Metal-insulator transition in the Hartree-Fock phase diagram of the fully polarized homogeneous electron gas in two dimensions

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We determine the ground state of the two-dimensional, fully polarized electron gas within the Hartree-Fock approximation without imposing any particular symmetries on the solutions. At low electronic densities, the Wigner crystal solution is stable, but for higher densities (r_s less than ~ 2.7) we obtain a ground state of different symmetry: the charge density forms a triangular lattice with about 11% more sites than electrons. We argue that this conducting state with broken translational symmetry remains the ground state of the high density region in the thermodynamic limit giving rise to a metal to insulator transition.

The two-dimensional homogeneous electron gas is one of the fundamental models in condensed matter physics. Despite its simplicity - the system consists of electrons interacting through a $1/r$-potential to which a uniform positive background is added for charge neutrality - the phase diagram at zero temperature is nontrivial[1, 2, 3]. In general, it is given in terms of the dimensionless parameter $r_s = 1/\sqrt{\pi n a_B^2}$, where n is the electronic density and a_B the Bohr radius. At low density (large r_s), the potential energy dominates over the kinetic energy and the system forms a perfect triangular lattice, the Wigner crystal (WC), whereas in the high density region ($r_s \to 0$) the kinetic energy favors a uniform Fermi gas (FG) phase[1]. Already Wigner[4] argued that the unpolarized FG is unstable even in the limit $r_s \to 0$. Later, Overhauser showed the instability of the unpolarized WC with respect to spin-density waves, even within the Hartree-Fock approximation (HF)[5]. It has further been conjectured that the Coulomb potential prevents any first order transition between the WC and a FG[6]. Despite these rather general instability theorems, we are not aware of any quantitative calculations establishing the true ground state of the electron gas within HF[7]. A previous HF study of the two and three dimensional electron gas with imposed symmetries considered only the FG and different crystal structures for the WC phase[8], and only recently an unrestricted HF 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 the high density region[9]. Indeed, establishing the precise HF phase diagram of the electron gas is a fundamental question, since many-body correlation effects can only be quantified with respect to the best HF solution.

In this letter, we consider the two-dimensional electron gas, and, for simplification, we concentrate on the HF ground state of the completely polarized system. At low densities, $r_s \gtrsim 2.7$, our simulations always lead to a WC, but for higher densities and large enough number of electrons, N, the solution is neither a FG nor a WC: the density modulation corresponds to a partially occupied crystal of different symmetry compared to the insulating WC phase (the number of sites is larger than N). We refer to this solution as a metallic phase.

To observe the metallic phase, the number of electrons has to exceed a threshold ranging from $N \gtrsim 10$ at $r_s \sim 2.7$ up to $N \gtrsim 10^2$ at $r_s \sim 1$. For sizes below the threshold, the solution is the FG [10]. However we can prove analytically that the metallic phase has a lower energy than the FG down to $r_s = 0$ in the thermodynamic limit. [11] This proof also indicates that the threshold size varies with r_s as $\exp(Cst/r_s)$, which may explain why this metallic phase has not been observed in previous simulations. It is possible to understand heuristically, why the metallic phase occurs at small r_s. One expects that the electrostatic energy is always lowered by a periodic triangular charge density. On the other hand, at small r_s the kinetic energy dominates and favors states close to the Fermi surface. The simplest solution is obtained by choosing a triangular modulation lattice with generators Q_i of modulus $2k_F$. This modulation is mainly carried by the wave vectors close to the Fermi surface. These new HF solutions open a new perspective for the qualitative understanding of the experimental observed metal to insulator transition[12] and should be considered in studies beyond the HF approximation.

The N-body Hamiltonian, $H = K + V$, contains the kinetic energy K and the $1/r$-periodic Coulomb potential V where a uniform positive charge background is subtracted. Within the HF approximation, the search of the true ground state of the quantum many-body system is reduced to the simpler problem of finding the lowest energy states in the subset of the Slater determinants. Let $\Phi = \varphi_1 \wedge \cdots \wedge \varphi_N$ be the Slater determinant associated with the single particle states $\{\varphi_i\}$ and $E(\varphi_1, \varphi_2, \ldots, \varphi_N)$ the corresponding energy expectation value. The varia-

tion of E with respect to a variation of the single particle state $\delta\varphi_i$ is then given by

$$\delta E = \sum_i \langle h_\Phi \varphi_i | \delta\varphi_i \rangle + \sum_i \langle \delta\varphi_i | h_\Phi \varphi_i \rangle. \qquad (1)$$

where h_Φ, the so-called HF Hamiltonian, is a single particle operator depending on the full state Φ (not on the particular choice of the φ_i's). Extremal states must satisfy the following equation

$$h_\Phi \varphi_i = \sum_j C_{ij} \varphi_j, \qquad (2)$$

where C_{ij} are the Lagrange coefficients associated with the normalization constraint $\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$. Conversely, if $\Phi = \varphi_1 \wedge \cdots \wedge \varphi_N$ is not an extremum, we have

$$h_\Phi \varphi_i = \sum_j C_{ij} \varphi_j + \theta_i \qquad (3)$$

where the θ_i's satisfy $\langle \varphi_i | \theta_j \rangle = 0, \forall i, j$. Within the steepest descent method one chooses first a $N \times N$ unitary transformation $A = (a_{ij})$ such that one obtains

$$\langle \varphi_i' | \theta_j' \rangle = 0, \quad \langle \theta_i' | \theta_j' \rangle \propto \langle \varphi_i' | \varphi_j' \rangle = \delta_{ij}, \quad \forall i, j \qquad (4)$$

for the transformed single particle states $\theta_i' = \sum_j a_{ij} \theta_j$, $\varphi_i' = \sum_j a_{ij} \varphi_j$. The energy $E(\varphi_1 + \lambda\theta_1, ..., \varphi_N + \lambda\theta_N)$ can be expressed as a sum of rational fractions whose numerators and denominators are polynomials of order four, at most. Thus, it is possible to find the best λ and to iterate the process until a stationary state is reached.

In fact, this method has the same drawbacks as the steepest decent method in linear optimization problems; in general, it converges slowly. For linear problems, conjugate gradient methods are preferable [13, 14]. However, since the HF states do not form a linear space, the genuine conjugate gradient method does not apply here. We have therefore adapted a variant of this method to the non-linear case. Let η_i be the previous variation $\delta\varphi_i$, and θ_i is obtained by Eq. (3). We then compute $E(\varphi_1 + \lambda\theta_1 + \mu\eta_1, \cdots, \varphi_n + \lambda\theta_N + \mu\eta_N)$ for six values of the pairs $\{\lambda, \mu\}$ in order to approximate E by a polynomial of order two in λ and μ. Minimizing the polynomial with respect to λ and μ, we obtain the new changes of the single particle states, $\delta\varphi_i$, and the corresponding energy change. This process is iterated until the relative variation of the energy, $\delta E/E$, is sufficiently small.

Since we expect the electrons to crystallize on a triangular lattice at low densities, we have chosen periodic conditions compatible with this geometry. Thus, the unit cell of our periodized system is given in terms of two vectors $\{\mathbf{L}_1, \mathbf{L}_2\}$ of length L and with an angle of 60 degrees between both; the volume of the unit cell is $\Omega = L^2\sqrt{3}/2$. We have restricted our study to system sizes which are compatible both with the triangular lattice and with a closed shell occupation in k-space. Any triangular crystal with unit-cell vectors $\{\mathbf{e}_1, \mathbf{e}_2\}$ is compatible with the
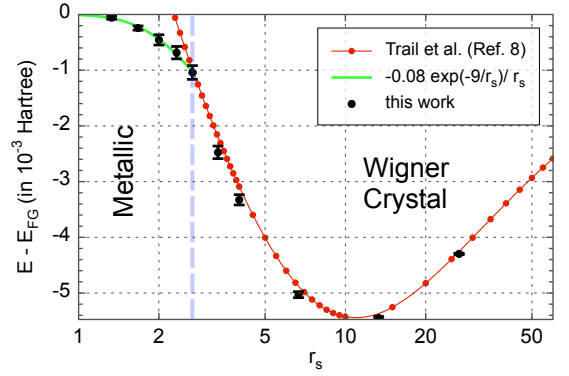

FIG. 1: Extrapolated energies $E_\infty - E_{FG}$ (milli-Hartree units) versus r_s. Points with error bars: present calculations, full line (red): data of Ref. [8], full line (green): fit to present results for ($r_s \lesssim 2.7$), vertical dash line (blue): $r_s \sim 2.7$.

boundary conditions if it satisfies $\mathbf{L}_1 = l\mathbf{e}_1 + m\mathbf{e}_2$ and $\mathbf{L}_2 = -m\mathbf{e}_1 + (l+m)\mathbf{e}_2$, where (l, m) are two non-negative integers. The number of sites of the lattice is given by $N_c = \det(\mathbf{L}_1, \mathbf{L}_2)/\det(\mathbf{e}_1, \mathbf{e}_2) = l^2 + m^2 + lm$. For a commensurate lattice $N = N_c$.

We compute the wavefunction on a $N_g \times N_g$ grid, the fast Fourier transform is used to switch between real and reciprocal space[15]. We have systematically checked the convergence of the solution with respect to the grid size. For the FG ground state, convergence is reached once all k-vectors up to $2k_F$ are represented in the grid ($N_g \sim 4\sqrt{N/\pi}$). At larger r_s, in the WC phase, the wave functions are essentially gaussians[16]. The width δ of the gaussians scales as $\delta/L \propto (r_s N)^{-1/2}$. For a correct resolution of the gaussians we need $L/N_g \propto \delta$, so that the number of grid points increases at low densities, $N_g \propto (Nr_s)^{1/2}$. Convergence was reached for $N_g = 32$ (resp. 64, 128) for $N \leq 43$ (resp. $N \leq 200$, $N \leq 500$) up to $r_s = 30$. Whenever the number of grid points was chosen too small, solutions without any particular symmetries have been obtained.

We have further studied the influence of the initial state on the final solution, choosing different types of wavefunction for initialization: a WC state, a converged state stored at larger or lower r_s, a state initialized with random numbers, or a "metallic state" as described below (this state has $N_c > N$ maxima in the charge density).

Typically, during the minimization procedure, the energies decrease exponentially; however, the rate of convergence depends on the initial state. The decrease in energy during transitions to a different symmetry is in general much smaller than the convergence within the same symmetry. We have often seen energy plateaus with changes of relative energy $\lesssim 10^{-4}$ just before the occurrence of a transition to a completely different state. For system sizes up to $N = 151$, the minimization is continued until a relative precision of 10^{-12} is reached, and
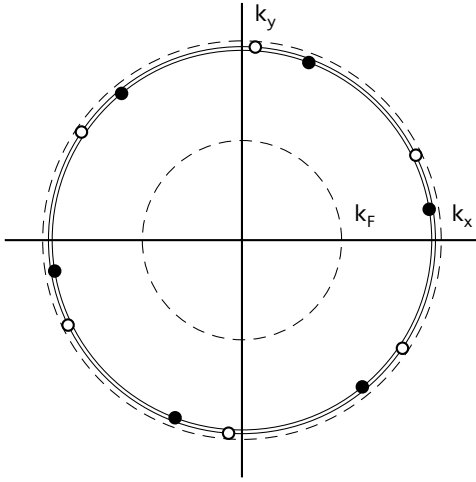
FIG. 2: Main points of $\tau(\mathbf{q})$ Eq. (7) for N=151. The black (resp. white) dots corresponds to $r_s = 3.33$ (resp. 2.7). The radii of the dashed circles are k_F and $2k_F$. The ratio of the radii of the solid circles is $\sqrt{157/151}$. The other points in $\tau(\mathbf{q})$ are several order of magnitude less.

FIG. 3: Charge density $\rho/\langle\rho\rangle - 1$, with $\rho(x) = \sum_{i=1}^{N} |\varphi_i(x)|^2$. Top: the number of maxima is $N_c = 9^2 + 5^2 + 9 \times 5 = 151$. Bottom: the number of maxima is $N_c = 12^2 + 1^2 + 12 \times 1 = 157$. Gray levels corresponds to the same density in both figures. Colored lines correspond to $\mathbf{L}_1 = l\mathbf{e}_1 + m\mathbf{e}_2$, where the numbers stands for l, m (see text).

for larger N a relative precision of 10^{-5} is used.

We have studied systems with up to 500 electrons at densities corresponding to $r_s = 1$ up to $r_s = 30$. In Figure 1, we report the energies of the obtained HF ground state $E_\infty(r_s)$, extrapolated to the thermodynamic limit, as a function of r_s. In the high density region, for $r_s > 3$, we obtain good agreement with the results of Trail *et al.*[8], which imposed the triangular WC symmetry. For $r_s < 3$, we find ground states of different symmetries than the WC which we describe below. These new states have been eventually found down to $r_s = 1$, at smaller r_s, the FG solution is stable for our finite system sizes with $N \leq 500$.

We now turn to a more detailed analysis of the different phases. It is instructive to follow the evolution of the Slater determinants in k-space as a function of r_s. In order to quantify the differences to the FG solution, we project each plane wave $\phi_{\mathbf{k}_0}$ of the FG ($k_0 \leq k_F$), on our HF solution $\{\varphi_i\}$,

$$\phi_{\mathbf{k}_0} = \phi_{\mathbf{k}_0}^{\parallel} + \phi_{\mathbf{k}_0}^{\perp}, \qquad (5)$$

$$\phi_{\mathbf{k}_0}^{\parallel} = \sum_i (\varphi_i, \phi_{\mathbf{k}_0})\varphi_i \qquad (6)$$

where $\phi_{\mathbf{k}_0}^{\parallel}$ is the projection of $\phi_{\mathbf{k}_0}$ on the subspace spanned by the φ_i's. The deviation of the HF solution from the FG can be measured by $\tau(\mathbf{q})$ as

$$\tau(\mathbf{q}) = \sum_{k_0 \leq k_F, k_0 \neq q} \left|\phi_{\mathbf{k}_0}^{\perp}(\mathbf{q} - \mathbf{k}_0)\right|^2 \qquad (7)$$

For the FG, $\tau(\mathbf{q})$ is 0. Remarkably, for the WC or the metallic ground states, $\tau(\mathbf{q})$ is non zero only for few $\mathbf{q}$-vectors (see Fig. 2). For the WC, $\tau(\mathbf{q})$ is nonzero on
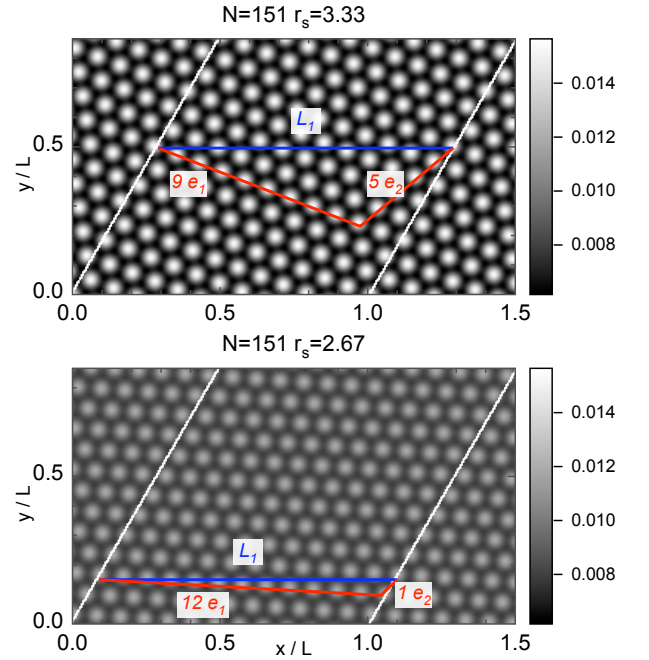
the points corresponding to the triangular reciprocal lattice: $a\mathbf{q}_1 + b\mathbf{q}_2$, with a, b integers and $\mathbf{q}_1 = l\mathbf{K}_1 - m\mathbf{K}_2$, $\mathbf{q}_2 = m\mathbf{K}_1 + (l+m)\mathbf{K}_2$ ($\mathbf{K}_\alpha \cdot \mathbf{L}_\beta = 2\pi\delta_{\alpha\beta}$) [17]. As r_s decreases from 26.7 down to 3, only the first layer of q-vectors corresponding to the triangular lattice remain important. In this region, only the hexagon of the 6 lowest q-vectors of the WC remains (see Fig. 2), and the shape of the charge-charge density in k-space is hexagonal instead of the circular shape at lower densities. This wavefunction has therefore a similar character as the hybrid wave functions studied in Ref. [3]. However, in contrast to Ref. [3], instead of a phase transition, we find a continuous change from many layers of k-vectors compatible with the WC at high r_s to only one layer (Figure 2) as r_s decreases. At the same time, $\tau(\mathbf{q})$ in Eq. (7) is dominated by the contribution of the FG vectors $\mathbf{k}_0$ close to Fermi surface. For $|\mathbf{k}_0| \approx k_F$, $\phi_{\mathbf{k}_0}^{\perp}(\mathbf{k})$ has essentially only one nonzero component at the vector $\mathbf{k} = \mathbf{k}_0 + \mathbf{q}$ closest to the Fermi surface, with $\mathbf{q}$ in the reciprocal lattice of the WC.

At $r_s \approx 2.7$, the system lowers its energy by delocalizing the electrons on a denser lattice with more sites than electrons (Figure 2 and 3). This denser lattice is characterized by integer numbers (l', m') different from the WC lattice (l, m). For some system sizes N, the maxima of $\tau(\mathbf{q})$ correspond to various couples of $\{l', m'\}$ leading
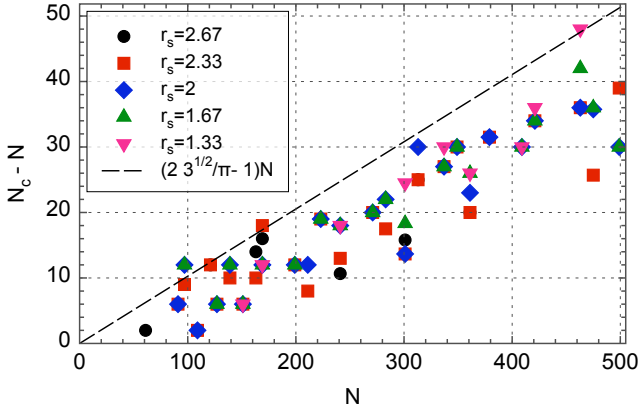
FIG. 4: $N_c - N$ versus the number N of electrons, where N_c is the number of maxima in the charge density. Remark that N_c never decreases with r_s. The line is from Eq. (8).

In conclusion, we have computed the ground state energy of the two dimensional fully polarized periodic electron gas in the HF approximation. We recover the WC at large r_s. For $r_s \lesssim 2.7$, the ground state changes symmetry. Still breaking translational symmetry, the crystal formed contains more lattice sites than particles and should therefore have metallic properties. For our finite systems, this solution disappears at small r_s in favor of the FG. The same metallic phase has also been numerically observed as the HF ground state both in the unpolarized system and in a model where the electrons interact with a screened Coulomb potential[11].

Post HF approaches, like the Quantum Monte Carlo method[1, 2, 3], have to be used in order to study the influence of correlation effects and to establish precisely the phase diagram of the electron gas.

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[15] In reciprocal space, the k-vectors of the WC fall on the grid.
[16] Indeed, a simple variational calculation with only one parameter, the width of the gaussians, gives the HF-energy with a relative precision better than 0.1%.
[17] In the triangular triangular, the magnitude of the reciprocal lattice vectors are scaled $\|\mathbf{K}_1\| = \|\mathbf{K}_2\| = (2/\sqrt{3})2\pi/L$, compared to a rectangular lattice.

to different number of lattice sites, $N' = l'^2 + m'^2 + l'm'$ (Fig.4). In this case, our system looks like a periodic crystal with an incomplete band in contrast to the WC solutions of fully occupied bands, studied in Ref. [8]. Therefore, our translational symmetry breaking HF solutions below $r_s \approx 2.7$, have a genuine metallic character. However, as r_s approaches zero, the energy gain of this metallic crystal compared to the FG gets more and more tiny. At the same time, as one can see in Fig.4, N_c is either constant or increases when r_s decreases (apart for one exception $N = 301$ at $r_s = 2.67$). For $r_s < 1$ and $N < 500$, the FG is always the ground state.

Now we show that the translational symmetry breaking, metallic states should exist at small r_s in the thermodynamic limit. Let us replace a plane wave state $\mathbf{k}$ of the free FG ($\|\mathbf{k}\| \le k_F$) by a superposition of two plane waves with wavevectors $\mathbf{k}$ and $\mathbf{k} + \mathbf{q}$ ($\|\mathbf{k} + \mathbf{q}\| > k_F$). Choosing $\mathbf{q}$ on the six-fold star of a triangular lattice we certainly obtain a gain in potential energy. The increase of kinetic energy is minimized if $\|\mathbf{k}\| \sim k_F$ and $\|\mathbf{k} + \mathbf{q}\| \sim k_F$. Then, the number of solutions for $\mathbf{k}$ is optimal if $\|\mathbf{q}\| \sim 2k_F$. This solution corresponds to a triangular lattice of length $L_c = 2\pi/(\sqrt{3}k_F)$ in real space leading to a unit cell of volume $\Omega_c = \sqrt{3}L_c^2/2$. Since our system is contained in the volume $\Omega = \sqrt{3}L^2/2$, we will obtain $N_c = \Omega_c/\Omega$ lattice sites, or

$$N_c = \frac{2\sqrt{3}}{\pi}N \approx 1.1N \qquad (8)$$

where we have used $n = N/\Omega = k_F^2/(4\pi)$. From Fig. 4 we see that, as r_s decreases, the number of sites of the HF ground state indeed approaches the limit of Eq. (8).

A simple model accounting for such a perturbation[11] (actually far in norm from the FG) gives an energy difference from the FG varying as $-\exp(-a/r_s)/r_s$ at the limit $r_s \to 0$. Our data are reasonably well represented by such a law (see Fig. 1).