Existence of a metallic phase and upper bounds of the Hartree-Fock energy in the homogeneous electron gas

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We consider the ground state of the homogeneous electron gas and we prove that a Hartree-Fock solution, motivated by previous simulations, has lower energy than the Fermi gas in the large density limit. This solution is a metallic phase: the density modulation corresponds to a partially occupied crystal (the number of sites is larger than the number of electrons).

I. INTRODUCTION

The homogeneous electron gas is one of the fundamental models in condensed matter physics. Despite its simplicity - the system consists of electrons interacting with each other through a $1/r$ potential to which a uniform positive background is added for charge neutrality - the phase diagram at zero temperature is nontrivial. In general, it is given in terms of the dimensionless parameter $r_s = (\alpha_D a_B R^{1/D})^{-1}$, where $D$ is the space dimension, $n$ is the electronic density, $a_B$ the Bohr radius and $\alpha_D$ is the volume of the sphere unity. At $r_s = 0$, the ground state is the Fermi gas. At large $r_s$, the Hartree-Fock ground state of the electron gas is a Wigner crystal, that is a state where the charge density forms a triangular crystal with exactly one electron per lattice site. In the intermediate region the Hartree-Fock approximation is not relevant and more sophisticated methods show that the ground state of the Hamiltonian is quite different.

At small $r_s$, the ground state of the electron gas within Hartree-Fock is still not known. Although the ground state of the ideal Fermi gas ($r_s = 0$) remains an eigenstate of the Hartree-Fock Hamiltonian of the electron gas at any density, already Wigner argued that the unpolarized Fermi gas is unstable even in the limit $r_s \to 0$. Later, Overhauser showed the instability of the unpolarized Fermi gas with respect to spin-density waves within the Hartree-Fock approximation. Only recently, a Hartree-Fock study of the unpolarized three-dimensional electron gas was performed which proposes a more complicated structure of a ground state with spin-density waves.

In Ref., we describe the results of our numerical simulations of the two-dimensional (2D), polarized electron gas at small $r_s$, and show that the ground state is neither a Fermi gas nor a Wigner crystal: the charge density modulation we find corresponds to a partially occupied crystal (the number of sites is larger than the number $N$ of electrons).

We refer to this solution as a metallic phase. The charge density of this metallic phase represents a triangular lattice with reciprocal generators $Q_i$ of modulus $2k_F$. This modulation is mainly carried by the wave vectors close to the Fermi surface. In order to observe the metallic phase, the number of electrons $N$ has to exceed a threshold ranging from $N \gtrsim 10$ at $r_s \sim 2.6$ up to $N \gtrsim 10^2$ at $r_s \sim 1$. As we shall see below, the threshold increases exponentially as $r_s$ goes to 0 which may explain why this metallic phase has not been observed in previous simulations.

In this study, we obtain rigorous upper bounds on the energy of the metallic phase in the two-dimensional polarized case with a class of states mimicking the real states obtained numerically. These bounds are obtained in the limit $r_s \to 0$ where the calculation is simplified by the long range behavior of the interaction potential. However, our numerical simulations show that this metallic phase also exists for screened potential, but strictly speaking we cannot prove in this case the existence of such a metallic phase in the limit $r_s \to 0$. These bounds are easily extended to the unpolarized 2D case. Then we show how this proof extends to the 3D case, whereas we have no numerical simulations indicating that this phase may correspond to the actual ground state of the 3D electron gas in Hartree-Fock.

Finally, let us point out that our bounds (for instance Eq. (12)) must be considered as mathematical bounds; they only give an understanding of the behavior of the energy of the ground state, but the actual constants involved in the expressions have to be evaluated by other means.

II. NUMERICAL RESULTS

In a previous paper, we have computed 2D Hartree-Fock states of lower energy than the Fermi gas for values of $r_s$ about 2.

Such a state $\Psi$ is obtained as a Slater determinant $\bigwedge_{i=1}^{N} \psi_i$ where $N$ is the number of electrons and $\{\psi_i\}$ is a set of orthonormal vectors. Only the space generated by the single particle wavefunctions $\psi_i$'s is relevant, and in order to
understand our numerical results we need to choose a canonical representation of the $\psi_i$'s.
The natural choice is to use the natural base of the Fermi gas $\{\phi_i\}_{i=1...N}$ corresponding to some indexation of the plane waves of the Fermi sphere.
Let $M$ be the square matrix defined by $M_{ij} = \langle \phi_i | \psi_j \rangle$. The Singular Value Decomposition (SVD) of $M$ is $M = U\sigma V$ where $U$ and $V$ are unitary matrices and $\sigma$ is a diagonal positive matrix.
Let us define
$$
\phi_i' = \sum_j U^{-1}_{ij} \phi_j \\
\psi_i' = \sum_j V^{-1}_{ji} \psi_j.
$$

Then $\{\phi_i'\}$ and $\{\psi_i'\}$ are also two sets of $N$ orthonormal vectors satisfying $\langle \phi_i' | \psi_j' \rangle = \delta_{ij} \sigma_i$.
They are the nearest bases of $\text{Span}(\{\phi_i\})$ and $\text{Span}(\{\psi_i\})$ and they define a canonical unitary operator $W$ from $\text{Span}(\{\phi_i\})$ onto $\text{Span}(\{\psi_i\})$ by:
$$
W \sum_i \lambda_i \phi_i' = \sum_i \lambda_i \psi_i'
$$

In particular, we have:
$$
W \phi_i = W \sum_j U_{ij} \phi_j' \\
= \sum_j U_{ij} \psi_j' \\
= \sum_j U_{ij} \sum_k V^{-1}_{kj} \psi_k \\
= \sum_j U V_{ik} \psi_k
$$

Thus the natural basis of $\text{Span}(\{\psi_i\})$ associated to the basis $\{\phi_i\}_{i=1...N}$ is $\{W \phi_i\}_{i=1...N}$.
Numerically we have chosen the $\psi_i$'s in this way and it appears that, if $r_s$ is not too large, $\psi_i$ is close to $\phi_i$ at least for $i$ associated to a wave vector not too close to the Fermi surface. Thus the largest amplitude of $\psi_i$, in the $k$ space, is for the $k_i$ corresponding to $\phi_i$. Fig.1 represents the next largest amplitude of $\psi_i$, that we denote $b_{k_i}$, for 499 electrons at $r_s = 2$ in 2D.
As $r_s$ decreases, the other amplitudes of the $\psi_i$'s become very small. Furthermore, the wave vector $k_i'$ corresponding to $b_{k_i}$ satisfies $k_i' - k_i = Q_\alpha$ where the generators $\{Q_\alpha\}_{\alpha=1...6}$ belong to the six-fold star of a triangular lattice.
Notice that the modulus of \( b_k \) is maximal for \( k \) on a six-fold star and close to the Fermi surface. In the direct space, the \( Q_\alpha \)'s induce a modulation corresponding to a triangular lattice for the charge density. But while this lattice forms a Wigner crystal with one electron per site for \( r_s > 2.6 \), for smaller \( r_s \) it is a denser lattice corresponding to a crystal with an incomplete band filling. Indeed, at any \( r_s \) the electrostatic interaction favors a periodic distribution of charges and at small \( r_s \) only \( k \)-vectors close to Fermi surface can be modulated. The optimal solution is to choose \( \| Q_\alpha \| = 2k_F \) which is larger than the reciprocal lattice vector of the Wigner case. In the following, we consider analytic solutions analogous to those of our numerical results and we prove that their energies are lower than the energies of the Fermi gas as \( r_s \) goes to 0.

### III. ENERGY OF THE FERMII GAS: POLARIZED CASE

We consider the Hamiltonian of \( N \) electrons in a 2D or 3D square box of volume \( \Omega \) with periodic boundary conditions.

\[
H = -\frac{\hbar^2}{2m} \Delta + e^2 \frac{V}{2}
\]

where \( V \) is the 2-body Coulomb potential \( \sum_{i \neq j} \frac{1}{|r_i - r_j|} \), the electron mass is \( m \), and \( e \) is its charge. It is convenient to choose Hartree as the unit of energy, \( H_a = \hbar^2/(ma_B^2) \), where \( a_B = \hbar^2/(me^2) \) is the Bohr radius. We get:

\[
H = \frac{a_B^2}{2} (\Delta + \frac{1}{a_B} V)
\]

Let \( \psi_n \) be an orthonormalized set of \( N \) vectors of \( L^2(\Omega) \). They define the \( N \)-particle Slater determinant \( \Psi = \wedge_n \psi_n \). And the energy of \( \Psi \) is:

\[
\mathcal{E} = \langle \Psi | H | \Psi \rangle = \frac{a_B^2}{2} \left( -\sum_n \langle \psi_n \Delta | \psi_n \rangle + \frac{1}{a_B} \sum_{n,n'} \langle \psi_n \wedge \psi_{n'} | v | \psi_n \wedge \psi_{n'} \rangle \right)
\]

(10)

where \( v \) is defined as:

\[
\langle \varphi_1 \otimes \varphi_2 | v | \psi_1 \otimes \psi_2 \rangle = \int dx dy \varphi_1(x)\varphi_2(y) \frac{1}{\|x - y\|} \psi_1(x)\psi_2(y).
\]

(11)

In order to avoid problems due to the Coulomb singularity, we introduce the jellium model and define the potential acting on the plane waves \( \phi_k \) as:

\[
\langle \phi_k \otimes \phi_{k'} | v | \phi_{k+q} \otimes \phi_{k'-q} \rangle = \pi \frac{2}{\Omega |q|} D^{-1}
\]

(12)

for \( q \neq 0 \) and 0 otherwise, so that the total charge of the electrons is compensated by a positive background charge. The Fermi gas is defined by \( \Phi = \bigwedge_{|k| < k_F} \phi_k \) where \( (k F)^D = (2\pi)^D N/\Omega \) and \( a_B^2 \) is the volume of the unit sphere.

\[
\mathcal{E}_{FG} = \langle \Phi | H | \Phi \rangle = \frac{a_B^2}{2} \left( \sum_{|k| < k_F} k^2 - \frac{2^{D-1} \pi}{a_B \Omega} \sum_{|k|,|k'| < k_F} \frac{1}{|k - k'|^{D-1}} \right)
\]

(13)

As \( \Omega \) goes to \( \infty \) with \( \Omega/N \) fixed, the thermodynamic limit for the energy per particle is obtained by the substitution \( \sum_k \to \frac{\Omega}{4\pi k^2} \int dk \):

\[
\frac{\mathcal{E}_{FG}}{N} = \frac{a_B^2}{2} \frac{\Omega}{N(2\pi)^D} \left( \int_{|k| < k_F} dk k^2 - \frac{1}{a_B 2\pi^{D-1}} \int_{|k|,|k'| < k_F} dk dk' \frac{1}{|k - k'|^{D-1}} \right)
\]

\[
= \frac{a_B^2}{2} \frac{\Omega}{N(2\pi)^D} k_F^{D+2} \left( \int_{|k| < 1} dk k^2 - \frac{1}{a_B k_F 2\pi^{D-1}} \int_{|k|,|k'| < 1} dk dk' \frac{1}{|k - k'|^{D-1}} \right)
\]

(14)
From the definition of \( r_s = (\alpha D a B n^{1/D})^{-1} \) and \( k_F \), it follows that \( k_F \alpha D r_s a_B = 2\pi \). Thus, we have:

\[
\frac{\mathcal{E}_{FG}}{N} = \frac{2\pi^2}{a_D^2 + 4\pi^2} \left( \int_{|k|<1} dk k^2 - \frac{r_s a_D^2}{4\pi D} \int_{|k||k'|<1} dk dk' \frac{1}{|k-k'|^{D-1}} \right)
\]  

(15)

which gives for \( D = 2 \) (\( \alpha^2 = \pi \)):

\[
\frac{\mathcal{E}_{FG}}{N} = \frac{2}{\pi r_s^2} \left( \int_{|k|<1} dk k^2 - \frac{r_s}{4\pi} \int_{|k||k'|<1} dk dk' \frac{1}{|k-k'|} \right)
\]  

(16)

**IV. HARTREE-FOCK UPPER BOUNDS: POLARIZED 2D CASE**

We restrict ourself to the 2D polarized case and we want to estimate the energy for a class of states inspired by our numerical results. Let us consider a state \( \Psi = \bigwedge_{|k|<k_F} \psi_k \) where:

\[
\psi_k = a_k \phi_k + b_k \phi_{k+Q_k}
\]

with \( Q_k \in \{-2k_F(\cos p\pi/3, \sin p\pi/3)\}_{p=0...5} \). For \( k = |k|(\cos \theta, \sin \theta) \) we choose \( Q_k \) such that \( |k + Q_k| \) is minimal; that is, we choose \( p \) as the integer part of \((3\theta/\pi + 1/2)\) and we must assume \( b_k \) is zero if \( k \) is zero or \( \theta = \pi/6 + n\pi/3 \). Furthermore, we assume that \( a_k \) and \( b_k \) are real positive number and invariant thru the rotation of \( 2n\pi/6 \) and the symmetry \( \theta \rightarrow -\theta \) (i.e. the dihedral group \( D_6 \)). The \( \psi_k \)'s are normalized, so that \( a_k^2 + b_k^2 = 1 \) and \( b_k = 0 \) if \( |k \cdot Q_k| < 2k_F^2 (1-\epsilon) \) (i.e. \( b_k \) is not zero only in the vicinity of \( \{k_F(\cos p\pi/3, \sin p\pi/3)\}_{p=0...5} \)), see Fig.2

Thus the limit energy per particle is given by:

\[
\frac{\mathcal{E}}{N} = \frac{2}{\pi r_s^2} \left( \int_{|k|<1} dk \langle \psi_k | -\Delta |\psi_k \rangle + \frac{r_s}{4\pi} \int_{|k||k'|<1} dk dk' \frac{\Omega}{2\pi} \langle \psi_k \wedge \psi_{k'} | v | \psi_k \wedge \psi_{k'} \rangle \right)
\]  

(17)

where, as in [10], the \( k \)'s have been renormalized by \( k_F \) and thus \( |Q_k| = 2 \).

We define \( \Delta E \) by:

\[
\frac{\mathcal{E} - \mathcal{E}_{FG}}{N} = \frac{2}{\pi r_s^2} \Delta E
\]  

(18)

Then

\[
\Delta E = \int_{|k|<1} dk \left[ \langle \psi_k | -\Delta |\psi_k \rangle - k^2 \right] + \frac{r_s}{4\pi} \Delta E_V
\]  

(19)
where
\[
\Delta E_V = \int_{|k|,|k'|<1} dkdk' \left( \frac{\Omega}{2\pi} \langle \psi_k \wedge \psi_{k'}|v|\psi_k \wedge \psi_{k'} \rangle + \frac{1}{|k - k'|} \right)
\] (20)

A. Potential energy contribution: $\Delta E_V$

Setting $v_q = 1/|q|$:
\[
\frac{\Omega}{2\pi} \langle \psi_k \wedge \psi_{k'}|v|\psi_k \wedge \psi_{k'} \rangle + v_{k-k'} = (v_{k-k'} - v_{k-k'-Q_{k'}})b_k^2 a_k^2
\]
\[
+ (v_{k-k'} - v_{k+Q_{k'}-k'})b_k^2 a_{k'}^2
\]
\[
+ (v_{k-k'} - v_{k+Q_{k'}-k'})b_k'^2 b_{k'}^2
\]
\[
+ 2v_{Q_{k}} a_k b_k a_{k'} b_{k'} (\delta_{Q_{k}+Q_{k'}} + \delta_{Q_{k'}-Q_{k'}})
\]
\[
- 2v_{k-k'} a_k b_k a_{k'} b_{k'} \delta_{Q_{k}+Q_{k'}}
\]
\[
- (v_{k+Q_{k}-k'} + v_{k-k'-Q_{k'}}) a_k a_{k'} b_k b_{k'} \delta_{Q_{k}+Q_{k'}}
\] (21)

Eq. (20), may be divided into 4 parts:

- $\{b_{k'} = 0, b_k = 0\}$: the contribution is zero.

- $\{b_{k'} = 0, b_k \neq 0\}, \{b_{k'} \neq 0, b_k = 0\}$: both cases are equivalent.

For $\{b_{k'} = 0, b_k \neq 0\}$, the integrant of Eq. (20) is:
\[
\frac{\Omega}{2\pi} \langle \psi_k \wedge \phi_{k'}|v|\psi_k \wedge \phi_{k'} \rangle + \frac{1}{|k - k'|} = (v_{k-k'} - v_{k+Q_{k'}-k'})b_k^2
\] (22)

Let $S_0$ be the sector of unit disk between $-\pi/6$ and $\pi/6$ (see Fig. 2); then in this sector $Q_k = (-2, 0)$ and by symmetry:
\[
\int_{b_{k'}=0} dkdk' (v_{k-k'} - v_{k+Q_{k}-k'})b_k^2 = 6 \int_{k \in S_0, b_{k'}=0} dkdk' (v_{k-k'} - v_{k+Q_{k}-k'})b_k^2
\] (23)
\[
= 6 \int_{k \in S_0, b_{k'}=0} dkdk' (v_{k-k'} - v_{k+Q_{k}-k'})b_k^2
\] (24)
\[
\leq Ce^3 + 6 \int_{k \in S_0, |k'|<1-\varepsilon} dkdk' (v_{k-k'} - v_{k+Q_{k}-k'})b_k^2
\] (25)

where $\tilde{k} = (2 - k_x, k_y)$. In $S_0$, $k = (k_x, k_y)$ where $k_x$ is close to 1 and setting $k_x = 1 - \varepsilon$, we assume from now that $b_k = b(x/\varepsilon)$.

In Appendix A we prove that:
\[
\int_{k \in S_0, |k'|<1-\varepsilon} dkdk' (v_{k-k'} - v_{k+Q_{k}-k'})b_k^2 \leq 8\varepsilon^2 \sqrt{2\varepsilon} \left[ \ln \varepsilon^{-1} + O(1) \right] \int_{0}^{1} dx b^2(x) x\sqrt{x}
\] (26)

- $\{b_{k'} \neq 0, b_k \neq 0\}$

By symmetry we can assume that $k$ belongs to $S_0$. If $k' \not\in S_0 \cup S_3$ all the $v$ appearing in (21) are uniformly bounded. And since the k-volume for each sector goes like $\varepsilon\sqrt{\varepsilon}$, the contribution of these terms is bounded by $C\varepsilon^3$. In the same way $v_{k-k'}$ is bounded when $k' \in S_3$ and $v_{k+Q_{k}-k'}$ is bounded when $k' \in S_0$. Thus setting:
\[
f := a_k^2 b_k^2 + b_k^2 a_{k'}^2 - 2a_k a_{k'} b_k b_{k'} = (a_k b_{k'} - b_k a_{k'})^2
\] (27)
\[
g := a_k^2 b_k^2 + b_k^2 a_{k'}^2 + 2a_k a_{k'} b_k b_{k'} = (a_k b_{k'} + b_k a_{k'})^2
\] (28)
one can check that:

\[
\int_{b_k b_k \neq 0} \frac{\Omega}{2\pi} \langle \psi_k \wedge \psi_{k'} \mid \psi_k \wedge \psi_{k'} \rangle + v_{k-k'} \leq C \epsilon^3 + 6 \int_{k,k' \in S_0} dk dk' \left( v_{k-k'} - v_{k+Q_k + k'} \right)
\]

(29)

In Appendix B we prove that

\[
\int_{k,k' \in S_0} dk dk' \left( v_{k-k'} - v_{k+Q_k + k'} \right) \leq 4e^2 \sqrt{2 \epsilon} \left[ \ln \epsilon^{-1} + O(1) \right] \int_0^1 dx \sqrt{x} \int_x^1 dx' \left( f(x, x') - g(x, x') \right)
\]

(30)

Thus, summing the four contribution gives:

\[
\Delta E_V \leq C \epsilon^3 + 6e^2 \sqrt{2 \epsilon} \left[ \ln \epsilon^{-1} + O(1) \right] \int_0^1 dx \sqrt{x} \left( 16b^2(x)x + 4 \int_x^1 dx' \left( f(x, x') - g(x, x') \right) \right)
\]

(31)

### B. Kinetic energy contribution:

The variation of the kinetic energy is given by:

\[
\int_{|\epsilon|<1} dk \left[ (|\psi_k| - \Delta|\psi_k|) - k^2 \right] = 6 \int_{k \in S_0} dk \left( (|\psi_k| - \Delta|\psi_k|) - k^2 \right)
\]

(32)

\[
= 6 \int_0^e dx \ 2y_m \ 4xb^2(x/\epsilon)
\]

(33)

\[
\leq 6 \times 8e^2 \sqrt{2 \epsilon} \int_0^1 dx \ \sqrt{x} \ xb^2(x)
\]

(34)

### C. Total energy:

Inserting Eqs.\([31,34]\) in Eq.\([18]\), the variation of the total energy from the Fermi gas energy becomes:

\[
\Delta E \leq 6e^2 \sqrt{2 \epsilon} \int_0^1 dx \sqrt{x} \left( 8xb^2(x) + \frac{r_s}{4\pi} \left[ \ln \epsilon^{-1} + O(1) \right] \left( 16b^2(x)x + 4 \int_x^1 dx' \left( f(x, x') - g(x, x') \right) \right) \right)
\]

\[
= 6 \times 8e^2 \sqrt{2 \epsilon} \int_0^1 dx \sqrt{x} \left( xb^2(x) + \frac{r_s}{2\pi} \left[ \ln \epsilon^{-1} + O(1) \right] \left( b^2(x)x - a(x)b(x) \int_x^1 dx' a(x')b(x') \right) \right)
\]

(35)

Let us set

\[
\delta = \epsilon^2 \sqrt{\epsilon}
\]

(36)

\[
I_1 = \int_0^1 dx \sqrt{x} xb^2(x)
\]

(37)

\[
I_2 = \frac{1}{5\pi} \int_0^1 dx \sqrt{x} \left( -b^2(x)x + a(x)b(x) \int_x^1 dx' a(x')b(x') \right)
\]

(38)

Then

\[
\Delta E \leq 6 \times 8\sqrt{2} \delta \left[ I_1 - r_s I_2 \left( \ln \delta^{-1} + O(1) \right) \right]
\]

(39)

If \(I_2 > 0\), as \(r_s\) goes to 0, \(\Delta E\) is minimal in Eq.\([39]\) for \(\delta\) defined by:

\[
\delta_{\text{min}} = \frac{1}{e} \exp \left( - \frac{I_1}{I_2 r_s} \right)
\]

(40)

and finally inserting \(\delta_{\text{min}}\) in Eq.\([39]\) gives:

\[
\Delta E \lesssim - \frac{6 \times 8\sqrt{2}}{e} \exp \left( - \frac{I_1}{I_2 r_s} \right) r_s I_2
\]

(41)
We now have to find a solution $b(x)$ such that $I_2$ is positive. Choosing $b(x) = b_0$ or $b(x) = b_0(1 - x)$ leads to negative $I_2$. In the Appendix C, as $r_s$ goes to 0 we find a family of $b$ leading to:

$$\Delta E \lesssim -r_s \exp \left( -\frac{5\pi}{3r_s} + O(1) \frac{r_s}{\sqrt{r_s}} \right)$$  \quad (42)$$

Though such a bound is correct in the thermodynamic limit, this behavior in not so relevant for finite systems. Indeed, numerical systems consider about $10^3$ electrons and, as we shall see later, the Fermi gas becomes then the ground state for $r_s \lesssim 1$. Thus the asymptotic bound (42) is not very helpful in the real word.

Nevertheless, for realistic $r_s$, one can choose a suitable function $b$ and evaluate numerically $I_1$ and $I_2$. For instance, with $b = b_\eta$ as in [88] of Appendix C and $\eta = 0.001$ we get

$$\Delta E \lesssim -2.6 \times 10^{-4} r_s \exp \left( -\frac{18.5}{r_s} \right)$$  \quad (43)$$

V. HF UPPER BOUNDS: UNPOLARIZED 2D CASE

We consider now the spin of the electrons, and we restrict to the case where half the electrons have a spin up and the others have a spin down.

We can choose a solution as the product of 2 Slaters $\Psi^+$ and $\Psi^-$ for the spins up and down.

$$\frac{2}{a_B^2} E^{NP} = -\sum_n \langle \psi_n^- | \Delta | \psi_n^+ \rangle + \frac{1}{a_B} \sum_{n,n'} \langle \psi_n^+ \wedge \psi_{n'}^+ | v | \psi_n^- \wedge \psi_{n'}^- \rangle \quad (44)$$

$$-\sum_n \langle \psi_n^- | \Delta | \psi_n^- \rangle + \frac{1}{a_B} \sum_{n,n'} \langle \psi_n^- \wedge \psi_{n'}^- | v | \psi_n^- \wedge \psi_{n'}^- \rangle \quad (45)$$

$$+ \frac{1}{a_B} \left( \sum_{n,n'} \langle \psi_n^+ \wedge \psi_{n'}^- | v | \psi_n^+ \wedge \psi_{n'}^- \rangle + \sum_{n,n'} \langle \psi_n^- \wedge \psi_{n'}^+ | v | \psi_n^- \wedge \psi_{n'}^+ \rangle \right) \quad (46)$$

The first terms (44) and (45) can be evaluated as in (18) noticing that the definition of $k_F$ becomes $k_F^2 = 4\pi N_{\pm}/\Omega = 2\pi N/\Omega$. So the $r_s$ in the evaluation of $\Delta E$ is now $r_s \sqrt{2}$ and:

$$\frac{E^{NP} - E_{FG}^{NP}}{N} = \frac{1}{\pi r_s} \Delta E(r_s \sqrt{2}) + [46]$$  \quad (47)$$

The extra terms (46) coming from the direct potential provide contributions like $a_n^+ b_n^- a_{n'}^- b_{n'}^+$ times a positive factor. These contributions are regular as $r_s$ goes to 0, and does not modify the asymptotic energy.

Nevertheless, these contributions depends on the signs of $b_n^+$ in the two Slaters $\Psi^+$ and $\Psi^-$. Thus, since the energy of one Slater does not depend on the global sign of the $b_n^+$’s, the minimal state is obtained by choosing $b_n^+ = -b_n^-$. For such a state, the main difference with the polarized case is that the charge density becomes flat, though the spin density is not.

Finally, we can compare our solutions with previous solutions proposed by Fedders and Martin. They consider a more complicated modulation of the states near the center of Fermi sphere. While their results may be correct, they missed the dominant contribution coming from the states near the Fermi surface. Indeed, our computations give nonzero contribution for the states near the center, but for $r_s = 1.5 b_k$ is about $10^{-5}$ and the energy benefit, following their formula, must be of order $10^{-20}$ of the energy benefit of the external states.

VI. THE METALLIC PHASE IN FINITE SYSTEMS

For finite systems of $N$ electrons, the minimum requirement is that the surface $|k \cdot Q_k| > 2k_F^2(1 - \epsilon)$, so that it contains at least one plane wave of the finite, discrete system. This gives the condition $N\epsilon/\sqrt{\tau} > 1$ and from Eqs. (36) [40], this leads to:

$$N > \exp \left( \frac{3I_1}{5I_2 r_s} \right)$$  \quad (48)$$
With our approximate behavior for $I_2/I_1$ in two dimensions, we find:

$$N > \exp \left( \frac{3\pi}{r_s} \right)$$

(49)

i.e. $N > 500$ for $r_s = 1.8$. This bound is compatible with our numerical simulations where the metallic phase disappears at $rs = 1$ for $N = 500$. Furthermore, this may explain why this metallic phase has not been observed in previous simulations.

VII. HARTREE-FOCK UPPER BOUNDS: POLARIZED 3D CASE

Mutatis mutandis, the 3D case works in the same way.

The potential term $v_k$ is now $1/||k||^2$ but the dominant terms are provide now from integrals like:

$$I(k_x, k_x') = \int_{||k||, ||k'|| \leq 1} dk_y dk_z dk_y' dk_z' \frac{1}{||k - k'||^2}$$

where $k_x$ is close to $k_x'$.

Let us suppose that $k_x > k_x'$, then

$$I(k_x, k_x') = \int_0^{\sqrt{2-k_x^2-k_x'^2}} \frac{du}{\mu(du)} \frac{1}{(k_x - k_x')^2 + u^2}$$

(51)

where $u$ stands for $((k_y - k_y')^2 + (k_z - k_z')^2)^{1/2}$ and $\mu(du)$ stands for the distribution of $u$. Here we are interested in small values of $u$. One can check that $\mu(u, u + \epsilon) \approx 2\pi^2(1 - k_x^2)\epsilon u$ provided that $u$ is sufficiently small ($k_y, k_z$ may be any point in disk of radius $\sqrt{1-k_x^2}$ and $(k_y', k_z')$ may belong to a thin ring around $(k_y, k_z)$).

$$I(k_x, k_x') \approx \pi^2(1-k_x^2) \int_0^{2\sqrt{2}} 2udu \frac{1}{(k_x - k_x')^2 + u^2}$$

$$\approx -\pi^2(1-k_x^2) \ln(k_x - k_x')^2$$

(52)

(53)

This must be compared with the 2D case $I(k_x, k_x') \approx -2\sqrt{1-k_x^2} \ln(k_x - k_x')^2$. Mutatis mutandis, (Eq. 19) becomes:

$$\Delta E = \int_{|k| < 1} dk \left( \langle \psi_k | - \Delta |\psi_k \rangle - k^2 \right) + \kappa r_s \Delta E_V$$

(54)

where $\kappa = \alpha^2/(4\pi^3)^2$ and $\alpha^3 = 4\pi/3$. Now, in $\Delta E_V$ the $2\epsilon x$ factors have to be replaced by $\pi^2 c x$:

$$\Delta E_V \leq C \epsilon^4 + 16 z \pi^2 c^3 \left[ \ln \epsilon^{-1} + O(1) \right] \int_0^1 dx \left( b^2(x) x - a(x)b(x) \int_x^1 dx' a(x')b(x') \right)$$

(55)

where $z$ is the number of sectors of the Fermi sphere. The variation of the kinetic energy is now

$$\int_{|k| < 1} dk \left( \langle \psi_k | - \Delta |\psi_k \rangle - k^2 \right) = 8\pi^3 \int_0^1 dx \ x^2b^2(x)$$

(56)

Thus setting

$$I_1 = \int_0^1 dx \ x^2b^2(x)$$

(57)

$$I_2 = \frac{2\kappa \pi}{3} \int_0^1 dx \ x \left( -b^2(x)x + a(x)b(x) \int_x^1 dx' a(x')b(x') \right)$$

(58)

$$\Delta E \leq z8\pi^3 \left( I_1 - 3r_s I_2 \left[ \ln \epsilon^{-1} + O(1) \right] \right)$$
that the asymptotic bound for small $r_s$ going beyond the simple Fermi gas states. The main interest of this proof is that it focuses on the small $r_s$ region where the Hartree-Fock approximation is relevant and that the upper bounds were obtained using metallic states which correspond to solutions obtained by numerical simulations.

In order to judge their relevance for the true ground state of the electron gas in the high density region, we have to consider correlation effects beyond the Hartree-Fock approximation. Due to the long-range, singular behavior of the Coulomb-potential, the perturbation expansion has to be rearranged which amounts to an effective screening of the electron interaction. Unfortunately a rigorous extension of our proof to the case of a screened Coulomb potential is not straightforward. However, numerical calculations provide evidence for the stability of the metallic states in the 2D polarized system within Hartree-Fock, so that these states are relevant candidates for the true ground state of the two-dimensional electron gas.

**VIII. CONCLUSION**

We have proven upper bounds for the energy of a metallic state below the Fermi gas energy. To our knowledge, it is the first time that rigorous upper bounds for the ground state energy of the polarized electron gas are obtained going beyond the simple Fermi gas states. The main interest of this proof is that it focuses on the small $r_s$ region where the Hartree-Fock approximation is relevant and that the upper bounds were obtained using metallic states which correspond to solutions obtained by numerical simulations.

We have to estimate

$$\Delta E \lesssim -\frac{z^8 \pi}{e} \exp \left( -\frac{I_1}{I_2 r_s} \right) r_s I_2$$

The operator $A$ of Appendix C is now modified. But the same analysis show that the spectrum of $A$ is still $(0, 4)$, so that the asymptotic bound for small $r_s$ is:

$$\Delta E \lesssim -\frac{z^8 \pi}{e} \exp \left( -\frac{1}{6 \kappa \pi r_s} + o(1/r_s) \right) r_s$$

**IX. APPENDIX A**

We have to estimate

$$I(f) = \int_{\|k\|,\|k'\| \leq 1} \int_{1-k_x \leq \epsilon, |k'_x| \leq 1-\epsilon} dk'k' (v_{k-k'} - v_{k-k'}) f(1-k_x)$$

where $k = (2-k_x, k_y)$ and $f$ is a positive function.

$$\int dk' (v_{k-k'} - v_{k-k'}) = \int dk'_x \text{asinh} \frac{y'_m - k_y}{k_x - k'_x} + \text{asinh} \frac{y'_m + k_y}{k_x - k'_x} - \text{asinh} \frac{y'_m - k_y}{2-k_x - k'_x} - \text{asinh} \frac{y'_m + k_y}{2-k_x - k'_x}$$

where $y'_m = \sqrt{1-k_x^2}$. And since asinh $x - \text{asinh} y \leq \ln x/y$ for $x > y > 0$:

$$\int dk' (v_{k-k'} - v_{k-k'}) \leq \int_{-1+\epsilon}^{1-\epsilon} dk'_x 2 \ln \frac{2-k_x - k'_x}{k_x - k'_x}$$

We set $k_x = 1-x$ and $y_m = \sqrt{2x-x^2}$,

$$I(f) \leq \int_0^x dx f(x) y_m \int_{-1+\epsilon}^{1-\epsilon} dk'_x 2 \ln \frac{1+x - k'_x}{1-x - k'_x}$$

$$= \frac{4}{\epsilon} \int_0^x dx f(x) y_m \int_{\epsilon}^{2-\epsilon} du \ln \frac{u + x}{u - x}$$

$$\leq \frac{4}{\epsilon} \int_0^x dx f(x) y_m \int_{\epsilon}^{2-\epsilon} du \frac{2x}{u - x}$$

$$= 8\epsilon^2 \sqrt{2e} [\ln \epsilon^{-1} + O(1)] \int_0^1 dx f(\epsilon x) x \sqrt{x}$$
X. APPENDIX B

We have to estimate

\[ I(f, g) = \int_{\|k\|, \|k'\| \leq 1} \int_{1 - k, 1 - k' < \epsilon} dkdk' (v_{k-k'} f - v_{k+k'} g) \tag{68} \]

where \( \tilde{k} = (k_x - 2, k_y) \) and \( f \) and \( g \) are positive functions of \( 1 - k_x \) and \( 1 - k'_x \).

Setting \( k_x = 1 - x, k'_x = 1 - x', k_y = y, k'_y = y', \) and \( r_x = \sqrt{(x \pm x')^2 + (y - y')^2} \), Eq. 68 can be rewritten:

\[ I(f, g) = \int dx \int f \int dy \int dy' \left( \frac{1}{r_-} f - \frac{1}{r_+} g \right) \]

\[ = 2 \int dx \int f \int dy \int dy' \left( \frac{1}{r_-} f - \frac{1}{r_+} g \right) \tag{69} \]

where \( y \) and \( y' \) must satisfy \((1 - x)^2 + y^2 \leq 1 \) and \((1 - x')^2 + y'^2 \leq 1 \).

Since \( \text{asinh} x \leq \ln(2(x + 1)) \), the first term in 69 is bounded by:

\[ 2 \int dx \int f \int dy \int dy' \left( \frac{1}{r_-} f - \frac{1}{r_+} g \right) \leq 2 \int dx \int f \int dy \int dy' \left( \frac{2y'_m}{x' - x} \right) \tag{70} \]

\[ \leq 4 \int dx \int f \int 2y_m \ln(2 + \frac{4y'_m}{x' - x}) \tag{71} \]

\[ \leq 4e^{2/2} \int \ln(\epsilon^{-1}) + O(1) \int dx \int f(\epsilon x, \epsilon x') \sqrt{x} \tag{72} \]

On the other hand, using \( \text{asinh} x \geq \ln 2x \), the last term of 69 is:

\[ 2 \int dx \int f \int dy \int dy' \left( \frac{1}{r_+} f - \frac{1}{r_-} g \right) \geq 2 \int dx \int f \int dy \int dy' \ln 4y'_m^2 - y^2 \]

\[ \geq 4 \int dx \int f \int g(y) \ln(\epsilon^{-1} + O(1)) \]

\[ \geq 4e^{2/2} \int \ln(\epsilon^{-1} + O(1)) \int dx \int f(\epsilon x, \epsilon x') \sqrt{x} \tag{73} \]

And we have:

\[ I(f, g) \leq 4e^{2/2} \int \ln(\epsilon^{-1} + O(1)) \int dx \int f(\epsilon x, \epsilon x') \sqrt{x} \tag{74} \]

XI. APPENDIX C

Here we provide exact bounds on \( I_1 \) and \( I_2 \) given by Eq. 37-57.

In order to estimate \( I_2 \) we introduce the linear operator \( A \):

\[ Af(x) = \frac{1}{2x} \int_x^1 f(y) dy + \frac{1}{2x\sqrt{x}} \int_0^x f(y) \sqrt{y} dy \tag{75} \]

defined on the Hilbert space of the functions on \([0, 1]\) with the scalar product:

\[ \langle f | g \rangle = \int_0^1 x \sqrt{x} \bar{f}(x)g(x) dx \tag{76} \]
Then $A$ is a bounded symmetric operator and:

$$I_2/I_1 = \frac{1}{5\pi} \left( \langle ab | Ab \rangle - 1 \right)$$

(81)

The unitary operator $f(x) \rightarrow g(y) = f(x^2)e^{-5/4y}$ from $L^2([0,1], x \sqrt{\int} dx)$ onto $L^2([0, +\infty], dx)$ maps the operator $A$ onto the operator $\tilde{A}$:

$$\tilde{A}g(x) = \frac{e^{-x/4}}{2} \int_0^x e^{y/4}g(y)dy + \frac{e^{x/4}}{2} \int_x^{+\infty} e^{-y/4}g(y)dy$$

Then

$$\tilde{A}e^{ikx} = \frac{1}{4(1/16 + k^2)}e^{ikx} - \frac{1}{1/2 + i2k}e^{-x/4}$$

(82)

Thus setting:

$$g_k(x) = \frac{1}{|1 + i4k|} \left[ (1 + i4k)e^{ikx} - (1 - i4k)e^{-ikx} \right]$$

(83)

(84)

$$\{g_k\}_{k>0}$$ is a full set of pseudo-eigenvectors satisfying:

$$\tilde{A}g_k = \frac{1}{4(1/16 + k^2)}g_k$$

Thus the spectrum of $\tilde{A}$ is $(0, 4)$ and the spectral measure is purely absolutely continuous; the largest spectral value is 4 with a pseudo-eigenvector $g_4(x) = x + 4$ corresponding to $f_4(x) = x^{-5/4}(4 - \ln x)$.

But $\|f_4\|$ is infinite and $f_4$ diverges at 0. The next step is to choose a family of functions $b_\eta$ such that $a_\eta = \sqrt{1 - b_\eta}$ is defined and $\langle a_\eta b_\eta | A a_\eta b_\eta \rangle / \|b_\eta\|^2$ is close to 4.

Thus setting $f_\eta(x) = \min(f_4(x), f_4(\eta))$ for $0 < \eta \ll 1$, we have:

$$\|f_\eta\|^2 = -\frac{1}{3} \left[ \ln^3 \eta - \frac{66}{5} \ln^2 \eta + O(\ln \eta) \right]$$

(85)

$$\langle f_\eta | A f_\eta \rangle = -\frac{4}{3} \left[ \ln^3 \eta - \frac{41}{5} \ln^2 \eta + O(\ln \eta) \right]$$

(86)

Then:

$$\frac{\langle f_\eta | A f_\eta \rangle}{\|f_\eta\|^2} = 4 - \frac{20}{\ln \eta} + O(\ln^{-2} \eta)$$

(87)

Thus $f_\eta$ is a good candidate for the linear part of the problem. Now, by the simple scaling:

$$b_\eta(x) = \frac{f_\eta(x)}{\sqrt{2}f_\eta(\eta)}$$

(88)

we get the nonlinear candidate satisfying $b_\eta(x) \leq 1/\sqrt{2}, a_\eta = \sqrt{1 - b_\eta^2}$ is well defined, $a_\eta(x) \geq 1/\sqrt{2}$ and $b_\eta$ satisfies (87).

We must now estimate the simultaneous convergence of $I_2/I_1$ (81) and $I_2$ as $\eta$ decreases.

$$\langle b_\eta | Ab_\eta \rangle - \langle b_\eta a_\eta | Ab_\eta a_\eta \rangle = -\langle b_\eta - b_\eta a_\eta | A | b_\eta - b_\eta a_\eta \rangle + 2 \langle b_\eta - b_\eta a_\eta | A | b_\eta \rangle \leq 2 \langle b_\eta - b_\eta a_\eta | A | b_\eta \rangle$$

$$= 8 \langle b_\eta - b_\eta a_\eta | b_\eta \rangle + 2 \langle b_\eta - b_\eta a_\eta | (A - 4) b_\eta \rangle \leq 8 \langle b_\eta - b_\eta a_\eta | b_\eta \rangle + 2 \|b_\eta - b_\eta a_\eta\| \|A - 4) b_\eta\|$$

$$\leq 8 \langle b_\eta - b_\eta a_\eta | b_\eta \rangle + 8 \|b_\eta - b_\eta a_\eta\| \sqrt{\langle b_\eta | (A - 4) b_\eta \rangle}$$
where:

\[
\langle \eta - \eta a_\eta | \eta \rangle = \int_0^1 \eta(x)^2 \left[ 1 - a_\eta(x) \right] x \sqrt{x} dx \\
\leq \int_0^1 \eta(x)^2 \left[ 1 - a_\eta(x) \right]^2 x \sqrt{x} dx \sup \frac{1}{1 - a_\eta} \\
\leq \| \eta - \eta a_\eta \|^2 \frac{\sqrt{2}}{\sqrt{2} - 1}
\]

and since \( \eta - \eta a_\eta > 0 \)

\[
\| \eta - \eta a_\eta \|^2 = \| \eta \|^2 - \| \eta a_\eta \|^2 - 2 \langle \eta - \eta a_\eta | \eta a_\eta \rangle \\
\leq \| \eta \|^2 - \| \eta a_\eta \|^2 \\
= \| \eta^2 \|^2
\]

By direct computation:

\[
\| \eta^2 \|^2 \leq \| \eta \|^2 \frac{6}{5|\ln \eta|}
\]

for \( \eta \) small enough, and thus:

\[
\frac{\langle \eta | A \eta \rangle}{\| \eta \|^2} - \frac{\langle \eta a_\eta | A \eta a_\eta \rangle}{\| \eta a_\eta \|^2} \leq \frac{8}{|\ln \eta|} \left( \frac{\sqrt{2}}{\sqrt{2} - 1} \frac{6}{5} + 2\sqrt{6} \right) \tag{89}
\]

And finally, from [87] for \( \eta \) and \( \| \eta \|^2 \), \( \| \eta a_\eta \|^2 \), \( \| \eta a_\eta \|^2 \) gives:

\[
I_2/I_1 \geq \frac{1}{5\pi} \left( 3 - \frac{C}{|\ln \eta|} \right) + O(\ln^{-2} \eta) \tag{90}
\]

\[
I_2 \leq \frac{2}{15\pi} \eta^{5/2} |\ln \eta|^3 \left[ 1 + O \left( \frac{1}{|\ln \eta|} \right) \right] \tag{91}
\]

where

\[
C = 20 + 8 \left( \frac{\sqrt{2}}{\sqrt{2} - 1} \frac{6}{5} + 2\sqrt{6} \right) \approx 92 \tag{92}
\]

Choosing \( \eta \) sufficiently small, this proves that \( \Delta E \) is strictly negative for any \( r_s > 0 \); furthermore choosing \( \eta \) to minimize \( \Delta E \) (Eq. 41), i.e. \( 9r_s |\ln \eta|^2 = 2C \pi \), we obtain as \( r_s \) goes to 0:

\[
\Delta E \lesssim -r_s \exp \left( -\frac{5\pi}{3r_s} + \frac{O(1)}{\sqrt{r_s}} \right) \tag{93}
\]

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