THE LOW DENSITY PHASES OF THE ELECTRON GAS*

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Résumé.- Nous avons généralisé la méthode de Monte Carlo quantique, utilisée par Kalos, Levesque et Verlet pour des bosons, pour simuler exactement les propriétés de l'état fondamental de systèmes de fermions. Nous avons effectué des simulations sur un plasma à une composante comportant jusqu'à 250 électrons et déterminé l'équation d'état des trois phases : le liquide de Fermi normal (non polarisé), le liquide de Fermi polarisé et le cristal de Wigner. Deux transitions de phase sont ainsi observées : entre le liquide normal et le liquide polarisé à $r_s = 75$ et entre le liquide polarisé et le cristal de Wigner à $r_s = 100$, r_s étant l'écart moyen entre particules exprimé en rayon de Bohr.

Abstract. - We have generalized the quantum Monte Carlo method for Bosons of Kalos, Levesque, and Verlet to exactly simulate the ground state of many-Fermion systems. We have carried out such simulations on the one component plasma with up to 250 electrons and determined the equation of state in three phases: the normal (unpolarized) Fermi liquid, the polarized Fermi liquid and the Wigner crystal. Two phase transitions are seen: from the normal liquid to the polarized at $r_s = 75$, and from the polarized liquid to the Wigner crystal at $r_s = 100$ where r_s is the mean interparticle spacing in Bohr radii.

For fifty years the phases of the electron gas (also known as jellium or the Fermion one component plasma) have been the object of theoretical interest, which began when Bloch[1] discovered that the Sommerfeld model for describing electrons in simple metals will exhibit a ferromagnetic state in the Hartree-Fock approximation for electron densities corresponding to cesium metal and lower. In this approximation, Pauli exclusion is the only mechanism for electrons to correlate so that a transition to a magnetic state is expected. A few years later, Wigner[2] pointed out, that as the electronic density is lowered, the potential energy dominates the kinetic energy, so that the electrons must crystallize. Since these early calculations, there have been numerous investigations[3,4,5] of the relative stabilities of these three states (paramagnetic, ferromagnetic, and crystal) without any consensus on when or if the ferromagnetic transition would occur and at what density Wigner crystallization would occur. The energies of the various phases are close to each other over a wide range of densities. To accurately compute the transition density one must be able to treat correlation effects equally well in each phase.

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Monte Carlo simulation is such a method for calculating the properties of many-body systems accurately. Only recently have computers been sufficiently powerful to tackle these quantum many-body problems. The work of Kalos, Levesque, and Verlet[7] on the ground state of hard sphere Bosons is a landmark calculation. Similar simulations of Lennard-Jones Bosons[8] have agreed very well with experimental data on the low temperature properties of Helium 4. Recently, we have generalized the quantum Monte Carlo method so as to treat Fermion systems and have performed simulations of the ground state of the electron gas. The details of the method will be given elsewhere. Here we wish to summarize the results that concern the phases of the electron gas at low density.

In the quantum Monte Carlo method, a trial function of the Slater-Jastrow form[9] (a product of pair correlation factors and a Slater determinant of orbitals) is employed to specify the symmetry of the particles, to keep the population of random walks in the important regions of phase space and to reduce the variance of the calculated energy. The mean value of the calculated energy will be exactly the ground state energy. It is in this statistical sense that the simulation is exact. As with most stochastic methods, the variance of the energy will be inversely proportional to the number of steps of the random walk.

For the fluid phases considered, the orbitals used were plane waves with vectors lying within the Fermi sea. In the paramagnetic fluid the spatial states are doubly occupied; in the ferromagnetic phase they are singly occupied. Hence, the ferromagnetic fluid is antisymmetric with respect to the interchange of all particles; the paramagnetic only with respect to like spins. In the Boson fluid, the Slater determinant is not used. For the crystalline phase, the orbits are Gaussians, centered around BCC lattice sites.

Table I contains the energy of the four phases that we have studied as a function of r_s, the mean interparticle spacing in units of Bohr radii. The energy difference between a Bose and Fermi crystal is less than the accuracy of our calculation. Hence, we cannot discuss the magnetic ordering within the crystal. In Fig. 1 are plotted the energies relative to the lowest Boson energy times r_s^2. Plotted in this manner one can see the small differences in energy amongst the phases. The Boson system crystalizes at $r_s = 160$. The Fermion system undergoes two phase transitions; polarization at $r_s = 75$ and Wigner crystallization at $r_s = 100$.

The melting of the Wigner crystal occurs because, as the density increases, the zero point motion of the electrons disrupts the lattice. Alternatively, the localization energy of the electrons about the lattice sites becomes larger than the kinetic energy of the liquid. Table II contains Lindemann's ratio, the rms deviation of an electron from the nearest lattice site in units of the nearest neighbor distance. This ratio equals 0.25 at melting for the Boson system and 0.30 for the Fermion system. This value at melting is about twice that found classically and very similar to that found[8] in solid Helium 4.

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Table I

r_s	E_{PMF}	E_{FMF}	E_{BF}	E_{BCC}
1.0	1.174(1)	----------	---------	----------
2.0	0.0041(4)	0.2517(6)	0.4531(1)	----------
5.0	-0.1512(1)	-0.1214(2)	-0.21663(6)	----------
10.0	-0.10675(5)	-0.1013(1)	-0.12150(3)	----------
20.0	-0.06329(3)	-0.06251(3)	-0.06666(2)	----------
50.0	-0.02884(1)	-0.02878(2)	-0.02927(1)	-0.02876(1)
100.0	-0.015321(5)	-0.015340(5)	-0.015427(4)	-0.015339(3)
130.0	----------	----------	-0.012072(4)	-0.012037(2)
200.0	----------	----------	-0.008007(3)	-0.008035(1)

The ground state energy of the charged Fermi and Bose systems. The density parameter, r_s, is the Wigner sphere radius in units of Bohr radii. The energies are Rydbergs and the digits in parenthesis represent the error bar in the last decimal place. The four phases are: paramagnetic or unpolarized Fermi fluid (PMF); the ferromagnetic or polarized Fermi fluid (FMF); the Bose fluid (BF); and the Bose crystal with a BCC lattice.

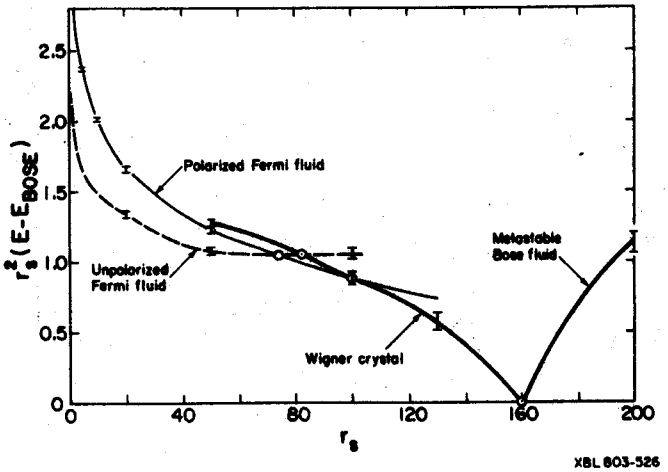

Fig. 1 The energy of the four phases studied relative to that of the lowest Boson state times r_s^2 in Rydbergs versus r_s in Bohr radii. Below r_s = 160 the Bose fluid is the most stable phase, while above, the Wigner crystal is most stable. The energies of the polarized and unpolarized Fermi fluid are seen to intersect of r_s = 75. The polarized (ferromagnetic) Fermi fluid will be stable between r_s = 75 and r_s = 100.

Table II

r_s	γ
50	0.423
100	0.300
130	0.283
200	0.248

Lindemann's ratio γ as a function of the density r_s in the Wigner crystal. The statistical error is approximately ±0.002.

magnetically order at low density can be ascribed to the fact that the localization caused by the increased antisymmetry lowers the potential energy. From the virial theorem, the potential energy is $r_s^{-1}\, d(r_s^2 E)/dr_s$. Hence, the potential energy relative to that of the Boson system is proportional to the slope of Fig. 1. One sees at high r_s (low density) the paramagnetic potential energy approaches that of the Bose fluid, while the ferromagnetic potential energy approaches that of the Wigner crystal. Thus, the ordering induced by the ferromagnetism is favored.

In Fig. 2, the radial distribution functions for the various phases at r_s = 50 are plotted. They are strikingly similar, the functions being only different by 10% at the peak. But the slight difference in potential energy is enough to cause a transition at this density. The corresponding momentum densities, n(k), defined as the number of electrons having momentum k are plotted in Fig. 3 at the same value of r_s. One can still see remnants of the discontinuities at the ideal gas Fermi surfaces as predicted by Midgal[10]. The momentum distributions of the ferromagnetic and paramagnetic fluids are quite different even at this density.

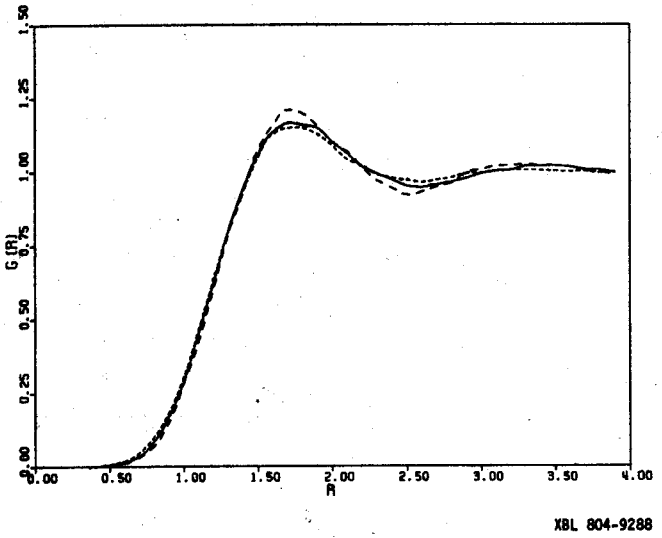

Fig. 2 The pair distribution functions for the electron gas at $r_s = 50$. ——— paramagnetic fluid, ---- Boson fluid, — — — ferromagnetic fluid. r is in units of the interparticle spacing.

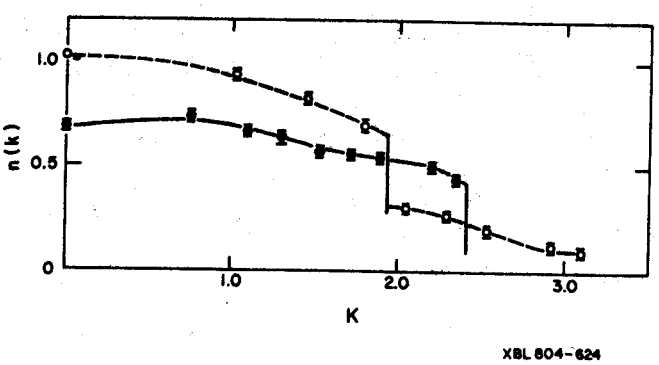

Fig. 3 The population of electrons in momentum states k at $r_s = 50$. The solid line is the ferromagnetic fluid; the dashed the paramagnetic fluid, k is in units of inverse interparticle spacings. The vertical lines represent the ideal gas Fermi wavevector.

The conclusions of this study are tentative given the very small energy differences between the potential and kinetic energies of the Wigner crystal and the ferromagnetic fluid in the density range $50 < r_s < 100$. Longer simulations with more particles (we have used a maximum of 242 to date) would be desirable to confirm these results, since the number dependence of the results is large compared to the energy difference between the various phases. Although the results are independent of the trial wavefunction, it would be useful to explore the effects of other trial functions with different symmetries, for example, one that describes spin density waves.

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