Eq. (55) above), for the metallic states of fermions interacting through the long-range Coulomb potential, \( \nabla \Sigma_\sigma^{ui}(k) \equiv (g/h) \nabla \varphi_{k,\sigma} \) (see Eq. (17)) is logarithmically divergent for \( k = k_{F,\sigma} \in S_{\gamma,\sigma} \). It follows therefore that the FL metallic states of Coulomb-interacting fermions fall into the category of systems dealt with in this Section. 16

From the expressions in Eqs. (99) and (101) it follows that to the leading order in \( (k - k_{F,\sigma}) \) we can write

\[ \eta_{k,\sigma} \sim \lambda_\sigma^+ \zeta_{k,\sigma} \quad k \in FS_\sigma, \quad (110) \]

where \( \lambda_\sigma^- \) and \( \lambda_\sigma^+ \) stand for finite constants specific to \( k = k_{F,\sigma} \). Thus, in view of the expressions in Eqs. (99) and (101), for \( \Gamma_\sigma(k) \), as presented in Eq. (97) above, we have

\[ \Gamma_\sigma(k) \sim \frac{-\gamma_{k,\sigma}}{(1 - \lambda_\sigma^+) \Lambda_\sigma(k) \zeta_{k,\sigma}} = \frac{1}{(1 - \lambda_\sigma^+) \Lambda_\sigma(k)}. \quad (111) \]

The requirement of the stability of the GS under consideration implies that

\[ \lambda_\sigma^+ \leq 1. \quad (112) \]

Solving Eq. (95) for \( k = k_{F,\sigma}^\pm, k_{F,\sigma} \in S_{\gamma,\sigma}, \) with \( \Gamma_\sigma(k) \) therein replaced by the asymptotic expression on the RHS of Eq. (111), we obtain

\[ \Lambda_\sigma(k_{F,\sigma}^\pm) = \frac{1}{\sqrt{1 - \lambda_\sigma^+}}, \quad (113) \]

which in conjunction with Eq. (32) yields

\[ n_\sigma(k_{F,\sigma}^\pm) = \frac{1}{1 + \sqrt{1 - \lambda_\sigma^+}}. \quad (114) \]

From this and Eq. (106) we have

\[ n_\sigma(k_{F,\sigma}) = \frac{1}{2}\left( \frac{1}{1 + \sqrt{1 - \lambda_\sigma^-}} + \frac{1}{1 + \sqrt{1 - \lambda_\sigma^+}} \right), \quad (115) \]

which is not necessarily equal to \( \frac{1}{2} \).

To gain insight into the quantitative values to be expected from \( \lambda_\sigma^+ \) and \( \lambda_\sigma^- \), we recall that in the weak-coupling limit for the Coulomb-interacting uniform-electron-gas system (and thus in the paramagnetic phase of this system) one has 17

\[ n_\sigma(k_{F,\sigma}) \sim 1 - \alpha_\sigma a \quad \text{for } r_s \downarrow 0, \quad (116) \]

where

\[ a := \frac{r_s}{\pi^{2/3}}. \quad (117) \]

\[ \uparrow \]

16 From the defining expression in Eq. (25) and the fact that \( \gamma_{k,\sigma} \sim 0 \) for \( k \rightarrow k_{F,\sigma} \in S_{\gamma,\sigma} \) (the latter rendering an assumption with regard to the boundedness of \( \varphi_{k,\sigma} \) for \( k \rightarrow k_{F,\sigma} \) redundant) it follows that a possible (logarithmic) divergence of \( \varphi_{k,\sigma} \) for \( k \rightarrow k_{F,\sigma} \) directly implies an analogous divergence of \( \nabla k \varphi_{k,\sigma} \) for \( k \rightarrow k_{F,\sigma} \).

17 Here we are relying on the fact that for \( r_s \downarrow 0 \) the leading-order asymptotic behaviour of the exact \( n_\sigma(k) = n_\sigma^{(0)}(k) \) is exactly reproduced by \( n_\sigma^{(\sigma)}(k) = n_\sigma^{(0)}(k), \forall k. \)
in which $\gamma_0$ has been defined in Eq. (88) above. The constants $\alpha_{\sigma}^\pm$ in Eq. (116) are in principle bounded functions of $r_s$; according to Daniel and Vosko \[95\], within the framework of the RPA, $\alpha_{\sigma}^- \equiv \alpha_{\sigma}^+ \approx 1.7$. As can be observed from the results in Fig. 3, $\alpha_{\sigma}^\pm$ are not constants; although for $r_s$ approaching zero, $\alpha_{\sigma}^-$ and $\alpha_{\sigma}^+$ tend towards the same value (which we denote by $\alpha_0$), for sufficiently small $r_s$, $\alpha_{\sigma}$ monotonically decreases towards zero, resulting in the fact that for $r_s \downarrow 0$, $n_{\sigma}(k_{F,\sigma})$, as defined in Eq. (106) above, approaches $\frac{1}{2}$ more rapidly than asserted in \[95\].

Making use of the results in Eqs. (116) and (117), from Eq. (114) we obtain

$$
\lambda_{\sigma}^- \sim 1 - \left( \frac{\alpha_{\sigma}^- \mathbf{a}}{1 - \alpha_{\sigma}^- \mathbf{a}} \right)^2 \sim 1 - (\alpha_{\sigma}^-)^2 \quad r_s \downarrow 0 \quad (118)
$$

$$
\lambda_{\sigma}^+ \sim 1 - \left( \frac{1 - \alpha_{\sigma}^+ \mathbf{a}}{\alpha_{\sigma}^+ \mathbf{a}} \right)^2 \sim 1 - \frac{1}{(\alpha_{\sigma}^+)^2} \quad \text{for} \quad r_s \downarrow 0 \quad (119)
$$

where

$$
\alpha_{\sigma}^\pm \sim \alpha_0 \quad \text{for} \quad r_s \downarrow 0.
$$

We observe that in the regime of weak interaction, corresponding to $r_s \ll 1$, $\lambda_{\sigma}^- \uparrow 1$ and $\lambda_{\sigma}^+ \downarrow 0$. We point out that similar expressions to Eqs. (114), (116) and (118) apply to anisotropic metallic GSs, with the parameters therein dependent on the direction in the $k$ space along which $S_{\sigma}$ is approached.

From the above considerations it follows that in the weak-coupling limit, corresponding to $0 \leq \alpha_{\sigma} \mathbf{a} \ll 1$, for $k \rightarrow S_{\sigma}$ one must have (see Eqs. (22) and (23) above)

$$
\frac{\xi_{k;\sigma} - (\varepsilon_{k} - \varepsilon_{k_{\sigma}})/\mathbf{g}}{\varepsilon_{k_{\sigma}} - (\varepsilon_{k} - \varepsilon_{k_{\sigma}})/\mathbf{g}} \sim \begin{cases} 
1 + \alpha_{\sigma} \mathbf{a}, & \text{for} \quad k \in \text{FS}_{\sigma}, \\
-\alpha_{\sigma} \mathbf{a}, & \text{for} \quad k \in \overline{\text{FS}}_{\sigma}.
\end{cases} \quad (120)
$$

In arriving at this result we have made use of Eqs. (27), (25), (110), (116) and (118).

### 6.2. The case when $\gamma = 1, \tau = 1$: general

Here we explicitly deal with the instances where the expressions in Eq. (98) and (100) apply. In the present case, for $k \rightarrow k_{F;\sigma} \in S_{\sigma}$ we have.

$$
\zeta_{k;\sigma} \sim b_{\sigma} \left( k_{F;\sigma}^+ \right) \cdot \left( k - k_{F;\sigma} \right), \quad k \in \left\{ \text{FS}_{\sigma}, \overline{\text{FS}}_{\sigma} \right\}, \quad (121)
$$

$$
\eta_{k;\sigma} \sim c_{\sigma} \left( k_{F;\sigma}^+ \right) \cdot \left( k - k_{F;\sigma} \right), \quad k \in \left\{ \text{FS}_{\sigma}, \overline{\text{FS}}_{\sigma} \right\}. \quad (122)
$$

With

$$
b_{\sigma} := b_{\sigma} \left( k_{F;\sigma}^+ \right) \cdot \hat{n}(k_{F;\sigma}), \quad (123)
$$

$$
d_{\sigma} := d_{\sigma} \left( k_{F;\sigma}^+ \right) \cdot \hat{n}(k_{F;\sigma}), \quad (124)
$$

in which

$$
d_{\sigma} \left( k_{F;\sigma}^+ \right) := b_{\sigma} \left( k_{F;\sigma}^+ \right) - c_{\sigma} \left( k_{F;\sigma}^+ \right), \quad (125)
$$

from Eq. (97) we obtain

$$
\Gamma_{\sigma}(k) \sim -\frac{(a_{\sigma} + \mathbf{g} \cdot \mathbf{b}_{\sigma}^+)}{a_{\sigma} - \mathbf{g} \cdot \Lambda_{\sigma}(k) \cdot \mathbf{d}_{\sigma}}, \quad k \rightarrow k_{F;\sigma} \in S_{\sigma}. \quad (126)
$$

The assumed stability of the GS of the system under consideration implies that both the numerator and the denominator of the function on the RHS of Eq. (97) must be non-negative. From this, considering $a_{\sigma} > 0$, $\mathbf{g} > 0$ and $\Lambda_{\sigma}(k) > 0$, we arrive at the following conditions

$$
b_{\sigma}^+ > -a_{\sigma}/\mathbf{g} < 0, \quad (I)
$$

$$
d_{\sigma} > a_{\sigma}/\mathbf{g} \Lambda_{\sigma} > 0, \quad (II)
$$

$$
b_{\sigma}^+ < -a_{\sigma}/\mathbf{g} < 0, \quad (III)
$$

$$
d_{\sigma}^+ > a_{\sigma}/\mathbf{g} \Lambda_{\sigma} > 0, \quad (IV)
$$

where

$$
\Lambda_{\sigma}^+ := \Lambda_{\sigma} \left( k_{F;\sigma}^+ \right). \quad (128)
$$

Making use of the expression in Eq. (126) above, the equation for $S_{\sigma}$ in Eq. (95) reduces to the following quadratic equation for $\Lambda_{\sigma}^+$:

$$
\mathbf{g} \cdot d_{\sigma}^+ \left( \Lambda_{\sigma}^+ \right)^2 - a_{\sigma} \Lambda_{\sigma}^+ - (a_{\sigma} + \mathbf{g} \cdot b_{\sigma}^+) = 0. \quad (129)
$$

For interaction potentials with non-vanishing range, in general $d_{\sigma}^+ \neq b_{\sigma}^+$ (see Eq. (125) above), whereby Eq. (129)
acquires a rich spectrum of solutions. Considering the second-order equation \( ax^2 + bx + c = 0 \), for which we have the solutions \( x = -b/2a \mp (b^2 - 4ac)^{1/2}/2a \), below in analogy we denote the possible two solutions of Eq. (129) by \( \Lambda_{\sigma \pm} \). From Eq. (129) we immediately obtain the following results

\[
\Lambda_{\sigma +} + \Lambda_{\sigma -} = \frac{a_\sigma}{g d^2_{\sigma}},
\]

\[
\Lambda_{\sigma +} - \Lambda_{\sigma -} = -\frac{a_\sigma + g b^2_{\sigma}}{g d^2_{\sigma}}.
\]

We note that for \( x_\pm = u \pm iv \), with \( u \) and \( v \) real, we have \( x_+ x_- = u^2 + v^2 \geq 0 \) from which it follows that in cases where the RHS of Eq. (131) is negative, the solutions (whether \( \Lambda_{\sigma +} \) and \( \Lambda_{\sigma -} \) or \( \Lambda_{\sigma +} \) and \( \Lambda_{\sigma -} \)) cannot be complex. In connection with \( x_\pm = u \pm iv \), we point out that, since \( g, a_\sigma, b_{\sigma} \) and \( d^2_{\sigma} \) are real, the possible complex solutions of Eq. (129) must indeed occur in complex-conjugate pairs.

Below we separately consider \( \Lambda_{\sigma +} \) and \( \Lambda_{\sigma -} \). In our following considerations we shall encounter \( c^\pm_{\sigma} \) which in analogy with \( b_{\sigma} \) and \( d^2_{\sigma} \) in Eqs. (123) and (124) respectively are defined according to

\[
c^\pm_{\sigma} := c_{\sigma}(k_{F,\rho}) \cdot \hat{n}(k_{F,\sigma}).
\]

### 6.2.1. Considering \( n_{\sigma}(k_{F,\rho}) \equiv \Lambda_{\sigma}/(1 + \Lambda_{\sigma}) \)

According to (II) in Eq. (127) above, \( d^-_{\sigma} > 0 \). Since according to (I) in Eq. (127), \( a_\sigma + g b_{\sigma} > 0 \), in view of \( d^-_{\sigma} > 0 \) from Eq. (131) it follows that \( \Lambda_{\sigma -} \), \( \Lambda_{\sigma -} < 0 \). Thus, of the possible two solutions of Eq. (129) for \( \Lambda_{\sigma} \) (which by our above argument, presented subsequent to Eq. (131), cannot be complex), one is positive and one is negative; with reference to Eq. (32) above, it is the positive solution, the ‘physical’ solution, that is of interest to our considerations that follow. Introducing

\[
L_{\pm}(x, y) := \frac{1 + (1 + 4x(1 + y)^{1/2})}{2x},
\]

for the physical solution of Eq. (129) for \( \Lambda_{\sigma} \) we have

\[
\Lambda^-_{\sigma} = \Lambda^{-}_{\sigma +} \equiv L_+(x^\pm_{\sigma}, y^\pm_{\sigma}),
\]

where

\[
x^\pm_{\sigma} := \frac{g d^-_{\sigma}}{a_\sigma}, \quad y^\pm_{\sigma} := \frac{g b^-_{\sigma}}{a_\sigma} = x^\pm_{\sigma} + \delta x^\pm_{\sigma},
\]

in which (see Eq. (125) above)

\[
\delta x^\pm_{\sigma} := \frac{g c^\pm_{\sigma}}{a_\sigma}.
\]

From (I) in Eq. (127) we deduce the following two identical relationships

\[
y^+_{\sigma} > -1 \iff 1 + x^+_{\sigma} + \delta x^+_{\sigma} > 0.
\]

From Eqs. (130) and (135) and the fact that \( \Lambda^-_{\sigma} = \Lambda^+_{\sigma} \) (see Eq. (134)) and \( \Lambda^-_{\sigma} < 0 \), we further have

\[
x^\sigma_{\sigma} = \frac{1}{\Lambda^+_{\sigma} + \Lambda^-_{\sigma}}, \quad x^\sigma_{\sigma} > \frac{1}{\Lambda^+_{\sigma}}.
\]

Making use of the exact result

\[
L_+(x, x + \delta x) = \frac{1}{2x} \left[ 1 + 2(x + \frac{1}{2}) \left( 1 + \frac{\delta x}{(x + 1/2)^2} \right)^{1/2} \right],
\]

from Eq. (134) we deduce the following inequalities (based on \( x^\sigma_{\sigma} > 0 \))

\[
\Lambda^-_{\sigma} < 1 \iff 1 + 2(x^\sigma_{\sigma} + \frac{1}{2}) \left( 1 + \frac{\delta x^\sigma_{\sigma}}{x^\sigma_{\sigma} + 1/2} \right)^{1/2} > 2 x^\sigma_{\sigma},
\]

which after some manipulations give rise to

\[
\Lambda^-_{\sigma} \leq 1 \iff \delta x^\sigma_{\sigma} \leq -2.
\]

From Eqs. (136), (141) and (32) we thus obtain

\[
c^-_{\sigma} \geq \frac{-2a_{\sigma}}{g} \iff \Lambda^-_{\sigma} \leq 1 \iff n_{\sigma}(k_{F,\sigma}) > \frac{1}{2}.
\]

Since \( -2a_{\sigma}/g \leq 0 \), it follows that in the event \( c^-_{\sigma} = 0 \) (as is the case with the single-band Hubbard Hamiltonian 20 [6]) we have \( \Lambda^-_{\sigma} \geq 1 \) or \( n_{\sigma}(k_{F,\sigma}) \geq \frac{1}{2} \). The more general result in Eq. (142), allowing for \( n_{\sigma}(k_{F,\sigma}) < \frac{1}{2} \), signifies the considerable influence that the (long) range of the interaction potential can have on the behaviour of \( n_{\sigma}(k_{F,\sigma}) \).

20 For instance, at half-filling, for \( d = 1 \) and \( \varepsilon = -2t \cos(k) \), \( t \not= 0 \) (here \( k \) is in units of the inverse lattice constant so that at half-filling \( \pm k_{F,\sigma} = \pm \pi/2 \), in the limit of large \( U/t \) one has the exact result 101) (see also 102) \( n_{\sigma}(k) \sim \frac{1}{2} + 4 \ln(2) \cos(k)t/U, \ k \in [-\pi, \pi] \); it is seen that in this limit indeed \( n_{\sigma}(k) \geq \frac{1}{2} \) for \( k \leq k_{F,\sigma} \) and \( n_{\sigma}(k) \leq \frac{1}{2} \) for \( k \geq k_{F,\sigma} \). Similar behaviours obtain for \( d = 2 \) (square lattice) and \( d = 3 \) (simple cubic lattice) 101. We point out that for \( d = 1 \) and \( \varepsilon = -2t \cos(k) \), \( t \not= 0 \), following the exact Bethe-Ansatz solution due to Lieb and Wu 103, at half-filling the GS is insulating for all \( U > 0 \), from which it follows that for the case at hand the absence of discontinuity in \( n_{\sigma}(k) \) at \( k = \pm \pi/2 \) is not specific to \( U/t \to \infty \), but to all \( U/t > 0 \) (in fact, in this case and so long as \( U/t > 0 \), \( d^n_{\sigma}(k)/dkm \) can be shown to be bounded at \( k = \pm \pi/2 \) for any finite value of \( m \)). Conversely, contrary to the statement in 101, the absence of the usual discontinuity in \( n_{\sigma}(k) \) (with reference to the above case, at \( k = \pm \pi/2 \)) does not necessarily imply absence of Fermi surface and thus an insulating underlying GS.
6.2.2. Considering \( n_\sigma(k_{\uparrow+}^+) \equiv \Lambda_\sigma^+/(1 + \Lambda_\sigma^+) \)

In contrast with \( d_\sigma^+ \), which is positive, \( d_\sigma^+ \) has no a priori sign; we know only that (see (IV) in Eq. (127) above) \( d_\sigma^+ < a_\sigma/(g \Lambda_\sigma^+) \). This necessitates us to consider separately the cases \( d_\sigma^+ > 0 \) and \( d_\sigma^+ < 0 \). Here we have however (see (III) in Eq. (127) above) \(- (a_\sigma + g b_\sigma^+ > 0). \) Thus following Eqs. (130) and (131), for \( g > 0 \) we have

\[
\Lambda_{\sigma+}^+ + \Lambda_{\sigma-}^+ \geq 0, \quad \Lambda_{\sigma+}^+, \Lambda_{\sigma-}^+ \geq 0 \quad \Leftrightarrow \quad d_\sigma^+ \geq 0, \quad (143)
\]

that is, the two solutions of Eq. (129) for \( \Lambda_\sigma^+ \) are positive when \( d_\sigma^+ > 0 \) while they have different signs when \( d_\sigma^+ < 0 \) (note that, by the argument presented following Eq. (131) above, in the case where \( d_\sigma^+ < 0 \) the solutions cannot be complex); in the latter case, the negative solution has a greater magnitude than the positive solution; in the former case \( (d_\sigma^+ > 0) \), where there are two positive solutions, we need to invoke the restriction \( \Lambda_\sigma \geq \Lambda_\sigma^+ \) (see Eq. (153) below) in order to guarantee \( n_\sigma(k_{\uparrow}^+ \sigma) - n_\sigma(k_{\uparrow}^+ \sigma) = Z_{k_{\uparrow}^+ \sigma} \geq 0 \). In this connection, we note that for the case when \( d_\sigma^+ < 0 \), where we have the single positive solution \( \Lambda_{\sigma-}^+ \) for \( \Lambda_{\sigma-}^+ \), the condition \( \Lambda_\sigma \geq \Lambda_{\sigma-}^+ \) is similarly not trivially fulfilled so that it necessarily restricts the ranges of variation of (some of) the parameters of the problem at hand.

6.2.2.1. The case when \( d_\sigma^+ < 0 \)

Here, in view of the requirement \( \Lambda_\sigma(k) \geq 0, \Lambda_{\sigma+} \) is to be identified with \( \Lambda_{\sigma-} \) (following Eq. (143), in the present case \( \Lambda_{\sigma+} < 0 \)), that is

\[
\Lambda_\sigma^+ = \Lambda_{\sigma-} \Leftrightarrow \Lambda_{\sigma-} \equiv \mathcal{L}_-(x_\sigma^+, y_\sigma^+), \quad (144)
\]

where \( \mathcal{L}_-(x, y) \) has been defined in Eq. (133) above, and

\[
x_\sigma^+ := g d_\sigma^+ / a_\sigma, \quad y_\sigma^+ := g b_\sigma^+ / a_\sigma \equiv x_\sigma^+ + \delta x_\sigma^+, \quad (145)
\]

in which

\[
\delta x_\sigma^+ := g c_\sigma^+ / a_\sigma. \quad (146)
\]

From (III) in Eq. (127) we deduce the following identical relationships (cf. Eq. (137) above)

\[
y_\sigma^+ < -1 \quad \Leftrightarrow \quad 1 + x_\sigma^+ + \delta x_\sigma^+ < 0. \quad (147)
\]

In addition, from Eqs. (130) and (145) and the fact that \( \Lambda_{\sigma+} = \Lambda_{\sigma-} \) (see Eq. (144)) and \( \Lambda_{\sigma+} < 0 \), we have

\[
x_\sigma^+ = \frac{1}{\Lambda_{\sigma+}^+ + \Lambda_{\sigma-}^+}, \quad x_\sigma^+ > \frac{1}{\Lambda_\sigma^+}. \quad (148)
\]

Making use of the exact result

\[
\mathcal{L}_-(x, x + \delta x) = \frac{1}{2x} \left[ 1 - 2|x| + \frac{1}{2} \left( 1 + \frac{x \delta x}{(x + 1/2)^2} \right)^{1/2} \right], \quad (149)
\]

from Eq. (144) we arrive at the following inequalities (based on \( x_\sigma^+ < 0 \)):

\[
\Lambda_\sigma^+ \geq 1 \quad \Leftrightarrow \quad -1 - 2|x_\sigma^+ + \frac{1}{2} \left( 1 + \frac{x_\sigma^+ \delta x_\sigma^+}{(x_\sigma^+ + 1/2)^2} \right)^{1/2} \geq -2 x_\sigma^+, \quad (150)
\]

which after some manipulations give rise to

\[
\Lambda_\sigma^+ \geq 1 \quad \Leftrightarrow \quad \delta x_\sigma^+ \leq -2. \quad (151)
\]

From Eqs. (146), (151) and (32) we thus obtain

\[
c_\sigma^+ \leq \frac{-2 a_\sigma}{g} \quad \Leftrightarrow \quad \Lambda_\sigma^+ \geq 1 \quad \Leftrightarrow \quad n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2}. \quad (152)
\]

The fact that here the condition \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \) is in principle feasible clearly signifies the considerable influence that a non-vanishing range of the two-body interaction potential can have on the behaviour of \( n_\sigma(k_{\uparrow}^+ \sigma) \). The requirement \( n_\sigma(k_{\uparrow}^+ \sigma) - n_\sigma(k_{\uparrow}^+ \sigma) = Z_{k_{\uparrow}^+ \sigma} \geq 0 \) implies the necessity for the following condition to be satisfied:

\[
\frac{\Lambda_{\sigma-}}{\Lambda_{\sigma+}} = \frac{\mathcal{L}_+(x_\sigma^+, y_\sigma^+)}{\mathcal{L}_-(x_\sigma^+, y_\sigma^+)} \geq 1 \quad \text{for} \quad \delta x_\sigma^- \leq -2 \land \delta x_\sigma^+ \geq -2. \quad (153)
\]

In connection with the above, we mention that the combinations \( \delta x_\sigma^- > 2 \), \( \delta x_\sigma^+ > 2 \) corresponds to \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \), \( n_\sigma(k_{\uparrow}^+ \sigma) < \frac{1}{2} \) so that it does not imply any further restriction; on the other hand, the combination \( \delta x_\sigma^- < -2 \), \( \delta x_\sigma^+ < -2 \) which corresponds to \( n_\sigma(k_{\uparrow}^+ \sigma) < \frac{1}{2} \), \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \), cannot be realized for stable GSs. It is for these reasons that only for the two combinations of \( \delta x_\sigma^- \) and \( \delta x_\sigma^+ \) explicitly presented in Eq. (153) can \( \Lambda_{\sigma^-} / \Lambda_{\sigma+} \geq 1 \) in principle amount to a non-trivial condition; below we shall demonstrate that indeed the latter cannot be trivially satisfied. For completeness, \( \delta x_\sigma^- = 0 \) and \( \delta x_\sigma^+ = 0 \) correspond to the general category of \( \delta x_\sigma^- > -2 \) and \( \delta x_\sigma^+ > -2 \) respectively for which, as indicated above, \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \) and \( n_\sigma(k_{\uparrow}^+ \sigma) < \frac{1}{2} \). In this connection, it is interesting to note that following Eqs. (146), (132), (122), (25), (26) and (17), \( \delta x_\sigma^- = \delta x_\sigma^+ = 0 \) corresponds to cases where (not exclusively) \( \Sigma_{\sigma}(k) \) is independent of \( k \) (such as is the case for the uniform metallic GSs of the single-band Hubbard Hamiltonian), so that with reference to the findings in [6], the results \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \) and \( n_\sigma(k_{\uparrow}^+ \sigma) < \frac{1}{2} \), obtained here, were in fact to be expected. The fact that, for \( \delta x_\sigma^+ \equiv g c_\sigma^+ / a_\sigma \rightarrow 0 \) one has \( n_\sigma(k_{\uparrow}^+ \sigma) > \frac{1}{2} \) and \( n_\sigma(k_{\uparrow}^+ \sigma) < \frac{1}{2} \) implies that, for interaction potentials of
non-vanishing range, $g/e_0$ must be greater than some finite value $g_\sigma/e_0$ in order for $n_\sigma(k_{\sigma}^-) < \frac{1}{2}$ or $n_\sigma(k_{\sigma}^+ > \frac{1}{2}$ to be realized (cf. footnote 15 above and footnote 23 below); here $e_0$ stands for an energy scale specific to the system under consideration.

We now demonstrate that the condition $\Lambda_\sigma^-/\Lambda_\sigma^+ \geq 1$ in Eq. (153) cannot be trivially satisfied; this we do through deducing restricted intervals in which various parameters of the problem at hand (such as $x_\sigma^\pm$ and $\sigma_\sigma^\pm$, and thereby $b_\sigma^\pm$, $c_\sigma^\pm$ and $d_\sigma^\pm$) have to be confined in order for the mentioned condition to be fulfilled. Readers who wish to take the validity of this statement for granted, may omit the remaining part of this Section.

Making use of the property $x_\sigma^- > 0$ (see Eq. (135) and (II) in Eq. (127) above) we re-write the expression in Eq. (153) as follows

$$f(x^-) \geq \alpha x^-,$$  
(154)

where

$$f(x):= 1 + (1 + 4x(1 + x + \delta x))^1/2,$$  
(155)

$$\alpha := \frac{1}{x^-} \left[ 1 - (1 + 4x^+ (1 + x^+ + \delta x^+))^1/2 \right].$$  
(156)

Above for clarity we have employed the short-hand notations $f(x^-)$ and $\alpha$ for $f(x^-, \delta x^-)$ and $\alpha(x^+, \delta x^+)$ respectively. When necessary, we shall employ the latter more complete notations. We have

$$f(x^-) \sim 2x^- + (2 + \delta x^-) := g(x^-) \quad \text{for} \quad x^- \to \infty. \quad (157)$$

For the considerations that follow it is crucial to realize that in consequence of Eq. (137) and (II) in Eq. (127), $x^- \to \infty$ is bound to satisfy

$$x^- > \tilde{x}^- \quad \text{where} \quad \tilde{x}^- := \max\{0, -(1 + \delta x^-)\}. \quad (158)$$

Consequently, unless indicated or implied otherwise, in what follows we implicitly assume that $x^- \sigma$ satisfies the condition in Eq. (158). We have

$$f(\tilde{x}^-) = 2.$$  
(159)

The graphical representation of the functions on both sides of Eq. (154) clearly reveals the conditions under which the inequality in Eq. (154) (or Eq. (153)) is satisfied. One readily verifies that, for $-2 \leq \delta x^- \sigma \leq 0$, $f(x^-) \sigma$ possesses a global minimum, equal to $1 + (1 - (1 + \delta x^-)^2)^{1/2}$, at $x^- = -(1 + \delta x^-)/2$; for $\delta x^- < -2$, $f(x^-)$ is complex-valued at $x^- = -(1 + \delta x^-)/2$. It is straightforwardly shown that for $\delta x^- < -2$ and $\delta x^- > 0$, $f(x^-)$ approaches the linear asymptote $g(x^-)$ (defined in Eq. (157) above) from below, whereas for $-2 < \delta x^- < 0$ it approaches $g(x^-)$ from above. From these observations we deduce that the inequality in Eq. (154) is always violated when the following conditions are satisfied:

$$\alpha \geq 2 \land \delta x^- < -2. \quad (160)$$

On the other hand, the relationship in Eq. (154) is always satisfied when either

$$\alpha \leq 2 \land \delta x^- > -2 \quad (161)$$

or

$$\alpha \leq \frac{2}{-(1 + \delta x^-)} \land \delta x^- < -2. \quad (162)$$

Note that, for $\delta x^- \leq -2$, we have $-2/(1 + \delta x^-) \in (0, 2]$. One trivially obtains the following for $\alpha \equiv \alpha(x^+ \sigma, \delta x^+)$

$$\alpha \geq 2 \quad \text{for} \quad \delta x^+ \sigma \leq -2. \quad (163)$$

In this connection, note that in general (see Eq. (147) above)

$$x^+ \sigma < -(1 + \delta x^+). \quad (164)$$

In the present case where $x^+ \sigma < 0$ (owing to $d^+ \sigma < 0$ considered here; see Eq. (145) above), $x^+ \sigma$ is bound to satisfy

$$x^+ < \min\{0, -(1 + \delta x^+)\}. \quad (165)$$

Combining the above results, we conclude that the inequality in Eq. (154) (or Eq. (153)) is violated when the following conditions are satisfied:

$$\delta x^- < -2 \land \delta x^+ < -2. \quad (166)$$

These conditions are precisely those we excluded for stable GSs in our discussions following Eq. (153) above.

Considering the case corresponding to (cf. Eq. (153) above) $\delta x^- > -2$ and $\delta x^+ < -2$ (the latter according to Eq. (163) implying $\alpha > 2$), from our above considerations we deduce that the condition in Eq. (154) (or, equivalently, that in Eq. (153)) is satisfied provided that (see Eq. (158) above)

$$\tilde{x}^- < x^- < \frac{2\alpha + 4(1 + \delta x^-)}{\alpha^2 - 4}, \quad \alpha > 2. \quad (167)$$

As for the case corresponding to (cf. Eq. (153) above) $\delta x^- < -2$ and $\delta x^+ > -2$ (the latter implying $\alpha < 2$; see above, and in particular Eq. (163)), from our above considerations we similarly deduce that the condition in Eq. (154) (or, equivalently, that in Eq. (153)) is satisfied provided that

$$x^- \geq \frac{-4(1 + \delta x^-) - 2\alpha}{4 - \alpha^2}, \quad \frac{2}{-(1 + \delta x^-)} \leq \alpha < 2. \quad (168)$$

Note that for $\alpha = -2/(1 + \delta x^-)$ the RHS of the above inequality for $x^- \sigma$ is, as expected, equal to $-(1 + \delta x^-) = 2/\alpha$; the condition considered here, namely $\delta x^- < -2$, implies that $-(1 + \delta x^-) > 1$. 

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6.2.2.2. The case when \( d^+ \sigma > 0 \)

As we have indicated above, in the present case both solutions \( \Lambda^+_{\sigma-} \) and \( \Lambda^+_{\sigma+} \) of Eq. (129) are positive, with \( \Lambda^+_{\sigma-} \leq \Lambda^+_{\sigma+} \). For these solutions we have

\[
\Lambda^+_{\sigma\pm} = \mathcal{L}_{\pm}(x_{\sigma}^+, y_{\sigma}^+),
\]

(169)

where \( x_{\sigma}^+ \) and \( y_{\sigma}^+ \) have been defined in Eq. (145) above. It is readily verified that

\[
\begin{align*}
\Lambda^+_{\sigma+} &> 1 \\
\Lambda^+_{\sigma-} &\leq 1
\end{align*}
\]

(170)

It is readily verified that, for \( \delta x_{\sigma}^+ \geq -2 \),

\[
0 < \Lambda^+_{\sigma-} \leq 1 \leq \Lambda^+_{\sigma+}
\]

(171)

which in fact shows the necessity for

\[
c^+_{\sigma} \geq \frac{-2a_{\sigma}}{\delta x_{\sigma}^-}.
\]

(172)

According to Eq. (142), for \( c^-_{\sigma} < -2a_{\sigma}/g \), \( n_\sigma(k_{\sigma,\sigma}^-) < \frac{1}{2} \) so that \( \Lambda^+_{\sigma+} \) (which according to Eq. (152) is greater than unity for \( c^+_{\sigma} > -2a_{\sigma}/g \) and thus following Eq. (32) corresponds to \( n_\sigma(k_{\sigma,\sigma}^+) > \frac{1}{2} \) is not permitted. It follows that \( \Lambda^+_{\sigma-} \) is the appropriate solution to Eq. (129) for \( \Lambda^+_{\sigma} \); for this solution to correspond to a non-negative \( Z_{k_{\sigma,\sigma}} \), it is required that the following condition be satisfied:

\[
\frac{\Lambda^+_{\sigma+}}{\Lambda^-_{\sigma}} \equiv \frac{\mathcal{L}_{-}(x_{\sigma}^+, y_{\sigma}^+)}{\mathcal{L}_{+}(x_{\sigma}^-, y_{\sigma}^-)} \leq 1 \quad \text{for} \quad \delta x_{\sigma}^- \leq -2 \land \delta x_{\sigma}^+ \geq -2.
\]

(173)

Here \( x_{\sigma}^- \) naturally satisfies the inequality in Eq. (158) above. On the other hand, since in this Section we deal with \( d^+ \sigma > 0 \), from Eqs. (145) and (147) we have (cf. Eq. (165) above)

\[
0 < x_{\sigma}^+ < -(1 + \delta x_{\sigma}^+)\).
\]

(174)

The inequalities in Eqs. (171) and (174) restrict the range of variation in \( \delta x_{\sigma}^+ \) as follows:

\[
-2 \leq \delta x_{\sigma}^+ < -(1 + \delta x_{\sigma}^+) < -1.
\]

(175)

The condition \( \Lambda^+_{\sigma-}/\Lambda^-_{\sigma} \leq 1 \) in Eq. (173) can be cast into the form \( f(x_{\sigma}^-) \geq \alpha x_{\sigma}^- \) presented in Eq. (154) above, with \( f(x) \) and \( \alpha \) as defined in Eqs. (155) and (156) respectively. In spite of this, one should realize that here \( x_{\sigma}^- > 0 \) (following \( d^+ \sigma > 0 \); see Eq. (145) above), whereas in our previous considerations \( x_{\sigma}^+ < 0 \).

As in the case of Eq. (153), below we show that the condition \( \Lambda^+_{\sigma-}/\Lambda^-_{\sigma} \leq 1 \) in Eq. (173) cannot be trivially satisfied. Readers who wish to take the validity of this statement for granted, may omit the following, up to and including Eq. (179) below.

Along the same lines as in the case of \( d^+ \sigma < 0 \), we deduce that the inequality in Eq. (173) is always violated when

\[
\alpha \geq 2 \land \delta x_{\sigma}^- < -2.
\]

(176)

On the other hand, the inequality in Eq. (173) is always satisfied when

\[
\alpha \leq \frac{2}{-(1 + \delta x_{\sigma}^-)} \land \delta x_{\sigma}^- < -2.
\]

(177)

From the defining expression for \( \alpha \) in Eq. (156) it can be readily deduced that for \( 0 < x_{\sigma}^+ < -(1 + \delta x_{\sigma}^+) \) (see Eq. (174) above), \( \alpha \) can take non-negative values only for \(-2 < \delta x_{\sigma}^- < -1 \). In fact we have

\[
0 \leq \alpha \leq 2 \quad \text{for} \quad -2 \leq \delta x_{\sigma}^- \leq -1 \land 0 \leq x_{\sigma}^+ \leq -(1 + \delta x_{\sigma}^+);
\]

(178)

\( \alpha = 2 \) applies only for \( \delta x_{\sigma}^+ = -2 \) and \( x_{\sigma}^+ \in [0, 1] \). Assuming that \( x_{\sigma}^+ \) and \( \delta x_{\sigma}^- \) are such that \( \alpha \geq -2/(1 + \delta x_{\sigma}^-) \), it is readily deduced that the inequality in Eq. (173) is satisfied provided that

\[
x_{\sigma}^+ \geq -4(1 + \delta x_{\sigma}^-) - 2\alpha \quad \frac{2}{4 - \alpha^2}, \quad \frac{2}{-(1 + \delta x_{\sigma}^-)} \leq \alpha < 2.
\]

(179)

Following Eq. (142), for \( c^-_{\sigma} < -2a_{\sigma}/g \) (or, equivalently, \( \delta x_{\sigma}^- > -2 \)), \( n_\sigma(k_{\sigma,\sigma}^-) > \frac{1}{2} \) so that, unless \( \Lambda^+_{\sigma+} > \Lambda^-_{\sigma} \) (which entails \( Z_{k_{\sigma,\sigma}} < 0 \)), \( \Lambda^+_{\sigma+} \) cannot be a priori discarded. Evidently, since here \( \Lambda^+_{\sigma-} > 0 \), in the event \( \Lambda^+_{\sigma-} \leq \Lambda^-_{\sigma} \), one will be confronted with a situation where there are two possible values to be taken by \( n_\sigma(k_{\sigma,\sigma}^+) \).

Which of the two is the correct value for \( n_\sigma(k_{\sigma,\sigma}^+) \) is a matter that has to be decided on the basis of a further consistency test. Below we shall present an example of such a test but, before doing so, we derive the conditions to be satisfied for the occurrence of \( \Lambda^+_{\sigma+} \leq \Lambda^-_{\sigma} \). Readers who do not wish to consider this aspect, may omit the following, up to the last paragraph of this Section.

It can be easily shown that for \( x_{\sigma}^- > 0 \) (which holds on account of (II) in Eq. (127) above) we have

\[
\Lambda^+_{\sigma+} \leq \Lambda^-_{\sigma} \iff f(x_{\sigma}^-) \geq \beta x_{\sigma}^+,
\]

(180)

where \( f(x) \) has been defined in Eq. (155) above and

\[
\beta := \frac{1}{x_{\sigma}^+} f(x_{\sigma}^+, \delta x_{\sigma}^+).
\]

(181)

It is readily verified that, for \( x_{\sigma}^+ > 0, \beta \geq 2 \). For \( x_{\sigma}^+ > 0 \) (which holds on account of our present assumption, namely \( d^+ \sigma > 0 \)) one equivalently has


\[ \Lambda^+_{\sigma +} \leq \Lambda^-_{\sigma} \iff f(x^>_x) \leq \beta' x^>_x, \quad (182) \]

where

\[ \beta' = \frac{1}{x} f(x^>_x, \delta x^>_x). \quad (183) \]

It is easily deduced that for \( x^>_x \geq 0, \beta' \geq 2 \). On account of \( \delta x^>_x > -2 \) (see the text following Eq. (179) above), along the lines of our earlier considerations we deduce

\[ f(x^-_x) \geq \beta x^<_x \iff x^-_x \geq \frac{2 \beta + 4(1 + \delta x^>_x)}{\beta^2 - 4}. \quad (184) \]

Similarly

\[ f(x^>_x) \leq \beta' x^>_x \iff x^>_x \geq \frac{2 \beta' + 4(1 + \delta x^>_x)}{\beta'^2 - 4}. \quad (185) \]

Note that from the defining expressions in Eqs. (181) and (183) and the expressions in Eqs. (169) and (134) respectively (see also Eq. (133) above) we have

\[ \beta = 2 \Lambda^+_{\sigma +}, \quad \beta' = 2 \Lambda^-_{\sigma} (\equiv 2 \Lambda^-_{\sigma}). \quad (186) \]

In order to establish the conditions under which \( \Lambda^+_{\sigma +} \leq \Lambda^-_{\sigma} \) is realized (if at all), it is natural first to establish the condition(s) required for the realization of \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \). For \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) to materialize, in which case \( \beta = \beta' \) (following Eq. (186)), we must have

\[ x^>_x = \frac{2 \beta + 4(1 + \delta x^>_x)}{\beta^2 - 4} \land x^>_x = \frac{2 \beta + 4(1 + \delta x^>_x)}{\beta^2 - 4}. \quad (187) \]

On the other hand, these expressions cannot be meaningful unless \( y^>_x > -1 \) (or \( x^>_x > \tilde{x}^>_x \); see Eqs. (137) and (158) above) and \( y^>_x < -1 \) (see Eq. (147) above), from which it follows that (note that \( \beta > 2 \))

\[ \delta x^>_x \geq -1 - \frac{2}{\beta} \land -2 \leq \delta x^>_x \leq -1 - \frac{2}{\beta}. \quad (188) \]

For \( \beta > 2 \), these inequalities are more restrictive than \( \delta x^>_x \geq -2 \) and \( -2 \leq \delta x^>_x \leq -1 \) respectively. Note in particular that the range of variation in \( \delta x^>_x \) as required for the satisfaction of \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) becomes narrower, the closer to 2 that \( \beta \) approaches. The inequalities in Eq. (188) imply the following intervals for \( x^>_x \) and \( x^>_x \) corresponding to \( \beta = \beta' \) (or \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \))

\[ x^>_x \geq \frac{2}{\beta} \land \frac{2}{\beta + 2} \leq x^>_x \leq \frac{2}{\beta}. \quad (189) \]

One observes that in the event \( x^>_x = x^>_x \), there is only one possibility for \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) to be realized, namely when \( x^>_x = x^>_x = 2/\beta \). In view of the results in Eqs. (138) and (148), \( x^>_x = x^>_x \) in combination with \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) (note that \( \Lambda_{\sigma} \equiv \Lambda^+_{\sigma +}, \) since \( \Lambda^-_{\sigma} \leq 0 \) imply \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} = 0 \). Since the choice of \( \Lambda^+_{\sigma +} \) for \( \Lambda^+_{\sigma +} \) (which is the unrivalled choice in cases where \( d^>_x < 0 \)) in the case when \( \Lambda^+_{\sigma +} = 0 \) implies that \( n_x(k^+_x) = 0 \), and this in turn amounts to the highly unusual condition for the single-particle spectral function, namely \( A_x(k^+_x; \varepsilon) = 0 \) for all \( \varepsilon < \mu \), we conclude that, in the event \( x^>_x = x^>_x \) and \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma}, \) \( \Lambda^+_{\sigma +} \) is to be identified with \( \Lambda^+_{\sigma +} \). If follows that, in such event, \( Z_{K_{\sigma}^x} = 0 \). Note that the inequalities in Eq. (189) show that \( x^>_x \geq x^>_x \) which in consequence of the results in Eq. (187) implies that, for \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) to be realized, it is necessary that \( \delta x^>_x \geq \delta x^>_x \); the equality \( x^>_x = x^>_x \) implies the equality \( \delta x^>_x = \delta x^>_x \), which following the inequalities in Eq. (188) is only possible if \( \delta x^>_x = \delta x^>_x = 2/\beta \).

It can be shown that \( f(x, \delta x)/x \) (and therefore \( \beta \) and \( \beta' \) for \( x = x^>_x, \delta x = \delta x^>_x \) and \( x = x^>_x, \delta x = \delta x^>_x \), respectively; see Eqs. (181) and (183)) is a monotonically decreasing function of \( x \) (here for \( x > 0 \)) and a monotonically increasing function of \( \delta x \) (here for \( \delta x \) satisfying the appropriate inequality in Eq. (188) above). These properties are properly reflected in the asymptotic expression

\[ \frac{1}{x} f(x, \delta x) \approx 2 + \frac{2 + \delta x}{x} \quad \text{for} \quad x \to \infty, \quad (190) \]

from which one further observes that so long as \( \delta x > -2 \), \( f(x, \delta x)/x \) (and thus \( \beta \) and \( \beta' \)) never attains the value 2 for any finite \( x \).

From the above properties it follows that, by starting from the set of values for \( x^>_x, \delta x^>_x, x^>_x \) and \( \delta x^>_x \) corresponding to \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \), one can achieve the inequality \( \Lambda^+_{\sigma +} < \Lambda^-_{\sigma} \) by (if possible; see the inequalities in Eq. (189) above) increasing \( x^>_x \) and/or (if possible) decreasing \( x^>_x \) while maintaining the values of \( \delta x^>_x \) and \( \delta x^>_x \) corresponding to \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \) (see Eq. (186) above according to which \( \beta = 2 \Lambda^+_{\sigma +}, \) and \( \beta' = 2 \Lambda^-_{\sigma} \)). Alternatively, \( \Lambda^+_{\sigma +} < \Lambda^-_{\sigma} \) can be achieved by maintaining the initial values of \( x^>_x \) and \( x^>_x \) while (if possible) increasing \( \delta x^>_x \) and/or decreasing \( \delta x^>_x \) from their initial values. Evidently, these choices are not unique, and one can obtain (if at all possible) \( \Lambda^+_{\sigma +} < \Lambda^-_{\sigma} \) by other apparent combinations of changes in the parameters corresponding to the condition \( \Lambda^+_{\sigma +} = \Lambda^-_{\sigma} \).

We now deal with a specific case which illustrates in how far the condition \( \Lambda^+_{\sigma +} < \Lambda^-_{\sigma} \) can be considered as feasible; it turns out that for the specific case that we consider, \( \Lambda^+_{\sigma +} < \Lambda^-_{\sigma} \) is never realized. In §6.3 below we investigate FL metallic states corresponding to two-body interaction potentials that are of shorter range than the Coulomb potential and arrive at two specific conditions (see Eqs. (195) and (196) below) which result in \( x^>_x = -g^b_x/(a_x \Lambda^>_{\sigma}) \) and \( x^>_x = -g^b_x/(a_x \Lambda^>_x) \). From these we deduce that

\[ \delta x^-_x = -x^>_x - \Lambda^-_x x^>_x, \quad \delta x^+_x = -x^>_x - \Lambda^-_x x^>_x, \quad (191) \]

which lead to

\[ \delta x^-_x = \delta x^+_x = (\Lambda^-_x - 1)x^>_x - (\Lambda^+ + 1)x^>_x. \quad (192) \]
From this it follows that, for \( \Lambda^e_\sigma = \Lambda^e_\tau \) and in the event \( \Lambda^e_\sigma \) were to be identified with \( \Lambda^e_\tau \equiv \beta/2 \), through employing the expressions for \( x^-_\sigma \) and \( x^+_\sigma \) in Eq. (187) one would have
\[
\delta x^-_\sigma - \delta x^+_\sigma = \frac{2}{\beta} (\delta x^-_\sigma - \delta x^+_\sigma); \tag{193}
\]
this and the fact that \( \beta > 2 \) imply that
\[
\delta x^-_\sigma = \delta x^+_\sigma = -1 - \frac{2}{\beta}. \tag{194}
\]
In arriving at the result on the RHS we have made use of the inequalities in Eq. (188) above, which uniquely determine the only common value that \( \delta x^-_\sigma \) and \( \delta x^+_\sigma \) can take in the case under consideration. From the expressions in Eq. (187) we observe that for \( \delta x^-_\sigma = \delta x^+_\sigma = -1 - 2/\beta \), indeed \( x^-_\sigma = x^+_\sigma = 2/\beta \) and consequently, through Eq. (191), \( \Lambda^-_\sigma = \Lambda^+_\sigma = \beta/2 \). For completeness, here \( \Lambda^-_\sigma = \Lambda^-_\tau, \Lambda^+_\sigma = \Lambda^+_\tau \) and \( \Lambda^-_\tau = \Lambda^+_\tau = 0 \). We observe that, because in the present case \( x^-_\sigma \) and \( x^+_\sigma \) achieve respectively the highest and the lowest values that are compatible with the inequalities in Eq. (189) (similarly and equivalently, for \( \delta x^-_\sigma \) and \( \delta x^+_\sigma \) according to the inequalities in Eq. (188) above), it is not possible to realize the strict inequality \( \Lambda^e_\sigma < \Lambda^-_\sigma \) by appropriately altering the parameters (as described above) \( x^\pm_\sigma, \delta x^\pm_\sigma \) corresponding to \( \Lambda^e_\tau = \Lambda^-_\tau \).

### 6.3. The case when \( \gamma = 1, \tau = 1 \): Fermi liquids

As we have indicated earlier (§ 3), for metallic states of fermions interacting through the long-range Coulomb potential, \( v_{k_F,\sigma} \) is not differentiable in the neighbourhood of \( S_{k_F,\sigma} \). For this reason, considerations in this Section should be viewed as not concerning the metallic GSs of the Coulomb-interacting fermion systems; the treatment appropriate to the latter systems is presented in § 6.1.3 above.

Along the lines of reasoning as in [6] concerning FL metallic states, we deduce that for such states we must have (compare with Eqs. (105) and (106) in [6])
\[
b^-_\sigma = -\Lambda^e_\sigma d^-_\sigma, \tag{195}
b^+_\sigma = -\Lambda^e_\sigma d^+_\sigma. \tag{196}
\]
In the case of the uniform GSs of the Hubbard Hamiltonian, where \( d^\pm_\sigma = d^\pm_\tau \), the results in Eqs. (195) and (196) lead to \( \Lambda^e_\sigma \Lambda^-_\sigma = 1 \) and consequently to \( n_\sigma(k_{F,\sigma}) = \frac{1}{2} \) for \( k_{F,\sigma} \in S_{k_F,\sigma} \) (cf. Eq. (110) in [6]). For two-body interaction potentials which have longer range than the contact potential in the conventional Hubbard Hamiltonian, \( c_\sigma(k_{F,\sigma}) \) cannot be identically vanishing for all \( k_{F,\sigma} \in S_{k_F,\sigma} \) so that, in general, \( b^\pm_\sigma \neq d^\pm_\sigma \) (see Eqs. (123) – (125) above) whereby it is not necessary that for FL metallic states \( n_\sigma(k_{F,\sigma}) = \frac{1}{2} \) should hold. Further, in contrast with the case of the Hubbard on-site interaction for which under all conditions considered in [6] one has \( n_\sigma(k_{F,\sigma}) \geq \frac{1}{2} \) and \( n_\sigma(k_{F,\sigma}) \leq \frac{1}{2} \), even for FL metallic states considered in this Section both \( n_\sigma(k_{F,\sigma}) \leq \frac{1}{2} \) and \( n_\sigma(k_{F,\sigma}) \geq \frac{1}{2} \); satisfying, however, the necessary stability condition \( n_\sigma(k_{F,\sigma}) - n_\sigma(k_{F,\sigma}) =: Z_{k_{F,\sigma}} \geq 0 \), are feasible. Below we explicitly demonstrate the feasibility of \( n_\sigma(k_{F,\sigma}) \leq \frac{1}{2} \).

From Eqs. (125), (132) and (196) we obtain
\[
c^-_\sigma \equiv b^-_\sigma - d^-_\sigma = b^+_\sigma + \frac{1}{\Lambda^e_\sigma} b^+_\sigma. \tag{197}
\]
From (I) and (III) in Eq. (127) we have \( b^-_\sigma > -a_\sigma/g \) and \( b^+_\sigma < -a_\sigma/g \) respectively so that we can write
\[
b^-_\sigma = -\frac{\lambda^-_\sigma a_\sigma}{g}, \lambda^-_\sigma < 1; \quad b^+_\sigma = -\frac{\lambda^+_\sigma a_\sigma}{g}, \lambda^+_\sigma > 1. \tag{198}
\]
On account of the expressions in Eqs. (197) and (198) it follows that, for
\[
\Lambda^-_\sigma \leq \frac{\lambda^+_\sigma}{2 - \lambda^+_\sigma}, \tag{199}
\]
one achieves the condition \( c^-_\sigma \leq -2a_\sigma/g \) required for \( \Lambda^-_\sigma \leq 1 \) (see Eq. (142) above) and thus \( n_\sigma(k_{F,\sigma}) \leq \frac{1}{2} \). Evidently, the consistency of the condition \( \Lambda^-_\sigma \leq 1 \) with that in Eq. (199) implies the further requirement that
\[
1 < \lambda^+_\sigma \leq 2 - \lambda^-_\sigma, \tag{200}
\]
which encompasses both \( \lambda^-_\sigma < 1 \) and \( \lambda^+_\sigma > 1 \) indicated in Eq. (198). It follows that, for two-body interaction potentials of non-vanishing range (corresponding to \( c^-_\sigma \neq 0 \)), \( n_\sigma(k_{F,\sigma}) \leq \frac{1}{2} \) is feasible even for FL metallic GSs considered in this Section.

### § 7. SUMMARY AND CONCLUDING REMARKS

In this paper we have considered some exact properties of the uniform metallic GSs of systems of fermions for arbitrary spatial dimensions interacting through arbitrary isotropic pair potentials that are capable of being Fourier transformed; thus, for instance, systems of fermions interacting through the Lennard-Jones 6 – 12 potential lie outside the domain of applicability of the considerations in this paper, however those interacting through the Aziz et al. potential [104] lie inside. 21 Our present work concerns natural extension of previous work [6] in which we

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21 Both of these potentials have been used for describing the inter-atomic interaction of 3He atoms, with the Aziz et al. potential as being the more superior; for a discussion of these and of a number of other available pair potentials see [104] and [105].
have explicitly dealt with the uniform single-band Hubbard Hamiltonian where the interaction is operative only between particles of opposite spin at the same lattice site.

In the present paper we have explicitly demonstrated that, for \( \mathbf{k} \) approaching the Fermi surface \( S_{F;\sigma} \) of the interacting metallic GS and \( \varepsilon \) approaching the Fermi energy \( \varepsilon_F \) of the interacting system, the self-energy \( \Sigma_\sigma(\mathbf{k};\varepsilon) \) continuously approaches the exact Hartree-Fock self-energy \( \Sigma_{HF}^\sigma(\mathbf{k}) \). On the basis of this and of an exact expression for the deviation of \( \Sigma_\sigma(\mathbf{k};\varepsilon) \) from \( \Sigma_{HF}^\sigma(\mathbf{k}) \), obtained from the Kramers-Krönig relation expressing the real part of the self-energy in terms of the imaginary part, we have deduced the subsidiary equation \( \sigma(\mathbf{k}) = 0 \) (Eqs. (52) and (51)), which in conjunction with the quasi-particle equation expressed in terms of \( \Sigma_\sigma(\mathbf{k};\varepsilon) \) (Eq. (45)) is not fulfilled; following the arguments presented in [6], the set of all such \( \mathbf{k} \) points constitutes the pseudogap regions of what otherwise would be constituent parts of the Fermi surface \( S_{F;\sigma} \).

Amongst others, the GS momentum distribution function \( n_\sigma(\mathbf{k}) \), though singular, is continuous for \( \mathbf{k} \) transposed from inside to outside the underlying Fermi sea through pseudogap regions. For \( \mathbf{k} \in S_{F;\sigma} \), the expression corresponding to \( S_\sigma(\mathbf{k}) = 0 \) amounts to a sum rule concerning \( \text{Im}[\Sigma_\sigma(\mathbf{k};\varepsilon)] \) (Eq. (54)); in this capacity, it can be of considerable relevance both for the purpose of both constraining theoretical models for \( \Sigma_\sigma(\mathbf{k};\varepsilon) \) and determining the consistency of experimental results that are directly related with \( \Sigma_\sigma(\mathbf{k};\varepsilon) \), or \( \text{Im}[\Sigma_\sigma(\mathbf{k};\varepsilon)] \) (such as those corresponding to photoemission and inverse-photoemission experiments). Owing to the generality of our considerations in this paper, the above-mentioned results equally apply to the uniform metallic GSs of the conventional single-band Hubbard Hamiltonian, a fact that can be explicitly verified.

In connection with the pseudogap phenomenon as observed in, for example, the angle-resolved photoemission data concerning the normal states of the cuprate compounds in the underdoped regime [106–110], it is relevant to mention that on general grounds it can be shown [78,6] (see in particular § 3.4 in [78]) that this phenomenon cannot be associated with the uniform GSs of systems for which \( \mathbf{k} \) is defined over the unbounded reciprocal space; thus the single-band Hubbard Hamiltonian (for which the reciprocal space is confined to the 1BZ of the underlying Bravais lattice), even in cases where the interaction is operative solely amongst particles of opposite spin on the same lattice site, is special in that, through the periodicity over the 1BZ of the corresponding functions of \( \mathbf{k} \), it takes account of Umklapp processes, albeit in some restricted form; this aspect is vital for the possibility of a uniform metallic GS of the single-band Hubbard Hamiltonian supporting the pseudogap phenomenon. With reference to the observations in [6], for such states \( S_{F;\sigma} \), \( S_{F;\sigma} \) is non-empty and, in view of our observations in the present work, \( S_\sigma(\mathbf{k}) \neq 0 \) for all \( \mathbf{k} \in S_{F;\sigma} \).

For the uniform and isotropic GSs of the uniform-electron-gas system, where on account of isotropy and of the Luttinger theorem concerning the ‘volume’ enclosed by \( S_{F;\sigma} \), one has \( S_{F;\sigma} \equiv S_{F;\sigma}^{(0)} \), through making use of \( \Sigma_\sigma(\mathbf{k};\varepsilon) \sim \Sigma_{HF}^\sigma(\mathbf{k}) \) for \( \mathbf{k} \) approaching \( S_{F;\sigma}^{(0)} \) and \( \varepsilon \to \varepsilon_F \), we have deduced (§ 5) exact expressions for the exchange potential \( \mu_{\sigma;\varepsilon} \) and correlation potential \( \mu_{\sigma;\varepsilon} \), contributing to the exchange-correlation potential \( \mu_{\sigma;\varepsilon;\varepsilon} \equiv \mu_{\sigma;\varepsilon} + \mu_{\sigma;\varepsilon} \) which plays a central role within the framework of the GS density-functional theory [75–77]. Our expression for \( \mu_{\sigma;\varepsilon} \), specialized to systems of electrons interacting through the Coulomb potential for \( d = 3 \), identically reproduces the well-known exact result for the exchange potential. Making use of the RPA for \( n_\sigma(\mathbf{k}) \) corresponding to the paramagnetic GSs of the uniform-electron-gas system (note that, for systems of Coulomb-interacting fermions, \( n_\sigma(\mathbf{k}) - n_\sigma^{(0)}(\mathbf{k}) \) reproduces the leading-order contribution to the exact \( n_\sigma(\mathbf{k}) - n_\sigma^{(0)}(\mathbf{k}) \) in the high-density limit), we have numerically calculated \( \mu_{\sigma;\varepsilon} \), which in the high-density limit, and up to densities corresponding to the dimensionless Wigner-Seitz radius \( r_s \lesssim 1 \), is in excellent agreement with the \( \mu_{\sigma;\varepsilon} \) deduced from the quantum Monte Carlo results for the GS correlation energy (see Figs. 1 and 2).

We have explicitly shown that interactions of non-zero range are of non-trivial consequence to a number of GS and excited-states properties of metallic systems. For instance, whereas for a strictly contact-type two-body interaction potential \( n_\sigma(\mathbf{k};\varepsilon) \geq \frac{1}{2} \) and \( n_\sigma(\mathbf{k};\varepsilon) \leq \frac{1}{2} \) for \( \mathbf{k} \in S_{F;\sigma} \) [6], for two-body interaction potentials of non-vanishing range in principle both \( n_\sigma(\mathbf{k};\varepsilon) \leq \frac{1}{2} \) and \( n_\sigma(\mathbf{k};\varepsilon) > \frac{1}{2} \) are feasible (in both cases, subject to the condition \( n_\sigma(\mathbf{k};\varepsilon) - n_\sigma(\mathbf{k};\varepsilon) \geq 0 \), implied by the assumed stability of the underlying GSs). This aspect is borne out by the quantum Monte Carlo results for ferromagnetically ordered uniform GSs one encounters direct spin gap even in models where \( \mathbf{k} \) is defined over the unbounded reciprocal space. It is interesting to note that the approximate solution of the Hubbard model, the so-called Hubbard-I solution [10], predicts an indirect (Mott-Hubbard) gap (see Fig. 1 in [10]).

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22 In these cases, indirect gap is not excluded. Further, for
$n_\sigma(k)$ pertaining to the uniform and isotropic GSs of the Coulomb-interacting electron-gas system for $d = 2$ [111] (see Fig. 5.9 herein) in the low-density regime 23 and of $^3$He in the normal liquid state at sufficiently large ambient pressures [105,113–116]. In the light of this and of the strict inequality $n_\sigma(k_F,\sigma) \geq \frac{1}{2}$ applicable to the $n_\sigma(k)$ pertaining to the uniform GSs of the conventional single-band Hubbard Hamiltonian [6], employed in studies of $^3$He [117–119], as well as to the uniform GSs of the Stoner Hamiltonian (involving contact interaction but defined on the continuum; likewise employed in studies of $^3$He within the framework of the paramagnon theory [120–124]; for a review of spin-fluctuation theories see [125]), one observes that such Hamiltonians cannot be capable of reliably describing the normal liquid state of $^3$He. In this connection, it is in place to refer to a series of papers by Hirsch (see [55] and references herein) in which the viewpoint has been consistently advocated that many (collective) phenomena for whose rationalization traditionally the conventional single-band Hubbard Hamiltonian has been invoked should in fact be accounted for by means of ‘extended’ Hubbard Hamiltonians (such as considered in [49–65], or in [126–129]), involving site off-diagonal (to be contrasted with on-site) interaction terms (including, e.g., the nearest-neighbour exchange). In [55], Hirsch referred to such phenomena as itinerant ferromagnetism [130,131] (see also [6]), 24 heavy-fermion superconductivity [132,133], high-temperature superconductivity in the cuprate compounds [44] (see also [134]), and superfluidity in liquid $^3$He [55].

Since for the (correlated) GS kinetic energy we have $\sum_{k,\sigma} \epsilon_k n_\sigma(k)$, by continuity it follows that in general the GS kinetic energy of systems in which $n_\sigma(k_F,\sigma) < \frac{1}{2}$, $k_{F,\sigma} \in S_{F,\sigma}$, exceeds that of comparable systems in which $n_\sigma(k_F,\sigma) \geq \frac{1}{2}$ (note that $n_\sigma(k) \geq 0$ and $\sum_{k,\sigma} n_\sigma(k) = N$, independent of interaction). We thus observe a direct relationship between the range of the two-body interaction potential and the magnitude of the corresponding GS kinetic energy, with the latter tending to increase (in the manner specified above) in consequence of increasing the range of the interaction potential. The existence of such a direct relationship between the range of the interaction potential and the value of the GS kinetic energy should be of relevance to a better understanding of the physics of the cuprate superconductors for which there

23 We recall that, for $d = 3$ and Coulomb-interacting fermions, $n_{\sigma^{\text{eff}}}(k_{F,\sigma})$ submerges below $\frac{1}{2}$ for densities corresponding to $r_s > 6.09887 \ldots$ (see footnote 15 above); the Monte Carlo results by Ortiz and Ballone [112] on the other hand show that, for $r_s = 10$, $n_\sigma(k_{F,\sigma}) \approx 0.09$. Interestingly, for $d = 2$, according to the quantum Monte Carlo results by Conti [111], for $r_s = 10$ one has $n_\sigma(k_{F,\sigma}) \approx 0.55$ and for $r_s = 20$, $n_\sigma(k_{F,\sigma}) \approx 0.42$. We observe that, for sufficiently large interaction strength, indeed the non-vanishing range of the interaction potential (here the Coulomb potential) gives rise to $n_\sigma(k_{F,\sigma}) < \frac{1}{2}$.

24 Concerning the role of interactions of longer range than the on-site repulsion in promoting specifically partial ferromagnetism, we refer the reader to the phase diagram in Fig. 4 of [62] which illustrates, albeit on the basis of a mean-field approximation, the consequence of a nearest-neighbour repulsive interaction energy $V$ (note that in the above-mentioned phase diagram the $U$ axis intersects the $V$ axis at some positive value of $V$). In this connection we mention that according to the analysis in [6], in the case of the conventional single-band Hubbard Hamiltonian, partially polarized uniform ferromagnetic states are often barred from qualifying as eigenstates through a kinematic constraint (see Eq. (63) in [6]); it can be readily verified that for longer-range interaction potentials no such a priori kinematic constraint exists, this in consequence of the $k$ dependence of $\Sigma_0^{\text{eff}}(k)$ in the case of the latter potentials.

25 We do not unreservedly subscribe to the assignments in [55] quoted above. For instance, in our opinion it is not the phenomenon of superconductivity in heavy-fermion compounds that has been rationalized by means of the conventional Hubbard model (explicitly, in [135], to which in [55] is referred, one does not explicitly rely on the Hubbard Hamiltonian). Rather, in considering the heavy-fermion compounds and superconductivity [132,133,136,137,135] in these, one has in essence solely relied on the so-called ‘almost-localized Fermi-liquid’ picture [117,118] of the charge carriers; the latter has its root in the Brinkman-Rice [138] scenario concerning the nature of the metallic states of the Hubbard Hamiltonian (for $d = 3$) at half-filling for the on-site $U$ approaching from below a critical value $U_c$, for which, according to the Gutzwiller Ansatz for the GS wavefunction of the Hubbard Hamiltonian combined with the Gutzwiller approximation [9,139], the jump in the GS momentum distribution function at $S_{F,\sigma}$ vanishes and thereby the inverse of the quasiparticle effective mass (hence the qualification ‘almost localized’). For completeness, we mention that the Gutzwiller approximation (to be distinguished from the Gutzwiller Ansatz) is a well-known source of uncertainty. For instance, the exact results corresponding to the Gutzwiller Ansatz for the GS wavefunction of the single-band Hubbard Hamiltonian for $d = 1$ [140] reveal that at half-filling the above-mentioned jump in the momentum distribution function does not vanish at any finite value of $U$; in contrast, according to the Gutzwiller approximation for $d = 1$, this jump vanishes for $U_c/t \approx 10$ (see Fig. 13 in [140]); these results should in turn be contrasted with the exact result indicated in footnote 20 above. Finally, insofar as the normal states of the heavy-fermion compounds are concerned, although the considerations in [141] are based on the Gutzwiller Ansatz (together with the Gutzwiller approximation) for the GS wavefunction of the Hubbard Hamiltonian, the work in [142], based on the periodic Anderson Hamiltonian, leaves no doubt that the analogies proposed in [141] have indeed been based on ‘intuitive grounds’.
is growing evidence indicating that in the normal state the kinetic-energy contribution to the GS total energy is relatively larger than in conventional metals and that superconductivity in the former is driven by a consequent decrease in the kinetic energy of these systems upon entering into the superconducting state. In the light of this and of our theoretical finding, we believe that any theoretical modelling of in particular the cuprate compounds is required to take account of the non-zero range of the interparticle interaction potential.

In addition to establishing the above-mentioned impact that a non-zero range of interaction has on the behaviour of $n_\sigma(k)$ in the vicinity of $S_{\gamma,\sigma}$, we have explicitly exposed (§ 6) some distinctive features associated with the actual range of the interaction potential; that is whether this range is sharply limited to a finite interparticle distance or it extents to arbitrary large distances. For instance, for interaction potentials $v(r-r')$ that possess power-law decay for $|r-r'| \to \infty$, the singular behaviour of $n_\sigma(k)$ in the neighbourhood of any $k$ directly implies a singular behaviour in the Fock part $\Sigma^\sigma_F(k)$ of the self-energy in the neighbourhood of the same $k$; the two singularities are, however, of different types. This observation is specifically significant for the $k$ points in the neighbourhood of $S_{\gamma,\sigma}$, where $n_\sigma(k)$ is unconditionally singular (and not necessarily discontinuous). From our considerations it follows that, for systems of fermions interacting through a potential $v(r-r')$ decaying, for instance, like $1/|r-r'|^m$ for $|r-r'| \to \infty$, a discontinuity in $n_\sigma(k)$ at a general $k = k_{\gamma,\sigma} \in S_{\gamma,\sigma}$ implies a logarithmic divergence at $k_{\gamma,\sigma}$ in the $m$th derivative (in the direction of the radius vector $k_{\gamma,\sigma}$) of $\Sigma^\sigma_F(k)$.

We believe that a detailed examination of $n_\sigma(k)$ determined experimentally (for $k$ in the close vicinity of $S_{\gamma,\sigma}$), in conjunction with the appropriate expressions for this function as presented in this paper, can shed light on some essential aspects of the two-body interaction potential to be employed within the framework of an extended single-band Hubbard Hamiltonian. The details presented in this paper can also with advantage be employed to constrain (approximate) theoretical frameworks concerning correlation functions (such as the self-energy $\Sigma_\sigma(k;\varepsilon)$) pertaining to the metallic GSs of the many-body Hamiltonians considered in this paper.

ACKNOWLEDGEMENTS

With pleasure I thank Dr R. J. Needs and Professor G. Senatore for discussions concerning the quantum Monte Carlo data for the ground-state momentum distribution function of liquid $^3$He; I am further indebted to Professor Senatore for kindly making Ref. [111] available to me prior to publication. With appreciation I thank Spinoza Institute for hospitality and support.

APPENDIX A: ESTIMATION OF ERROR IN $S_\sigma(k)$ WITHIN THE FRAMEWORK OF A FINITE-ORDER MANY-BODY PERTURBATION THEORY FOR $\Sigma_\sigma(k;\varepsilon)$

In the defining expression for $S_\sigma(k)$ in Eq. (51) we encounter $\text{Im}\{\Sigma_\sigma(k;\varepsilon_f \pm \varepsilon)\}$ in which for definiteness we assume $\Sigma_\sigma(k;\varepsilon) \in (-\infty, \infty)$, to have been calculated within the framework of a finite-order perturbation theory based on skeleton self-energy diagrams (for the definition see [92]) evaluated in terms of the exact single-particle Green function. With the latter assumption we wish to estimate the error in $S_\sigma(k)$ as arising from the truncation of the set of skeleton self-energy diagrams and not from the further approximation corresponding to using an approximate single-particle Green function.

We proceed by writing $S_\sigma(k)$ as follows

$$S_\sigma(k) = S^{(1)}_\sigma(k;\Delta) + S^{(2)}_\sigma(k;\Delta),$$

(A1)

where

$$S^{(1)}_\sigma(k;\Delta) := \frac{1}{\pi} \int_0^\Delta \frac{d\varepsilon}{\varepsilon} \text{Im}\{\Sigma_\sigma(k;\varepsilon_f + \varepsilon) + \Sigma_\sigma(k;\varepsilon_f - \varepsilon)\},$$

(A2)

$$S^{(2)}_\sigma(k;\Delta) := \frac{1}{\pi} \int^\infty_\Delta \frac{d\varepsilon}{\varepsilon} \text{Im}\{\Sigma_\sigma(k;\varepsilon_f + \varepsilon) + \Sigma_\sigma(k;\varepsilon_f - \varepsilon)\},$$

(A3)

in which $\Delta > 0$ stands for an energy sufficiently large with respect to a relevant energy scale in the system under consideration [78] so that a finite-order large-$|\varepsilon|$ asymptotic series for $\text{Im}\{\Sigma_\sigma(k;\varepsilon_f \pm \varepsilon)\}$ is accurate for $|\varepsilon| \geq \Delta$. Later in our considerations we shall consider the case in which the latter series is formally summed to all orders whereby it is possible to effect the limit $\Delta \downarrow 0$. To avoid unnecessary technical complication, in what follows we assume that the two-body interaction potential $v(r-r')$ is of shorter range than the Coulomb potential and moreover that the single-particle excitation spectrum $\varepsilon_k$ is unbounded from above so that the single-particle spectral function $A_\sigma(k;\varepsilon)$ is of unbounded support. For such cases we have [78]

$$\text{Im}\{\Sigma_\sigma(k;\varepsilon)\} \sim \frac{\Xi_\sigma(k)}{\varepsilon} + \frac{\Pi_\sigma(k)}{\varepsilon^2} + \ldots \text{ for } |\varepsilon| \to \infty,$$

(A4)

where

\begin{itemize}
  \item \textsuperscript{26} For the stability of the GS of the system under consideration it is required that $\Xi_\sigma(k) \geq 0$, $\forall k, \sigma$ [78].
\end{itemize}
\( \Xi_{\sigma}(k) := -\frac{1}{\pi} \int_{0}^{\infty} d\varepsilon' \left\{ \text{Re}[\Sigma_{\sigma}(k; \varepsilon') + \Sigma_{\sigma}(k; -\varepsilon')] \right\} - 2\Sigma_{\sigma;\infty}(k) \}, \quad (A5) \\
\Pi_{\sigma}(k) := -\frac{1}{\pi} \int_{0}^{\infty} d\varepsilon' \left\{ \varepsilon' \text{Re}[\Sigma_{\sigma}(k; \varepsilon') - \Sigma_{\sigma}(k; -\varepsilon')] \right\} - 2\Sigma_{\sigma;\infty}(k) \}, \quad (A6) \\

In Eqs. (A5) and (A6) the real-valued functions \( \Sigma_{\sigma;\infty}(k) \), \( m = 0, 1 \), are the coefficients of the first two leading terms in the large-\( |z| \) asymptotic series of \( \Sigma_{\bar{\sigma}}(k; z) \), with \( \text{Im}(z) \neq 0 \), that is

\[ \Sigma_{\bar{\sigma}}(k; z) \sim \Sigma_{\sigma;\infty}(k) + \frac{\Sigma_{\sigma;\infty}(k)}{z} + \ldots, \quad |z| \to \infty. \]  

(A7)

Here \( \Sigma_{\bar{\sigma}}(k; z) \) stands for the analytic continuation of \( \Sigma_{\sigma}(k; \varepsilon) \) into the physical Riemann sheet of the complex \( z \) plane, for which we have \( \Sigma_{\sigma}(k; \varepsilon) = \lim_{\mu \to \infty} \Sigma_{\sigma}(k; \varepsilon \pm i\mu) \), \( \varepsilon \geq \mu \). We point out that, even for cases where \( \Sigma_{\sigma;\infty}(k) \) is bounded for all finite values of \( m \), use of a complex \( z \) in Eq. (A7) is necessary when the series on the RHS of this equation is taken account of to some infinite order, because \( \Sigma_{\bar{\sigma}}(k; z) \) possesses a branch-cut discontinuity along the real \( \varepsilon \) axis. It can be shown that \([82,78]\)

\[ \Sigma_{\sigma;\infty}(k) \equiv \Sigma_{\bar{\sigma}}^\text{fr}(k). \]  

(A8)

We write

\[ \Xi_{\sigma}(k) \equiv \Xi_{\sigma}^{(1)}(k; \Delta) + \Xi_{\sigma}^{(2)}(k; \Delta), \]  

(A9)

\[ \Pi_{\sigma}(k) \equiv \Pi_{\sigma}^{(1)}(k; \Delta) + \Pi_{\sigma}^{(2)}(k; \Delta), \]  

(A10)

where \( \Xi_{\sigma}^{(1)}(k; \Delta) \), \( \Xi_{\sigma}^{(2)}(k; \Delta) \), \( \Pi_{\sigma}^{(1)}(k; \Delta) \) and \( \Pi_{\sigma}^{(2)}(k; \Delta) \) stand in relation to \( \Xi_{\sigma}(k) \) and \( \Pi_{\sigma}(k) \), defined in Eqs. (A5) and (A6), as \( S_{\sigma}^{(1)}(k) \) and \( S_{\sigma}^{(2)}(k) \) in Eqs. (A2) and (A3) in relation to \( S_{\sigma}(k) \), defined in Eq. (51). From the defining expressions for the functions on the RHSs of Eqs. (A9) and (A10), making use of the asymptotic series for \( \Sigma_{\sigma}(k; z) \) in Eq. (A7), for \( \Delta \to \infty \) one straightforwardly obtains

\[ \Xi_{\sigma}^{(2)}(k; \Delta) \sim \frac{2\Sigma_{\sigma;\infty}(k)}{\pi \Delta} - \frac{2\Sigma_{\sigma;\infty}(k)}{3\pi \Delta^3} - \ldots, \]  

(A11)

\[ \Pi_{\sigma}^{(2)}(k; \Delta) \sim \frac{2\Sigma_{\sigma;\infty}(k)}{\pi \Delta} - \frac{2\Sigma_{\sigma;\infty}(k)}{3\pi \Delta^3} - \ldots. \]  

(A12)

From the above results we deduce

\[
\text{Im}[\Sigma_{\sigma}(k; \varepsilon_{\varphi} + \varepsilon) + \Sigma_{\sigma}(k; \varepsilon_{\varphi} - \varepsilon)] \\
\sim 2 \left[ \Pi_{\sigma}^{(1)}(k; \Delta) - \varepsilon_{\varphi} \Xi_{\sigma}^{(1)}(k; \Delta) \right] + \frac{2}{\pi \Delta} \left( \Sigma_{\sigma;\infty}(k) - \varepsilon_{\varphi} \Sigma_{\sigma;\infty}(k) \right) \frac{1}{\varepsilon_{\varphi}}, \quad |\varepsilon|, \Delta \to \infty. \]

(A13)

Making use of this expression, from the defining expression for \( S_{\sigma}^{(2)}(k) \) in Eq. (A3) we obtain

\[
S_{\sigma}^{(2)}(k; \Delta) \sim \frac{\Pi_{\sigma}^{(1)}(k; \Delta) - \varepsilon_{\varphi} \Xi_{\sigma}^{(1)}(k; \Delta)}{\pi} + \frac{2\Sigma_{\sigma;\infty}(k) - \varepsilon_{\varphi} \Sigma_{\sigma;\infty}(k)}{\pi^2} + \ldots, \quad \Delta \to \infty. \]  

(A14)

It is interesting to note the occurrence in Eq. (A14) (in particular in the second term on the RHS) of \( \varepsilon_{\varphi} \), the energy with respect to which the energies of the lowest-lying single-particle excitations are measured, in conjunction with coefficients that determine the behaviour of \( \Sigma_{\sigma}(k; \varepsilon) \) at large values of \( |\varepsilon| \).

The expression on the RHS of Eq. (A14) is not a well-ordered asymptotic series, as the first term involves contributions to terms of higher order in \( 1/\Delta \) than \( 1/\Delta^2 \). Since \( \left( \Pi_{\sigma}^{(1)}(k; \Delta) - \Pi_{\sigma}(k) \right) = o(1) \) and \( \left( \Xi_{\sigma}^{(1)}(k; \Delta) - \Xi_{\sigma}(k) \right) = o(1) \) for \( \Delta \to \infty \), to the leading-order in \( 1/\Delta \) we have

\[
S_{\sigma}^{(2)}(k; \Delta) \sim \frac{\Pi_{\sigma}(k) - \varepsilon_{\varphi} \Xi_{\sigma}(k)}{\Delta^2} \quad \text{for} \quad \Delta \to \infty. \]  

(A15)

Note that by replacing \( \Pi_{\sigma}(k) \) and \( \Xi_{\sigma}(k) \) on the RHS of this expression by the expressions on the RHSs of Eqs. (A9) and (A10) respectively and using the leading-order terms in the asymptotic series on the RHSs of Eqs. (A11) and (A12) respectively, we recover the expression on the RHS of Eq. (A14).

From our perspective, the most important aspect of the asymptotic expression in Eq. (A14) is the explicit dependence on \( \Sigma_{\sigma;\infty}(k) \) and \( \Sigma_{\sigma;\infty}(k) \) of the second term on the RHS. This in view of the fact that according to the analysis in [78], the reproduction of the exact \( \Sigma_{\sigma;\infty}(k) \) requires calculation of \( \Sigma_{\sigma}(k; \varepsilon) \) to third order and that of \( \Sigma_{\sigma;\infty}(k) \) to fourth order in the perturbation series in terms of skeleton self-energy diagrams, with these in turn evaluated in terms of the bare particle-particle interaction function and the exact interacting single-particle Green function. Thus the second term on the RHS of Eq. (A14) associated with the \( \Sigma_{\sigma}(k; \varepsilon) \) evaluated in terms of the full set of first- and second-order skeleton diagrams deviates from its exact counterpart. In connection with the result in Eq. (A15) (or Eq. (A14)), it is important to realize that since \( S_{\sigma}^{(1)}(k; \Delta) \) and \( S_{\sigma}^{(2)}(k; \Delta) \) as defined in Eqs. (A2) and (A3) respectively exist for \( \Delta \downarrow 0 \), and since \( S_{\sigma}^{(1)}(k; \Delta) \to 0 \) for \( \Delta \downarrow 0 \), one can in principle recover the entire \( S_{\sigma}(k) \) by evaluating the large-\( \Delta \) asymptotic series of \( S_{\sigma}^{(2)}(k; \Delta) \) to all orders in \( 1/\Delta \) and, subsequent to its full summation, taking the limit \( \Delta \downarrow 0 \). Although this approach is of no practical use, the fact that the formal infinite-order large-\( \Delta \) asymptotic series of \( S_{\sigma}^{(2)}(k; \Delta) \) is capable of exactly reproducing \( S_{\sigma}(k) \) is significant in it that sheds light on
the way (as in Eq. (A14) above) in which the coefficients \( \{ \Sigma_{\sigma;\infty_{m}}(k) \} \) of the large-\( |\varepsilon| \) asymptotic series of \( \Sigma_{\sigma}(k;\varepsilon) \) contribute to those of the former asymptotic series; by the further knowledge that for \( m \geq 1 \) all skeleton self-energy diagrams from order 2 up to and including order \( m+1 \) contribute to \( \Sigma_{\sigma;\infty_{m}}(k) \) [78], one gains insight into the consequences for \( \Sigma_{\sigma}(k;\varepsilon) \) of employing a finite-order perturbation series for \( \Sigma_{\sigma}(k;\varepsilon) \). The same line of reasoning applies to \( \Xi_{(2)}^{(2)}(k;\Delta) \) and \( \Pi_{\sigma}^{(2)}(k;\Delta) \) from whose complete large-\( \Delta \) asymptotic series the exact \( \Xi_{\sigma}(k) \) and \( \Pi_{\sigma}(k) \) respectively can be deduced; these asymptotic series are evidently fully determined by \( \{ \Sigma_{\sigma;\infty_{m}}(k) \} \) (see Eqs. (A11) and (A12) above). In this connection note that according to Eq. (A15) the leading-order term in the large-\( \Delta \) asymptotic series of \( \Sigma_{\sigma}^{(2)}(k) \) is in addition to \( \varepsilon_{F} \) fully determined by \( \Xi_{\sigma}(k) \) and \( \Pi_{\sigma}(k) \). Concerning \( \varepsilon_{F} \), in view of Eqs. (46) and (A8) one observes that this constant is determined by the first-order (skeleton) self-energy diagram; its exact determination is, however, dependent on the knowledge of the exact interacting single-particle Green function \( G_{\sigma}(k;\varepsilon) \) or, what in this context is the same, \( n_{\sigma}(k) \).

The inaccuracy in a calculated \( S_{\sigma}(k) \), which in practice arises from use of both a finite set of (skeleton) self-energy diagrams and an approximate single-particle Green function (either a non-interacting single-particle Green function or one determined self-consistently), combined with the inaccuracy in \( \Sigma_{\sigma}^{\text{HF}}(k) \) arising from use of an approximate single-particle Green function (or \( \sigma_{\sigma}(k) \); see Eqs. (12), (16) and (17)), leads through Eqs. (45) and (50) to deviation of a calculated Fermi surface from its exact counterpart \( S_{\sigma}^{\text{HF}}(k) \). For the uniform paramagnetic metallic GSs of the single-band Hubbard Hamiltonian where \( \Sigma_{\sigma}^{\text{HF}}(k) \) is equal to the exactly-known constant value \( U_{n}/(2\hbar) \), in which \( n = N/N_{L} \) (the total number of fermions per lattice site), the inaccuracy in a calculated Fermi surface based on the use of Eq. (45) is entirely attributable to that in the underlying \( S_{\sigma}(k) \) (see Eq. (50)). The apparent violation (albeit very slightly) of the exact result \( S_{\sigma}^{\text{HF}} \subseteq S_{\sigma}^{(0)} \), deduced in [6], by the \( S_{\sigma}^{\text{HF}} \) (pertaining to the uniform paramagnetic GS of the single-particle Hubbard Hamiltonian, with \( U/t = 4 \) determined from a self-consistently evaluated \( \Sigma_{\sigma}(k;\varepsilon) \) (based on the second-order expansion of \( \Sigma_{\sigma}(k;\varepsilon) \)) is thus attributable to the fact that none of \( \Sigma_{\sigma;\infty_{m}}(k;\varepsilon) \) is correct [78]. For our criticism of non-selfconsistently calculated Fermi surfaces pertaining to the metallic states of the single-band Hubbard Hamiltonian we refer the reader to [6]. Note the principal advantage of the expression for \( S_{\sigma}^{\text{HF}} \) in Eq. (53) in comparison with that in Eq. (45); following the evident fact that \( \Sigma_{\sigma}^{\text{HF}}(k) \) is in principle exactly determined by the first-order self-energy operator (i.e. leaving aside the necessity for the knowledge of the exact \( n_{\sigma}(k) \)), use of the expression in Eq. (53) in conjunction with a first-order expression for the self-energy operator guarantees the exact reproduction of the skeleton of the underlying Fermi surface (if not the entire Fermi surface).

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explicit analysis of the eight presented data points for
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the value presented above. For this reason, we do not consider
a somewhat more accurate, but vastly time-consuming, calcula-
ation shows that through these are cubic-splines interpolations.
Explicit calculation of \( \bar{\mu}_{c; \sigma} \) for \( r_s \) \( \leq 0 \).
A least-squares fit of the expression \( a \ln(r_s) + b \) to
curve QMC over the range presented yields \( a = 0.0308213 \),
\( b = -0.0589913 \); a similar least-squares fit to curve RPA over
the range presented yields \( a = 0.0304144 \), \( b = -0.170157 \).
Explicit analysis of the eight presented data points for \( \bar{\mu}_{c; \sigma} \)
and \( \bar{\mu}_{QMC} \) yields \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{QMC} = 0.107 \pm 0.002 \), to be compared with
\( b_{QMC} - b_{RPA} = 0.111 \). The constancy of \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{QMC} \) over the entire
range presented is consistent with the fact that the potential
\( \bar{\mu}_{c; \sigma} \) is determined up to an additive constant. For completeness,
a somewhat more accurate, but vastly time-consuming, calculation
of \( \mu_{c; \sigma}^{RPA} \) at four different \( r_s \) values inside \( 10^{-9}, 10^{-3} \) reveals
that while \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{RPA} \) remains independent of \( r_s \), the absolute
value of \( b_{RPA} \) decreases slightly (by about 0.003) with respect to
the value presented above. For this reason, we do not consider
\( b_{RPA} = -0.170157 \) as being the converged value.

FIG. 1. The correlation potential \( \bar{\mu}_{c; \sigma} \) (in Hartree
atomic units) pertaining to the paramagnetic GS of the
Coulomb-interacting uniform-electron-gas system for \( d = 3 \) as
calculated through the expression in Eq. (87) with \( n_x(k_F x) \)
herein replaced by \( n_x^{qmc}(k_F x) \), due to Daniel and Vosko [95],
and the \( \bar{\mu}_{c; \sigma} \) determined through \( \bar{\mu}_{c; \sigma} = \hat{\varepsilon}_c - (r_s/3)\partial \hat{\varepsilon}_c / \partial r_s \)
(cf. Eq. (92)) with \( \hat{\varepsilon}_c \) herein replaced by a parametrized expression
due to Vosko et al. [97] based on the quantum Monte Carlo results (curve QMC) due to Ceperley and Adler [99].
The open circles indicate the explicitly calculated data and the lines through these are cubic-splines interpolations.
Explicit calculation shows that \( \bar{\mu}_{c; \sigma} \sim 0.0310907 \ln(r_s) - 0.0570205 \) for
\( r_s \downarrow 0 \). A least-squares fit of the expression \( a \ln(r_s) + b \) to
curve QMC over the range presented yields \( a = 0.0308213 \),
\( b = -0.0589913 \); a similar least-squares fit to curve RPA over
the range presented yields \( a = 0.0304144 \), \( b = -0.170157 \).
Explicit analysis of the eight presented data points for \( \bar{\mu}_{c; \sigma} \) and
\( \mu_{c; \sigma}^{QMC} \) yields \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{QMC} = 0.107 \pm 0.002 \), to be compared with
\( b_{QMC} - b_{RPA} = 0.111 \). The constancy of \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{QMC} \) over the entire
range presented is consistent with the fact that the potential
\( \bar{\mu}_{c; \sigma} \) is determined up to an additive constant. For completeness,
a somewhat more accurate, but vastly time-consuming, calculation
of \( \mu_{c; \sigma}^{RPA} \) at four different \( r_s \) values inside \( 10^{-9}, 10^{-3} \) reveals
that while \( \bar{\mu}_{c; \sigma} - \mu_{c; \sigma}^{RPA} \) remains independent of \( r_s \), the absolute
value of \( b_{RPA} \) decreases slightly (by about 0.003) with respect to
the value presented above. For this reason, we do not consider
\( b_{RPA} = -0.170157 \) as being the converged value.

FIG. 2. The correlation potentials \( \bar{\mu}_{c; \sigma} \) and \( \bar{\mu}_{c; \sigma}^{QMC} \) over a larger range than in Fig. 1 (for details of the underlying calculations see the caption of Fig. 1). The vertical broken line at \( \ln(r_s) = 7.769269 \ldots = 2.050176 \ldots \) indicates the boundary beyond which \( Z_{RPA} = n_{\sigma}^{RPA}(k_F r_s) - n_{\sigma}^{QMC}(k_F r_s) \) is negative, indicative of the instability of the uniform paramagnetic GS of the system under consideration according to the RPA (see footnote 15). Note the remarkable near-constant behaviour of \( \bar{\mu}_{c; \sigma} - \bar{\mu}_{c; \sigma}^{QMC} \) over the range of validity of the RPA. That this aspect cannot be due to smallness of higher-order correlation effects is evident from the behaviour of finite-order asymptotic series of \( \bar{\mu}_{c; \sigma} \), for \( r_s \downarrow 0 \), at large values of \( r_s \), for which we employ (broken curves) \( \bar{\mu}_{c; \sigma} \sim 0.0310907 \ln(r_s) - 0.0570205 \) for curve (a),
\( \bar{\mu}_{c; \sigma} \sim 0.0310907 \ln(r_s) - 0.0570205 - 0.0585 r_s \) for curve (b) and
\( \bar{\mu}_{c; \sigma} \sim 0.0310907 \ln(r_s) - 0.0570205 - 0.0585 r_s + 0.2794 r_s^{1/2} \) for curve (c). These asymptotic series correspond to \( \mu_{c; \sigma}^{QMC} \). Our calculation of \( \bar{\mu}_{c; \sigma} \) based on the expression in Eq. (87) with \( n_x(k_F x) \)
therein replaced by a parametrized expression due to Gori-Giorgi and Ziesche [100] yields values between approximately \( -5 \times 10^{-7} \) and \( 7 \times 10^{-3} \) over the range \( r_s \lesssim 12 \) where this expression is as-
serted reliably to represent the momentum distribution function.

The reason underlying this shortcoming is discussed in the text.
FIG. 3. The behaviours of \( \alpha_{\sigma} := [1 - n_{\sigma}(k_f, \sigma)]/a \) (curve (a)) and \( \alpha_{\sigma}^+ := n_{\sigma}(k_{f, \sigma})/a \) (curve (b)), where \( a := r_s/(\pi^2 \gamma_0) \), in which \( \gamma_0 \) is defined in Eq. (88); the results presented here correspond to \( n_{\sigma}(k) \equiv n_{\sigma}^{\text{ext}}(k) \) [95]. One observes that, although for sufficiently small \( r_s \), \( \alpha_{\sigma}^- \) and \( \alpha_{\sigma}^+ \) approach towards the same value \( \alpha_{\sigma} \), in contrast with the finding by Daniel and Vosko [95] this value is not equal to approximately 1.7, a value to which \( \alpha_{\sigma}^- \) and \( \alpha_{\sigma}^+ \) are indeed relatively close for \( 10^{-4} \lesssim r_s \lesssim 1 \). From the results depicted in this figure, one further observes that, for \( r_s \downarrow 0 \) (explicitly, for \( r_s \lesssim 10^{-4} \)) \( n_{\sigma}^{\text{ext}}(k_f, \sigma) \), as defined according to Eq. (106), approaches \( \frac{1}{2} \) more rapidly than would be expected from the above-mentioned finding in [95].