Coulomb Correlations and Instability of Spinless Fermion Gas in 1D and 2D

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Abstract

We study the stability of the ordinary Landau Fermi liquid phase for interacting, spinless electrons. We require causality and demand that the Pauli principle be obeyed. We find a phase diagram determined by two parameters: the particle density and the interaction strength. We find that the homogeneous, constant density Fermi liquid phase of a spinless Fermion gas is never stable in 1D, but that it may have a restricted domain of stability in 2D.

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INTRODUCTION The theory of the homogeneous electron gas, the “Fermi liquid”, plays a very important role in study of metallic properties in real solids. For even within the continuous jellium model, Wigner [1] argued long ago that at low density, the translational symmetry of this phase is broken and electrons are localized in a lattice to lower the potential energy. Qualitatively speaking, as the mean interparticle distance \( r_s \propto 1/n^{1/d} \) increases, i.e. density \( n \) decreases, the Coulomb potential energy (\( \propto 1/r_s \)) of such an electron gas will eventually dominate the kinetic energy (\( \propto 1/r_s^2 \)). As a result, the homogeneous Fermi liquid phase with a well-defined Fermi surface is unstable in the low density limit. The nature of the phase which replaces it is, however, a matter of conjecture. The localized particles in a Wigner lattice are one possibility. A two-phase regime (high density/low density) is another. The marginal Fermi liquid [2] and the quantum Fermi liquid [3] in addition to a variety of “anyons” are distinct possibilities in low dimensions. In 3D, there have been a number of estimates of the critical \( r_s \), as summarized by Care and March [4].

Sometime ago Mattis [5] proposed a lattice model which incorporates the “granular” nature of electronic states, reflecting the finite size of the Wannier orbitals of the conduction band of a simple metal. He found that Coulomb interactions alone could lead to instability of ordinary paramagnetic Fermi liquid against various interesting phases, including charge-density waves. Following a theorem of Ginzburg and Kirzhnits [6], he proposed a loose but general stability criterion, viz.: the effective two-body interaction \( v(q) \) is required to be non-negative for all wave vector \( q \).

In this paper, we propose a refinement taking into account the short-range correlation in addition to the causality requirement considered previously. The application is to spinless electrons living on a simple \( d \)-dimensional cubic structure undergoing
mutual Coulomb interactions. In contrast to the jellium model where the only length scale is \(r_s\), there appears an additional parameter in the lattice length \(a\). (In the case of real electrons with spins, the magnetic degrees of freedom interfere with the charge dynamics to make the analysis much more complicated.)

The stability criterion of a spinless Fermi liquid will be based on simultaneously satisfying two requirements: (a) by causality, the inverse static dielectric function \(1/\varepsilon(q,0) < 1\); (b) by the Pauli principle, the zero-range pair correlation function of spinless Fermions \(g(0) = 0\). Condition (a), the “Ginzburg-Kirzhnits criterion” [6], is proved using the Kramers-Kronig relation:

\[
\text{Re}\left\{ \frac{1}{\varepsilon(q, \omega)} \right\} = 1 + \frac{1}{\pi} \int_0^\infty P. \frac{d\omega'^2}{\omega'^2 - \omega^2} \text{Im}\left\{ \frac{1}{\varepsilon(q, \omega')} \right\}
\]

where “P.” stands for principal value. As \(\text{Im}\{\varepsilon(q, \omega)\} \geq 0\), it follows that the reciprocal static dielectric function \(1/\varepsilon(q,0) < 1\).

The function \(g(r)\) is defined [7] as the probability of finding two particles separated by a distance \(r\), normalized to be 1 asymptotically at large \(r\). Fortunately \(g(r)\) can also be determined by the dielectric function according to a well-known many-body identity (see Eq.(1.6.2), (5.4.12) in reference [7]):

\[
g(r) = 1 + \frac{1}{n} \left( \frac{1}{N} \sum_q e^{i\vec{q} \cdot \vec{r}} S(q) - 1 \right)
\]

where

\[
S(q) = \int_0^\infty \frac{d\omega}{\pi} \cdot \frac{1}{nv(q)} \text{Im}\left\{ \frac{-1}{\varepsilon(q, \omega)} \right\}
\]

and \(v(q)\) is the two-body vertex function.

It is well-known that condition (b) is never satisfied within the jellium model at low density. The calculated [7,8] pair correlation function \(g(r)\) of the continuum
theory inevitably turns out to be negative at small $r$, evidence of an unphysical excess of exchange and correlation holes around each electron. However, this defect is easily cured when electrons live on a discrete lattice where the short-range, on-site interaction and the long-range, off-site Coulomb interaction can be treated separately. For we have observed that within RPA, condition (b) is equivalent to the requirement that the ground state energy be stationary with respect to a fictitious zero-range interaction parametrized by a new coupling constant $\alpha$. This appears to cure a major flaw in the RPA, allowing it to be used for semi-quantitative purposes.

**SPINLESS FERMIONS** The extended Hamiltonian is:

\begin{equation}
H = \sum_k (\epsilon_k - \mu) c_k^\dagger c_k + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{2} \sum_i \alpha n_i (n_i - 1) \tag{4}
\end{equation}

The third term $\sum_i n_i (n_i - 1) = 0$ vanishes for spinless Fermions and $\alpha$ is the corresponding undetermined Lagrange multiplier. The $c's$ are Fermion operators and $n_i = c_i^\dagger c_i$ is the particle number operator on site $i$. In 1D, $\epsilon_k = -2t \cos k a$ ($a$ the lattice length) and $t$ is the transfer integral. The chemical potential $\mu = \epsilon_F$, the Fermi level. The two-body Coulomb interaction $U_{ij} = e^2 / r_{ij}$, $r_{ij} = |i - j| a$; generalization to higher dimensional hypercubic lattices is straightforward.

To find the ground state energy, we rewrite $H$ in momentum space keeping careful track of all the terms:

\begin{equation}
H = \sum_k (\epsilon_k - \mu) c_k^\dagger c_k + \frac{1}{2N} \sum_{q \neq 0} (\alpha + \Delta V(q)) \rho(q) \rho(-q) - \frac{1}{2} \alpha N n (1 - n) \tag{5}
\end{equation}

where the generalized Ewald sum

\begin{equation}
\Delta V(q) = \sum_{i \neq 0} e^{i \vec{q} \cdot \vec{r}_i} \frac{e^2}{r_i} \tag{6}
\end{equation}

and charge density operator $\rho(q) = \sum_k c_k^\dagger c_{k+q}$. $N_e$ is the total particle number, $N$ the total number of cells and $n = N_e / N$ is the particle density. In the usual way, we
estimate the correlation function

\[ < \rho(q)\rho(-q) >_\omega = \frac{-\Pi(q,\omega)}{1 - (\alpha + \Delta V(q))\Pi(q,\omega)} \]  

(7)

within the RPA approximation by taking \( \Pi \approx \Pi^0 \), the Lindhard polarization function [7]. Then the ground state energy is given by an integral over the coupling constant yielding:

\[ E_G = E_0 + \frac{1}{2} \text{Im} \sum_{q \neq 0} \int_0^\infty \frac{d\omega}{\pi} \log(1 - (\alpha + \Delta V(q))\Pi^0(q,\omega)) - \frac{1}{2} \alpha N n(1 - n) \]  

(8)

with \( E_0 \) the energy of free Fermions. Optimizing \( E_G \) with respect to \( \alpha \),

\[ \frac{\partial E_G}{\partial \alpha} = 0 \]  

(9)

we find:

\[ \frac{1}{N} \sum_{q \neq 0} S_\alpha(q) = 1 - n \]  

(10)

where

\[ S_\alpha(q) = \int_0^\infty \frac{d\omega}{\pi} \cdot \frac{1}{n(\alpha + \Delta V(q))} \text{Im} \frac{-1}{1 - (\alpha + \Delta V(q))\Pi^0(q,\omega)} \]  

(11)

is the structure function. The dielectric function which appears in Eqs.(1)-(3) is:

\[ \varepsilon_\alpha(q,\omega) = 1 - (\alpha + \Delta V(q))\Pi^0(q,\omega), \quad \text{in RPA.} \]  

(12)

By combining Eqs.(2) and (10) we find:

\[ g_\alpha(0) = 1 + \frac{1}{n} \left( \frac{1}{N} \sum_{q \neq 0} S(q) - 1 \right) = 0 \]  

(13)

Therefore

\[ \frac{\partial E_G}{\partial \alpha} = 0 \quad \Leftrightarrow \quad g_\alpha(0) = 0 \]  

(14)
and the stationary condition enforces the Pauli principle. Using the value of $\alpha$ which satisfies this criterion, we now identify $V_\alpha(q) = \alpha + \Delta V(q)$ as the “best” effective two-body vertex function. Since $\Pi^0(q,0) < 0$, Ginzburg and Kirzhnits’ criterion $\varepsilon_\alpha(q,0) = 1 - V_\alpha(q)\Pi^0(q,0) = 1 + V_\alpha(q)|\Pi^0(q,0)| > 1$ implies $V_\alpha(q) > 0$ for all $q$ for the system in the Fermi liquid phase, just as in reference [5]. The interpretation of our result is that the “best” choice of $\alpha$ compensates for the errors in RPA at short distances, and transforms it into a more reliable procedure.

**NUMERICAL RESULTS** The problem has thus been reduced to to find a solution for $\alpha$ which satisfies both

$$V_\alpha(q) = \alpha + \Delta V(q) > 0, \quad \forall q, \quad \text{and} \quad g_\alpha(0) = 0 \quad (15)$$

We will first solve for $\alpha$, then plug it into the inequality to check whether it is satisfied. If not, *some* symmetry breaking must occur.

We present the numerical results in 1D and 2D. In 1D, the generalized Ewald summation is:

$$\Delta V(q) = \sum_{n \neq 0} e^{i q n a} \frac{e^2}{|n a|} = -\frac{e^2}{a} \ln |4 \sin^2 \frac{qa}{2}| \quad (16)$$

and it has a minimum $\Delta V(\pi/a) = -1.386e^2/a$. In addition, the retarded polarization function $\Pi^0(q,\omega)$ can also be evaluated analytically, using the tight-binding spectrum $\epsilon_k = -\cos ka$ (taking $2t = 1$ as our unit from now on). By symmetries $\Pi^0(q,\omega) = \Pi^0(-q,\omega)$, $\Re \Pi^0(q,-\omega) = \Re \Pi^0(q,\omega)$, $\Im \Pi^0(q,-\omega) = -\Im \Pi^0(q,\omega)$, and because of periodicity in $q$, we only need to consider $\omega > 0$ and $0 < qa < \pi$. For $\omega > 2 \sin \frac{qa}{2}$:

$$\Re \Pi^0(q,\omega) = \frac{1}{2\pi \sin \frac{qa}{2} \sqrt{(\omega/2 \sin \frac{qa}{2})^2 - 1}}.$$
\[
\frac{\arctan\left(\frac{-\cos\left(\frac{qa}{2} - k_F\right)}{\sqrt{\left(\omega/2\sin\frac{qa}{2}\right)^2 - 1}}\right) - \arctan\left(\frac{-\cos\left(\frac{qa}{2} + k_F\right)}{\sqrt{\left(\omega/2\sin\frac{qa}{2}\right)^2 - 1}}\right)}{2}\] (17)

For \(\omega = 2 \sin \frac{qa}{2}\):

\[
\text{Re}\Pi^0(q, \omega) = \frac{1}{2\pi \sin \frac{qa}{2}} \left(\frac{1}{\cos\left(\frac{qa}{2} + k_F\right)} - \frac{1}{\cos\left(\frac{qa}{2} - k_F\right)}\right)\] (18)

For \(0 < \omega < 2 \sin \frac{qa}{2}\):

\[
\text{Re}\Pi^0(q, \omega) = \frac{1}{2\pi \sin \frac{qa}{2} \sqrt{1 - (\omega/2 \sin \frac{qa}{2})^2}} \ln \left|\frac{\cos\left(\frac{qa}{2} - k_F\right) - \sqrt{1 - (\omega/2 \sin \frac{qa}{2})^2}}{\cos\left(\frac{qa}{2} - k_F\right) + \sqrt{1 - (\omega/2 \sin \frac{qa}{2})^2}}\right|\] (19)

The imaginary part is:

\[
\text{Im}\Pi^0(q, \omega) = \frac{-i}{2\sqrt{4 \sin^2 \frac{qa}{2} - \omega^2}} \cdot \theta(\cos p \cos \frac{qa}{2} + \sin p \sin \frac{qa}{2} - \cos k_F) \theta(\cos k_F - \cos p \cos \frac{qa}{2} + \sin p \sin \frac{qa}{2}) \cdot \theta(2 \sin \frac{qa}{2} - \omega)\bigg|_{\cos p = \pm \sqrt{1 - (\omega/2 \sin \frac{qa}{2})^2}}\] (20)

In 2D, the Ewald sum \(\Delta V(q_x, q_y)\) has been given by Glasser [9]. But it was expedient to input a slightly “screened” form of \(\Delta V(q_x, q_y)\). This does not affect the physics but simplifies the numerical work:

\[
\Delta V(q_x, q_y) = \sum_{(m,n) \neq (0,0)}^{(\pm M, \pm M)} \frac{e^{2}}{\sqrt{m^2 + n^2}} e^{i(mq_x a + nq_y a - q_c \sqrt{m^2 + n^2}} (21)

\] having a minimum \(\Delta V(\pi, \pi) = -1.024e^2/a\) for \(M = 10, q_c = 0.69\) (the numbers adopted in our numerical simulations.) Similarly, the lattice \(\Pi^0(q_x, q_y, \omega)\) (a generalized Watson integral) is replaced by the isotropic 2D Lindhard polarization function \(\Pi^0(\sqrt{q_x^2 + q_y^2}, \omega)\) [10] evaluated in the effective mass approximation, and the filling factor is determined by \(n = k_F^2/4\pi\) for \(n < \frac{1}{2}\) (electrons) and \(1 - k_F^2/4\pi\) for \(n > \frac{1}{2}\)
(holes.) These approximations should be good for all almost empty or almost full band, but should not be considered accurate at or near half-filling.

Only two parameters govern our problem: one is the particle density \( n \). The other is \( U/W = e^2/2ta \), measuring the Coulomb interaction strength \( U \) relative to half band width \( W \).

The solution \( \alpha \) is presented in Fig.1 for 1D case, and Fig.2 for 2D case for \( n < \frac{1}{2} \). The results are symmetric about \( n = \frac{1}{2} \), so \( n > \frac{1}{2} \) is not shown.

As we see in Fig.1, solutions \( \alpha \)'s never reach 1.386, the maximum of \( -\Delta V \) in 1D. This implies that causality can not be satisfied as there always exist some \( q_c < \pi/a \) such that for \( q > q_c \), \( V(q) < 0 \) for all density \( n \) and interaction \( U/W \). Thus we see that the 1D spinless homogeneous Fermion gas is unstable. This instability is already known by way of the exact solution by Mattis and Lieb [11] of the Luttinger model. At arbitrarily small values of the interaction energy, these authors found that the discontinuity of \( < n_k > \) at the Fermi surface disappears, and the Fermi liquid is transmuted into a “Luttinger liquid” with a corresponding charge in correlation functions.

Fig.2 shows the situation in 2D; the \( \alpha \)'s increase along with \( n \), and finally exceed 1.024, the maximum of \( -\Delta V \) in our calculations, after which they satisfy causality. Hence, at a given interaction strength \( U/W \), the spinless Fermion gas is unstable only at density \( n \) lower than some critical \( n_c \). The phase diagram in Fig.3 shows \( n_c \) v.s. \( U/W \). As \( U/W \) increases, \( n_c \) approaches \( \frac{1}{2} \). An additional possible region of instability against dimerization near \( n = \frac{1}{2} \) can not be investigated within the effective mass approximation. Thus it is possible that at sufficiently large \( U/W \), the 2D Fermi liquid becomes altogether unstable, but due to the errors in obtaining the optimum
\(\alpha\) at large \(n\) using the effective mass approximation, and because of the systematic and inherent errors in the RPA at large \(U/W\), we can only speculate on the strong-coupled behavior.Efros [12], who has studied the strong-coupling limit of the 2D electron liquid (in a strong magnetic field which effectively quenches the spin degree of freedom) has found that in the absence of motional energy, the electron-electron interaction leads to a very inhomogeneous phase. His result may be complementary to our RPA approach, which was predicated on the weak-coupling regime.

The effects of introducing a local field correction [8] \(G(q)\) were also investigated, but were found to have no qualitative influence on our results.

In conclusion, we find for spinless Fermions that the Landau Fermi-Liquid phase, characterized by a one-to-one correspondence with the Fermi gas, including the discontinuity in \(<n_k>\) at \(k_F\), has only a restricted region of validity in 2D, and that it is never applicable in 1D. This last result was already anticipated in the solution of the 1D Luttinger liquid [11], albeit from a different point of view. In the present paper, we reach these conclusions by optimizing RPA using a Lagrange multiplier \(\alpha\). At the optimum \(\alpha\), the RPA is found to satisfy the Pauli principle, thereby becoming a simple and satisfactory tool with which to study the stability of the Fermi liquid.

The phase diagrams for \(SU(2)\) Fermions in 2D and in 3D are more complex and require a subtler analysis. They will be examined separately.
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Figure Captions

FIG.1
Solution $\alpha$ (in unit of $e^2/a$) required to satisfy $g_\alpha(0) = 0$ in 1D. Solid line is for $U/W = 1.0$, dash line for $U/W = 0.1$. Causality requires $\alpha > 1.386$, which can never be satisfied.

FIG.2
Solution $\alpha$ (in unit of $e^2/a$) for $g_\alpha(0) = 0$ in 2D. Solid line is for $U/W = 1.0$, dash line for $U/W = 0.1$. Causality requires $\alpha > 1.024$, as shown by horizontal dash line. It fails to be satisfied at low density.

FIG.3
Phase diagram in 2D, indicating maximum region of stability of Fermi liquid (there may be an additional dimerization instability near $n = \frac{1}{2}$ which we are unable to examine by our methods.)