Effective interactions between parallel-spin electrons in
two-dimensional jellium approaching the magnetic phase
transition

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Abstract

We evaluate the effective interactions in a fluid of electrons moving in a plane, on the approach to the quantum phase transition from the paramagnetic to the fully spin-polarized phase that has been reported from Quantum Monte Carlo runs. We use the approach of Kukkonen and Overhauser to treat exchange and correlations under close constraints imposed by sum rules. We show that, as the paramagnetic fluid approaches the phase transition, the effective interactions at low momenta develop an attractive region between parallel-spin electrons and a corresponding repulsive region for antiparallel-spin electron pairs. A connection with the Hubbard model is made and used to estimate the magnetic energy gap and hence the temperature at which the phase transition may become observable with varying electron density in a semiconductor quantum well.

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Electronic fluids with an essentially two-dimensional (2D) dynamics, as are realized in semiconductor heterostructures, present a very rich phenomenology especially at low density, where the interactions between carriers come to play a crucial role [1]. This fact continues to motivate theoretical studies of the simplified system consisting of a gas of electrons described by the basic Coulomb Hamiltonian with a uniform neutralizing background (EG). More generally, this has been for many decades a basic reference model for calculations of electronic structure in molecular and condensed-matter systems [2].

Quantum Monte Carlo (QMC) simulation studies have been highlighting the formation of spontaneous spin polarization in the EG at strong coupling. A continuous transition from the paramagnetic to spin-polarized states has been reported to take place in the 3D EG with increasing coupling strength [3, 4], before a first-order transition into a ferromagnetic Wigner electron crystal occurs. Spontaneous partial spin polarization ("weak ferromagnetism") has been observed in doped hexaborides [5]. In the 2D EG, on the other hand, the quantum simulation studies indicate a first-order transition to a fully spin-polarized ("ferromagnetic") fluid before crystallization, no evidence being found for partially spin-polarized states [6 - 8].

Theoretical studies of the equation of state described by the ground-state energy \( E(n, \zeta) \) of the EG with spin densities \( n_\uparrow \) and \( n_\downarrow \) as a function of the electron density \( n = n_\uparrow + n_\downarrow \) and of the spin polarization \( \zeta = (n_\uparrow - n_\downarrow)/n \) are clearly called for in both dimensionalities. The ground-state energy is in turn determined by the pair distribution functions, stressing the importance of two-body electron-electron scattering via effective interactions in the many-body system [9, 10].

Exchange between parallel-spin electrons and correlations from the Coulomb repulsions are crucial in determining the pair distribution functions. These effects are embodied in the so-called local-field factors (LFF) entering the expressions of the charge and spin susceptibil-
ities of the EG [11]. The LFF play the same role as vertex corrections in accounting for the difference between the effective potentials experienced by an electron and their mean-field value. From their knowledge one can also calculate the quasi-particle self-energies and the effective electron-electron interactions, as is well known from work on the unpolarized EG [12].

In this letter we are concerned with the effective electron-electron interactions in the paramagnetic phase of the 2D EG as functions of the coupling strength on the approach to the magnetic quantum phase transition. We adopt the linear-response approach of Kukkonen and Overhauser [9] to construct these interactions from recent determinations of the LFF [13, 14], embodying their asymptotic behaviours from exact sum rules and information from QMC studies. The difference between the $↑↑$ and $↑↓$ effective interactions is related to the magnetic susceptibility and in the low scattering-momentum region most strikingly reflects the approaching phase transition in its behaviour with increasing coupling strength. After pointing out how these results could be used to reveal the magnetic phase transition in a theoretical calculation based on the solution of Schrödinger equations for two-electron problems, we establish an approximate connection with a simple mean-field solution of the Hubbard model for itinerant electrons and use it to estimate the temperature of the magnetic transition in the 2D EG at the density predicted by the QMC studies.

Following, therefore, Kukkonen and Overhauser [9], the effective interaction potential between two electrons with spin indices $\sigma_1$ and $\sigma_2$ is written in momentum space as

$$V_{\sigma_1\sigma_2}(q) = V_0(q) - J(q)\sigma_1 \cdot \sigma_2$$

where by convention the product $\sigma_1 \cdot \sigma_2$ equals +1 for parallel spins and -1 for antiparallel spins. The functions $V_0(q)$ and $J(q)$ are expressed in terms of the bare Coulomb potential $v(q) = 2\pi e^2/q$ and of the ideal-gas Lindhard susceptibility $\chi_0(q)$ as

$$V_0(q) = v(q) \frac{1 + [1 - G_{\pm}(q)]G_{\pm}(q)v(q)\chi_0(q)}{1 + [1 - G_{\pm}(q)]v(q)\chi_0(q)}$$

$$J(q) = \frac{1}{4\pi} \frac{1}{v(q)} \left( \frac{\chi_0(q)}{\chi_0(q) + \frac{1}{v(q)}} \right)$$
and

\[ J(q) = v(q) \frac{G_+^2(q)v(q)\chi_0(q)}{1 - G_+(q)v(q)\chi_0(q)} \]  (3)

Here, \( G_+(q) \) and \( G_-(q) \) are the charge-charge and spin-spin LFF in the paramagnetic 2D EG. It is important to remark for later use that the denominator in Eq. (3) also enters the microscopic magnetic susceptibility \( \chi(q) \) of the EG, which is given by

\[ \chi(q) = \frac{\chi_0(q)}{1 - G_-(q)v(q)\chi_0(q)} \]  (4)
in units such that the Bohr magneton equals unity.

The limiting behaviours of the LFF at low and high momenta are determined by a set of exact sum rules [15, 16]. Considering first \( G_+(q) \), these are the compressibility sum rule yielding

\[ \lim_{q \to 0} G_+(q) = \left\{ \frac{1}{\pi} - \frac{r_s^3}{8\sqrt{2}} \left[ \frac{d^2\varepsilon_c(r_s)}{dr_s^2} - \frac{1}{r_s} \frac{d\varepsilon_c(r_s)}{dr_s} \right] \right\} \frac{q}{k_F} \]  (5)

with the Fermi momentum given by \( k_F = \sqrt{2\pi n} \) in terms of the areal density \( n \), and the Kimball-Niklasson-Holas relation yielding

\[ \lim_{q \to \infty} G_+(q) = [1 - g(0)] - \frac{r_s}{2\sqrt{2}} \frac{d[r_s\varepsilon_c(r_s)]}{dr_s} \frac{q}{k_F} . \]  (6)

In these equations \( \varepsilon_c(r_s) \) is the correlation energy per particle as a function of the density parameter \( r_s = (\pi na_B^2)^{-1/2} \) with \( a_B \) the effective Bohr radius, and \( g(0) \) is the pair distribution function at contact. The corresponding limiting values of \( G_-(q) \) are determined by the magnetic susceptibility sum rule,

\[ \lim_{q \to 0} G_-(q) = \left[ \frac{1}{\pi} - \frac{r_s}{2\sqrt{2}} \frac{\partial^2\varepsilon_c(r_s)}{\partial\xi^2} \bigg|_{\xi=0} \right] \frac{q}{k_F} \]  (7)

and by the Santoro-Giuliani-Holas relation,

\[ \lim_{q \to \infty} G_-(q) = g(0) - \frac{r_s}{2\sqrt{2}} \frac{d[r_s\varepsilon_c(r_s)]}{dr_s} \frac{q}{k_F} . \]  (8)
Ample data from QMC studies are available for the correlation energy of the 2D EG as a function of density [7, 17] and for its long-wavelength magnetic susceptibility determining the coefficient in Eq. (7) [8, 18 - 20]. The value of $g(0)$ is also known over a wide range of density [21], from the solution of the two-body scattering problem and from many-body calculations in the ladder approximation.

Complete analytical expressions for both LFF have been obtained in the density range $r_s \leq 10$ [13, 14], using all the above information and further QMC data from [18 - 20] to describe their behaviour in the region of intermediate wave number. We have now extended this work to determine the LFF at $r_s = 20$, with the results that are shown in Figure 1. Especially relevant for this purpose have been the newly available QMC data on the magnetic susceptibility [8], which reaches the value $\chi(0)/\chi_0(0) \approx 25$ at $r_s = 20$. The corresponding values of the effective interactions between parallel-spin and antiparallel-spin electrons at several values of $r_s$ are shown in Figures 2 and 3, respectively. Some smoothing of apparently noisy features has been made in obtaining these results.

As was shown in Ref. [13, 14] and as again assumed in constructing $G_{-}(q)$ in Figure 1, the long-wavelength behaviour reported for this LFF in Eq. (7) holds over a rather wide range of scattering momentum $q$, extending almost up to $q = 2k_F$. The plateau shown by the effective interactions in this range of momentum is, therefore, essentially determined by the value of the magnetic susceptibility $\chi(0)$. As already noted, this thermodynamic parameter is approaching very large values as the paramagnetic phase of the 2D EG approaches the quantum phase transition to a fully spin-polarized state, that the latest QMC evidence places at $r_s \approx 25$ [8]. The effective interaction between parallel-spin electrons in Figure 2 becomes correspondingly strongly attractive in the momentum range $q \leq 2k_F$, while a repulsive structure grows at momenta above $2k_F$. In parallel to this behaviour, and as is evident from Eq. (1), the effective interaction between antiparallel-spin electrons in Figure 3 becomes strongly repulsive in the momentum range $q \leq 2k_F$. Although the quantitative
details of these results are rather sensitive to the precise value of $\chi(0)$, their significance is evidently correct: the approach to the transition into an ordered phase having a space-independent order parameter is driven by the emergence of effective interactions favouring spin alignments over a scale of distances which is becoming long compared with $(2k_F)^{-1}$.

In Figure 2 we have also reported the values of $V_{\uparrow\uparrow}(q)$ as calculated in the fully spin-polarized state at $r_s = 40[22]$, to show that the effective interactions regain a ”standard shape” after the magnetic phase transition has taken place. That is, the electron-electron interactions in momentum space are repulsive and show a rapid variation as $q$ goes through $2k_F$, corresponding to Friedel oscillations in coordinate space.

As was shown in the work of Takada [23] (see also Richardson and Ashcroft [24]), the effective electron-electron interactions may be used to assess the possibility of superconductive s-wave or p-wave pairing in the EG through the solution of an Eliashberg equation in the absence of phonons. It is natural to ask whether they may play a similarly useful role in regard to a magnetic phase transition. In fact, Ortiz et al. have stressed in their work [4] that a precise signal of the transition of an electron fluid to a magnetically ordered state is carried by the spin-spin radial distribution function, which is proportional to the difference $g_{\uparrow\uparrow}(r) - g_{\uparrow\downarrow}(r)$ between the radial distribution functions for the two spin populations. Near a magnetic transition the function $g_{\uparrow\uparrow}(r) - g_{\uparrow\downarrow}(r)$ can be expected to change sign at short range, going from negative in the deep paramagnetic phase (where it reflects a preference for spin alternation) to positive as magnetically ordered domains emerge. Methods to evaluate pair distribution functions in a many-body system through the solution of a Schrödinger equation for a two-body scattering problems have drawn some attention in the recent literature [10, 21, 25] and could easily be adapted to the study of magnetic phase transitions with the help of the effective potentials that we have determined in this work.

Here we adopt a much simpler and cruder route in order to estimate the magnetic
energy gap $\Delta$ which would be required for spin flips at zero momentum transfer in the magnetically ordered phase. This estimate is based on the remark that Eq. (4) for the magnetic susceptibility takes at low momenta the form that is obtained in the Hubbard model for a system of itinerant electrons [26]. The value of the Hubbard parameter $U$ appropriate for the 2D EG near the magnetic transition can therefore be estimated as

$$U \approx \lim_{k \to 0} [G_-(k)v(k)] = \chi_0^{-1}(0) - \chi^{-1}(0)$$

Setting $\Delta \approx nU$ for a fully spin-polarized state we estimate

$$\Delta \approx k_B T_c \approx \frac{2}{r_s^2} \left( 1 - \frac{\chi(0)}{\chi_0(0)} \right) \text{Ryd},$$

that is, taking $r_s \approx 25$ and $\chi(0)/\chi_0(0) \approx 25$ as from Ref. [8], $\Delta \approx 3.10^{-3}$ Ryd and $T_c \approx 400$ K for the EG model. This value is reduced by about three orders of magnitude when one takes account of an effective mass correction and of screening by a background dielectric constant in a semiconducting material. For instance, for the high-mobility GaAs/GaAlAs heterostructures studied by Yoon et al.[27] we estimate $T_c \approx 1$ K.

In summary, we have evaluated the effective interactions in momentum space between electrons in the paramagnetic phase of the 2D EG at various densities and shown how their shape reflects the emergence of magnetically ordered domains on the approach to the quantum phase transition into a fully spin-polarized phase. We have also given an estimate for the transition temperature at the density predicted by the QMC runs.

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FIG. 1. Charge-charge and spin-spin local field factors, $G_+(q)$ and $G_-(q)$, as functions of $q/k_F$ in the 2D EG in the paramagnetic state at $r_s = 20$. The straight dashed lines show the asymptotic behaviours determined by sum rules and exact relations (Eqs. (5) - (8)), while the full line show an approximate interpolation suggested by earlier studies at lower $r_s[13, 14]$. 
FIG. 2. Effective interaction potential in momentum space for parallel-spin electrons in the 2D EG in the paramagnetic state at various values of $r_s$ from 5 to 20. The dots report the effective interaction in the fully spin-polarized 2D EG at $r_s = 40$[22].

FIG. 3. Effective interaction potential in momentum space for antiparallel-spin electrons in the 2D EG in the paramagnetic state at various values of $r_s$ from 5 to 20.