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Hartree–Fock energy of a density wave in a spin-polarized two-dimensional electron gas

Juana Moreno and D C Marinescu

Department of Physics, Clemson University, Clemson, SC 29634, USA

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Abstract

We calculate the Hartree–Fock energy of a density-wave state in a spin-polarized two-dimensional electron system with short-range repulsive interactions. We find that the ground state is *always* either normal (nonmagnetic) or ferromagnetic. However, the energy of a density-wave state approaches the energy of the ferromagnetic ground state by a factor proportional to $(1-\zeta^2)$ (ζ is the polarization of the electron gas). Based on this result, we comment on the possible existence of a density-wave ground state when a more realistic interaction that includes electron correlations is considered.

The possible existence of a nonuniform ground state for a two-dimensional (2D) electron system in the presence of a magnetic field has been recently proposed in explaining the results of different experiments. Several examples of such puzzling data are the unidirectional charge-density-wave states that appear in partially filled Landau levels [1, 2], the incompressible, inhomogeneous insulating phase in p-GaAs/AlGaAs heterostructures displaying metal–insulator transition [3, 4], and the unusual magneto-optical properties of the ferromagnetic phase of p-type $Cd_{1-x}Mn_xTe$ quantum wells [5].

The idea of a nonuniform ground state in a paramagnetic 2D electron system had surfaced before. Prior to the discovery of the quantum Hall effect, it was argued that in 2D GaAs-type structures the ground state was a charge-density wave [6]. More recent experimental [1, 2] and theoretical [7, 8] results point, indeed, to the existence of charge-density-wave states in partially filled higher Landau levels on account of the quasi-one-dimensional electron motion.

In the case of an unpolarized electron gas recent numerical calculations [9] show that as the density is lowered the electron gas first undergoes a ferromagnetic transition followed by Wigner crystallization. However, a study of point defects in the 2D Wigner crystal suggests that the quantum melting could be continuous rather than first order [10], leaving open the possibility of inhomogeneous intermediate phases.

In this work we analyse the possible formation of density waves in an interacting 2D electron system that exhibits a very large Zeeman splitting. This situation occurs in II–VI dilute-magnetic semiconductor structures where the effective Landé factor is up to thousands

of times the band value. This is exactly opposite to the case in GaAs, where the cyclotron energy is dominant[1]. Within the Hartree–Fock (HF) approximation, we estimate the energy of a density-wave state for a delta-function repulsive interaction, the most unfavourable situation for the development of a density-wave instability in an isotropic system. Under these circumstances, obtaining a result that points toward a density instability bolsters the idea of finding a nonuniform ground state in a spin-polarized electron system when higher many-body corrections are incorporated within the Coulomb interaction. Such an assumption seems to be supported by quantum Monte Carlo calculations that show an enlargement of the exchange–correlation hole in polarized systems [11, 12], suggesting a propensity for density instabilities. Whether or not the instability develops before the Wigner crystallization and its dependence on the degree of polarization has not been studied yet.

It is well known that in three dimensions, within the HF approximation and for an unscreened Coulomb interaction, the paramagnetic state is unstable with respect to the formation of a spin density wave with wavevector near $2k_{\mathrm{F}}$ [13]. However, for a short-range potential the stable HF solution is *always* either the normal nonmagnetic state or the uniform ferromagnetic state [14]. We find that this result also holds in the 2D polarized system. In this case, however, the difference in energy between a density-wave state with momentum $\mathbf{q}$, $E(\mathbf{q})/N$, and the ferromagnetic state, $E(\mathbf{q}=0)/N$, is reduced by a factor proportional to $(1-\zeta^2)$, where $\zeta=(n_\uparrow-n_\downarrow)/n$ is the polarization of the electron gas,

$$\frac{E(\mathbf{q})-E(\mathbf{q}=0)}{N}=\mathbf{q}^2\frac{1-\zeta^2}{4}. \tag{1}$$

If the background charge is allowed to relax, as in the deformable jellium model, our result applies to both spin- and charge-density waves [15].

Since the effective electronic interaction in real systems is somewhere in between the short-range delta-function and the unscreened Coulomb potential our result suggests the possibility of an inhomogeneous density-wave ground state in highly polarized two-dimensional electron systems. If this inhomogeneous state exists it will be most probably a charge-density wave, since electronic correlations in real systems favour charge-density over spin-density wave instabilities [15]. Below we present the details of our analysis.

A density wave develops when the correlation function between an electron with momentum $\mathbf{k}$ and spin σ and another electron with momentum $\mathbf{k}+\mathbf{q}$ and spin σ', $\langle\psi^{\dagger}_{\mathbf{k}\sigma}\psi_{\mathbf{k}+\mathbf{q}\sigma'}\rangle$ becomes finite. When $\sigma=\sigma'$, a charge-density wave is formed, while $\sigma\neq\sigma'$ corresponds to a spin-density wave [15]. The interacting electron system Hamiltonian is diagonalized by a canonical transformation that introduces a new set of operators:

$$\psi^{\mathrm{lower}}_{\mathbf{k}}=\cos(\theta_{\mathbf{k}}/2)\psi_{\mathbf{k}-\frac{\mathbf{q}}{2}\sigma}+\sin(\theta_{\mathbf{k}}/2)\psi_{\mathbf{k}+\frac{\mathbf{q}}{2}\sigma'} \tag{2}$$

$$\psi^{\mathrm{upper}}_{\mathbf{k}}=-\sin(\theta_{\mathbf{k}}/2)\psi_{\mathbf{k}-\frac{\mathbf{q}}{2}\sigma}+\cos(\theta_{\mathbf{k}}/2)\psi_{\mathbf{k}+\frac{\mathbf{q}}{2}\sigma'}, \tag{3}$$

where $\theta_{\mathbf{k}}$ is the coupling parameter and $\psi^{\mathrm{lower}}_{\mathbf{k}}$ ($\psi^{\mathrm{upper}}_{\mathbf{k}}$) refers to the new lower (upper) band excitations.

The Hartree–Fock ground state energy is a function of $\mathbf{q}$ and the parameters $\theta_{\mathbf{k}}$ [14]. For a system with N electrons, volume V and polarization ζ the total ground state energy is

$$E(\mathbf{q})=\frac{1}{2m}\sum_{\mathbf{k}}\left[\mathbf{k}^2+\frac{\mathbf{q}^2}{4}-(\mathbf{k}\cdot\mathbf{q})\cos\theta_{\mathbf{k}}\right]-\frac{H}{2}\left[\sum_{\mathbf{k}}\cos\theta_{\mathbf{k}}-N\zeta\right]$$
$$-\frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'}v(\mathbf{k}-\mathbf{k}')\cos^2[(\theta_{\mathbf{k}}-\theta_{\mathbf{k}'})/2] \tag{4}$$

[1] For example, in GaAs the ratio of the cyclotron frequency to the Zeeman splitting is around 14, while the same ratio is close to $1/20$ in $Zn_{1-x}Cd_xSe$.

where the first term is the kinetic energy, the second is the effective Zeeman energy[2], needed to fulfil the constraint of constant polarization, and the last one the Coulomb and exchange energies.

For a delta-function interaction with strength $v(\mathbf{k}-\mathbf{k}') = v_0$ the total ground state energy in atomic units[3] becomes

$$E(\mathbf{q}) = \sum_{\mathbf{k}} \left[\mathbf{k}^2 + \frac{\mathbf{q}^2}{4} - (\mathbf{k}\cdot\mathbf{q})\cos\theta_{\mathbf{k}} \right] - \frac{H}{2}\left[\sum_{\mathbf{k}} \cos\theta_{\mathbf{k}} - N\zeta \right] - \frac{v_0}{4V}\left[\left(\sum_{\mathbf{k}} \cos\theta_{\mathbf{k}} \right)^2 + \left(\sum_{\mathbf{k}} \sin\theta_{\mathbf{k}} \right)^2 - N^2 \right]. \tag{5}$$

$E(\mathbf{q})$ reaches a minimum with respect to $\theta_{\mathbf{k}}$ when

$$\tan\theta_{\mathbf{k}} = \frac{\kappa(v_0,\zeta)}{2\mathbf{k}\cdot\mathbf{q} + H'(v_0,\zeta)} \qquad \text{and} \qquad \kappa(v_0,\zeta) = \frac{v_0}{V}\sum_k \sin\theta_k \tag{6}$$

where $n = N/V$, $\zeta = \frac{1}{N}\sum_k \cos\theta_k$ and $H' = H + v_0\zeta n$.

The quasi-particle energy in the ground state when only the lower band is occupied is given by

$$\epsilon_k^{\text{lower}} = \mathbf{k}^2 + \frac{\mathbf{q}^2}{4} + \frac{nv_0}{2} - \frac{1}{2}\sqrt{[2\mathbf{k}\cdot\mathbf{q} + H'(v_0,\zeta)]^2 + \kappa^2(v_0,\zeta)}. \tag{7}$$

The solution for $\mathbf{q}' = \lambda\mathbf{q}$, $v_0' = v_0/\lambda$, $V' = V/\lambda^3$ is homologous to that for $\mathbf{q}$, v_0, V, and results in $\kappa' = \lambda^2\kappa$ and $H' = \lambda^2 H$. From a numerical point of view, a simple way to minimize the total energy is to take $\kappa(v_0,\zeta) = 1$ and, for a fixed value of the parameter H', select the maximum occupied energy in the lower band. Then, n, ζ, v_0 and $E(\mathbf{q})$ are computed for these values by using equations (5) and (6).

Figure 1 displays our results for the normalized energy per particle of the density-wave state, $E(\mathbf{q})/(NE_{\text{F}})$, as a function of normalized momentum, $\mathbf{q}/k_{\text{F}}$, for $\zeta = 0.5$ and several values of the effective potential strength, $v_{\text{eff}} = \frac{nv_0}{E_{\text{F}}} = \frac{v_0}{2\pi}$. The energy is measured with respect to the energy of the normal paramagnetic state with the same density and polarization, $\frac{E^{\text{PARA}}}{NE_{\text{F}}} = \frac{1}{2}(1+\zeta^2) + \frac{v_{\text{eff}}}{4}(1-\zeta^2)$. For values of $v_{\text{eff}} > 2$ there is a range of momenta where the density-wave states are lower in energy than the nonmagnetic state. However, the absolute minimum is *always* at $\mathbf{q} = 0$, the ferromagnetic state. The range of momenta where the density-wave states are stable increases with the strength of the interaction, while their energies are reduced.

Figure 2 shows the normalized energy for $v_{\text{eff}} = 2.15$ and three values of the polarization, $\zeta = 0, 0.5, 0.9$. The range of momenta where the density-wave state is lower in energy is the same for all values of polarization. However, the energies increase with polarization.

By scaling the energies and momenta we find that all our numerical results overlap on a single curve. Figure 3 displays our results for the ratio of the energy per particle relative to the energy of the paramagnetic state $\Delta\epsilon(\mathbf{q}) = (E(\mathbf{q}) - E^{\text{PARA}})/(NE_{\text{F}})$ to $\epsilon_{\text{scl}} = (v_{\text{eff}}-2)(1-\zeta^2)/4$ as a function of the scaled momentum $\tilde{q} = \frac{q}{k_{\text{F}}\sqrt{v_{\text{eff}}-2}}$. We have studied a full range of values of v_0 and ζ. All the data are in excellent agreement with the simple scaling relation

$$\frac{\Delta\epsilon(\mathbf{q})}{\epsilon_{\text{scl}}} = \tilde{q}^2 - 1. \tag{8}$$

[2] The spin magnetization is written as $M = \frac{N\zeta}{2} = \frac{1}{2}\sum_k \cos\theta_{\mathbf{k}}$.

[3] $\mathbf{k}$ and $\mathbf{q}$ are in units of inverse Bohr radius (a_0^{-1}) and the energy in Rydbergs.

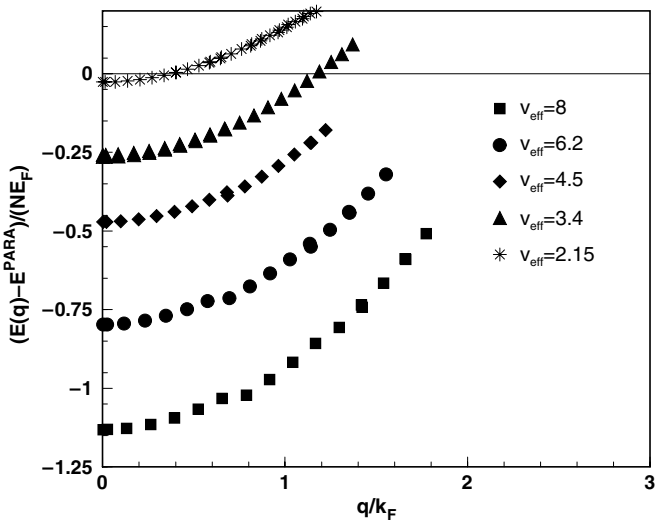

Figure 1. Normalized Hartree–Fock energy of the density-wave state, $(E(\mathbf{q}) - E^{\mathrm{PARA}})/(NE_{\mathrm{F}})$ versus its normalized momentum, $\mathbf{q}/k_{\mathrm{F}}$, for $\zeta = 0.5$ and different values of the effective potential strength, v_{eff}, as indicated in the legend.

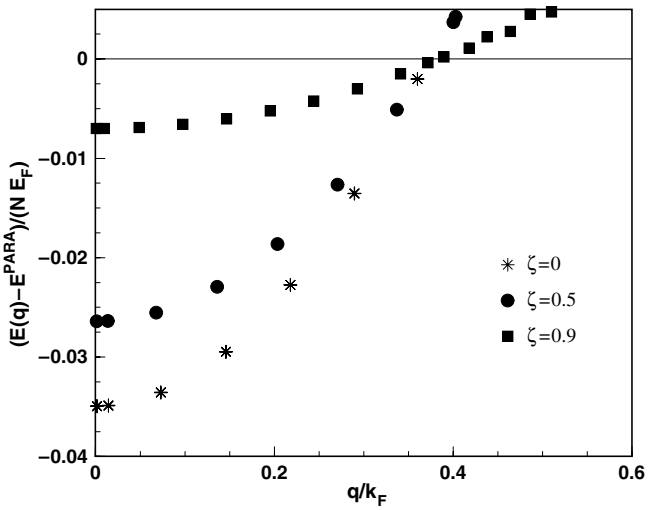

Figure 2. Normalized Hartree–Fock energy of the density-wave state, $(E(\mathbf{q}) - E^{\mathrm{PARA}})/(NE_{\mathrm{F}})$, versus its normalized momentum, $\mathbf{q}/k_{\mathrm{F}}$, for an effective interaction strength of $v_{\mathrm{eff}} = 2.15$ and $\zeta = 0$ (stars), $\zeta = 0.5$ (circles) and $\zeta = 0.9$ (squares).

Therefore, the HF energy of a two-dimensional density wave (equation (5)) is a quadratic function of the wavevector for any value of the polarization and strength interaction. The difference in energy between the ferromagnetic ground state and the density-wave states decreases by a factor proportional to $(1-\zeta^2)$. Since a short-range repulsive potential is the most unfavourable situation for the development of density instabilities, it is conceivable that upon

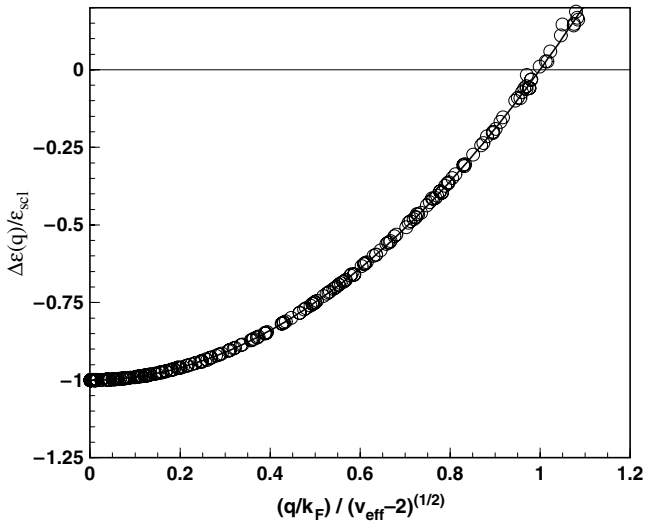

Figure 3. Scaled Hartree–Fock energy per particle of the density-wave state, $\Delta\epsilon(\mathbf{q})/\epsilon_{\rm scl}$, as a function of the scaled momentum, $\tilde{q} = q/(k_{\rm F}\sqrt{v_{\rm eff}-2})$. Circles correspond to different values of $v_{\rm eff}$ (between 2 and 8) and polarization $\zeta = 0, 0.5$ and 0.9. The solid line corresponds to the scaling relation equation (8).

the inclusion of higher-order many-body corrections to the electron interaction the ground state might be a density-wave state in some range of densities and spin polarizations. The self-consistent nature of the density-wave equation makes the incorporation of higher-order, many-body effects a nontrivial task. In a different approach, one can search for signs of ground state density instabilities by studying the poles of the magnetic and electric susceptibilities of the system, the many-body effects being included in the latter as local field corrections. The results of this analysis will be reported elsewhere [16].

In conclusion, we have found that, independent of the polarization, for $v_{\rm eff} > 2$ and wavevector $\mathbf{q} < k_{\rm F}\sqrt{v_{\rm eff}-2}$ the density-wave ground state is lower in energy than the paramagnetic state. In all cases, the absolute minimum is realized at $\mathbf{q} = 0$ in the ferromagnetic state. However, the difference in energy between a density-wave state with wavevector $\mathbf{q}$ and the ferromagnetic state is reduced by a factor proportional to $\mathbf{q}^2(1-\zeta^2)$. As a consequence, in a highly polarized electron gas the density-wave states are very close in energy to the ferromagnetic instability and many-body corrections can make this energy difference negative, leading to nonuniform ground states.

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