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

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Abstract.
We calculate the Hartree-Fock energy of a density-wave in a spin polarized two-dimensional electron gas using a short-range repulsive interaction. We find that the stable ground state for a short-range potential is *always* either the paramagnetic state or the uniform ferromagnetic state. The energy of a density-wave state is, however, reduced by a factor proportional to $(1 - \zeta^2)$, where ζ is the polarization of the electron gas. Since this situation occurs in the most unfavorable conditions (short-range repulsive interaction) it is therefore conceivable that by including higher order many-body corrections to the interaction a density-wave ground state is indeed found to be stable.

The possible existence of a non-uniform ground state for a two-dimensional (2D) electron system in the presence of a magnetic field has been proposed in explaining the results of a number of recent 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].

Numerical calculations[6] have definitely proved that at low densities an unpolarized electron gas forms a Wigner crystal. However, a study of point defects in the two-dimensional Wigner crystal suggests that the quantum melting could be continuous rather than first order[7], leaving open the possibility of inhomogeneous intermediate phases.

The idea of a non-uniform ground state in a paramagnetic 2D electron system has 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 [8]. More recent experimental[1, 2] and theoretical[9, 10] 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 this work we are interested in the possible formation of density waves in a 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. 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 $Zn_{1-x}Cd_xSe$.

Quantum Monte Carlo results show that the exchange-correlation hole is larger in the polarized electron gas[11, 12] suggesting that a highly polarized system is prone to 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. Here, we calculate the Hartree-Fock (HF) energy of a spin density wave state in a spin polarized system for a delta-function repulsive interaction, the most unfavorable situation for the development of a density-wave instability in an isotropic system.

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 formation of a spin density wave with wave vector near $2k_F$ [13]. However, for a short-range potential the stable HF solution is *always* either the usual paramagnetic state or the uniform ferromagnetic state [14]. We find that this result holds also 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 suggest 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 favor 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', $\langle \psi_{\mathbf{k}\sigma}^\dagger \psi_{\mathbf{k}+\mathbf{q}\sigma'} \rangle$ becomes finite. When $\sigma = \sigma'$, a charge-density wave is formed, while $\sigma \neq \sigma'$ corresponds to a spin-density wave. The interacting electron system Hamiltonian is diagonalized by a canonical transformation that introduces a new set of operators:

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

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

where $\theta_{\mathbf{k}}$ is the coupling parameter and $\psi_{\mathbf{k}}^{lower}(\psi_{\mathbf{k}}^{upper})$ 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:

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

$$-\frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'}v(\mathbf{k}-\mathbf{k}')\cos^2\left[(\theta_{\mathbf{k}} - \theta_{\mathbf{k}'})/2\right] \tag{4}$$

where the first term is the kinetic energy, the second is the effective Zeeman energy‡, needed to fulfill 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 § becomes:

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

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

‡ The spin magnetization is written as $M = \dfrac{N\zeta}{2} = \dfrac{1}{2}\sum_{k}\cos\theta_{\mathbf{k}}$.

§ $\mathbf{k}$ and $\mathbf{q}$ are in units of inverse Bohr radius (a_0^{-1}) and the energy in rydbergs.
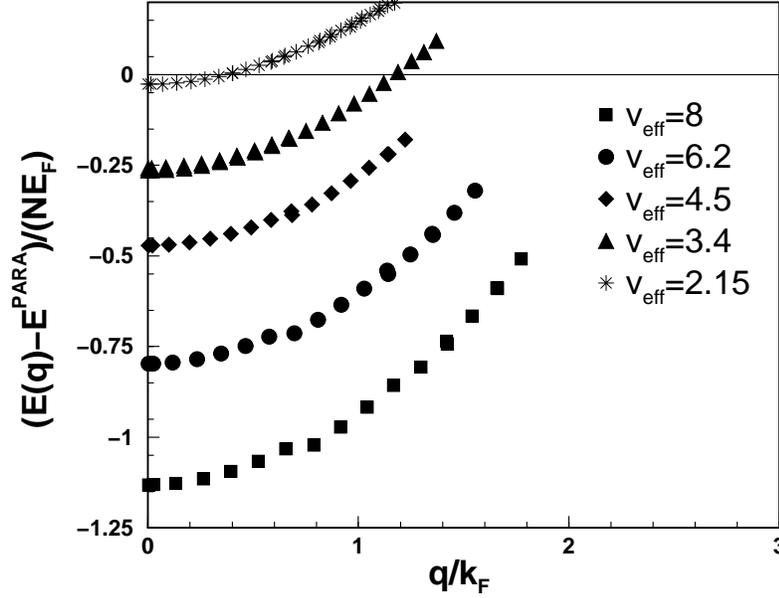
Figure 1. Normalized Hartree-Fock energy of the spin density wave state, $(E(\mathbf{q}) - E^{PARA})/(NE_F)$ versus its normalized momentum, $\mathbf{q}/k_F$, for $\zeta = 0.5$ and different values of the effective potential strength, v_{eff}, as indicated in the legend.

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

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

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:

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

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 $H' = \lambda^2 H$. Then, from a numerical point of view, the simpler way to minimize the total energy is to take $\kappa(v_0, \zeta) = 1$ and a fixed value for the parameter H', select the maximum occupied energy in the lower band, and then compute n, ζ, v_0 and $E(\mathbf{q})$ for this choice of parameters using Eqs. (5) and (6).

Fig. 1 displays our results for the normalized energy per particle of the spin density wave state, $E(\mathbf{q})/(NE_F)$, as function of normalized momentum, $\mathbf{q}/k_F$, for $\zeta = 0.5$ and several values of the effective potential strength, $v_{eff} = \dfrac{nv_0}{E_F} = \dfrac{v_0}{2\pi}$. The energy is measured with respect to the energy of the paramagnetic state with the same density and polarization, $\dfrac{E^{PARA}}{NE_F} = \dfrac{1}{2}(1 + \zeta^2) + \dfrac{v_{eff}}{4}(1 - \zeta^2)$. For values of $v_{eff} > 2$ there is a range of momenta where the density wave states are lowest in energy than the non-magnetic state. However, *always* the absolute minimum is at $\mathbf{q} = 0$, the ferromagnetic
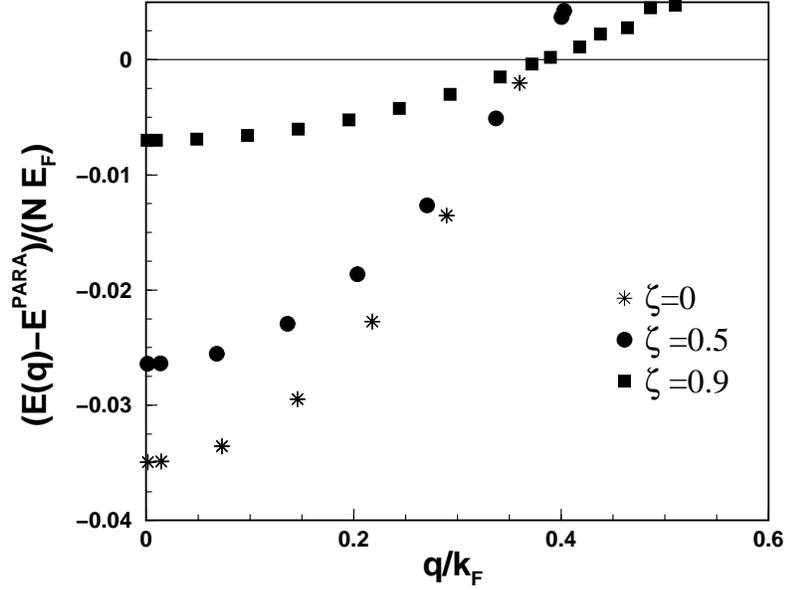
Figure 2. Normalized Hartree-Fock energy of the spin density wave state, $(E(\mathbf{q}) - E^{PARA})/(NE_F)$ versus its normalized momentum, $\mathbf{q}/k_F$, for an effective interaction strength of $v_{eff} = 2.15$ and $\zeta = 0$ (stars), $\zeta = 0.5$ (circles) and $\zeta = 1$ (squares).

state. The range of momenta where the density wave states are stable increases with the strength of the interactions, while the energies get reduced.

Fig. 2 shows the normalized energy for $v_{eff} = 2.15$ 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. Fig. (3) displays our results for the energy per particle relative to the energy of the paramagnetic state $\Delta\epsilon(\mathbf{q}) = (E(\mathbf{q}) - E^{PARA})/(NE_F)$ divided over $\epsilon_{scl} = (v_{eff} - 2)(1 - \zeta^2)/4$ as a function of the scaled momentum $\tilde{q} = \dfrac{q}{k_F\sqrt{v_{eff} - 2}}$. We have studied a full range of values of v_0 and ζ. All the data are in excellent agreement with the surprising simple scaling relation:

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

Therefore, the HF energy of a two-dimensional density wave (Eq. (5)) is a quadratic function of the wave-vector for any value of the polarization and strength interaction.

In conclusion, we have found that independently of the polarization, for $v_{eff} > 2$ and wave-vector $\mathbf{q} < k_F\sqrt{v_{eff} - 2}$ the density wave ground state is lower in energy than the paramagnetic state. In all cases, the absolute minima is the ferromagnetic state with $\mathbf{q} = 0$, but the depth of the minima scales with the polarization as $(1 - \zeta^2)$. As a consequence, in a highly polarized electron gas the density wave states are very close in energy to the ferromagnetic instability. Because a short range potential is the most unfavorable for the development of density instabilities, that fact suggests that in
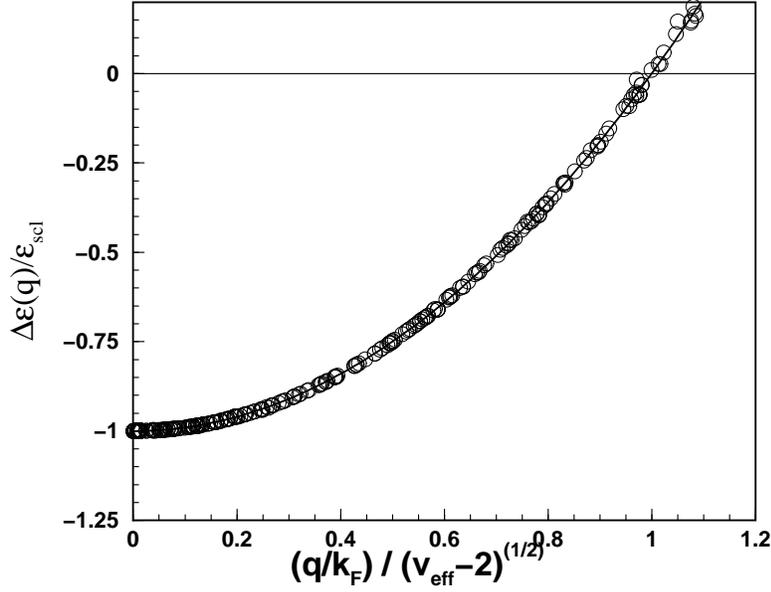
Figure 3. Scaled Hartree-Fock energy per particle of the spin density wave state, $\Delta\epsilon(\mathbf{q})/\epsilon_{scl}$, as a function of the scaled momentum, $\tilde{q} = q/(k_F\sqrt{v_{eff}-2})$. Circles correspond to different values of v_{eff} (between 2 and 8) and polarization $\zeta = 0, 0.5$ and 0.9. The solid line corresponds to the scaling relation Eq. (8).

real systems the ground state might be a density wave state in some range of densities and spin polarizations [16]. Since in two dimensions transitions to long-range order phases take place at zero temperature, the extension of our arguments to the geometry of real systems, quasi-two-dimensional heterostructures, thus allowing direct comparison with experimental results [5], is currently being investigated.

Acknowledgments

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