Two dimensional electron liquid in the presence of Rashba spin-orbit coupling: symmetrical momentum space occupation states

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The orientation of the local electron spin quantization axis in momentum space is identified as the most significant physical variable in determining the states of a two-dimensional electron liquid in the presence of Rashba spin-orbit coupling. Within mean field theory several phases can be identified that are characterized by a simple symmetric momentum space occupation. The problem admits uniform paramagnetic as well as spin polarized chiral solutions. The latter have a nontrivial spin texture in momentum space and are constructed out of states that are not solutions of the non interacting Hamiltonian. The concept of generalized chirality as well as the stability of spatially homogeneous states are also discussed.

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Recent interest in the physics of two dimensional electronic systems subject to the effects of Rashba spin-orbit interaction makes the corresponding many-body problem one of timely interest. Since it is well known that interaction effects in modern quasi-two dimensional electron liquid devices are quite strong in a wide range of accessible densities, it is clearly of fundamental importance to establish a sound set of theoretical notions about the effects of the electron-electron interactions in this problem. Patterning the general approach on that followed for the familiar case of the electron liquid in the absence of spin-orbit the first step in tackling the many-electron problem is to establish a meaningful mean field theory. Once this step is successfully taken, and the relevant dynamical variables and symmetries identified, correlation corrections can be eventually approximately calculated by a variety of methods. The purpose of this paper is to describe some of the general results of the mean field theory of the two dimensional electron liquid in the presence of Rashba spin-orbit. The present analysis is limited to the simple case of symmetric momentum space occupation states that, as we will show, can be completely and elegantly classified in terms of what we will refer to as the generalized chirality.

The problem is defined by the following model Hamiltonian:

\begin{equation}
\hat{H} = \sum_i \hat{H}_0^{(i)} + \frac{1}{2} \sum_{i\neq j} \frac{e^2}{|r_i - r_j|},
\end{equation}

where the electronic motion is limited to the \(x-y\) plane and the single particle terms contain a spin-orbit interaction of the Rashba type \(\alpha \hat{x} \hat{p}_y - \hat{y} \hat{p}_x\),

\begin{equation}
\hat{H}_0 = \frac{\hat{p}^2}{2m} + \alpha (\hat{\sigma}_x \hat{p}_y - \hat{\sigma}_y \hat{p}_x),
\end{equation}

where \(\alpha\) is assumed positive and terms corresponding to an homogeneous neutralizing background are understood. In the homogeneous case \(\hat{H}_0\) has eigenfunctions and eigenvalues given by

\[ \varphi_{k,\pm}(r) = \frac{e^{i k \cdot r}}{\sqrt{2L^2}} \left( \pm 1 \right) \left( \frac{\mp 1}{ie \phi_k} \right), \quad \epsilon_{k\pm} = \frac{\hbar^2 k^2}{2m} \mp \alpha \hbar k, \]

where \(L\) is the linear size of the system and \(\phi_k\) is the angle between the direction of the wave vector and the \(x\)-axis. Interestingly spin-orbit forces each state in momentum space to have its own spin quantization axis. This direction lies in the \(x-y\) plane and makes an angle of \(\frac{\pi}{4}\) with \(k\). The corresponding unit vector will be denoted by \(\hat{\phi}_k\). These states form two split bands characterized by opposite chirality which are schematized in Fig. 1.

Since the mean field theory involves, but as we shall see is not limited to, single Slater determinants obtained by occupying the single particle states \(\mid \psi \rangle\), it proves necessary to establish a complete yet manageable classification scheme. We have found that for states with isotropic, compact occupation in momentum space the following quantity,

\[ \chi = \left\{ \begin{array}{ll}
\frac{k_{\text{in}}^2 + k_{\text{out}}^2}{k_{\text{out}}^2 - k_{\text{in}}^2} & \text{for } 0 \leq \chi_0 < 1 \\
1 & \text{for } \chi_0 = 1
\end{array} \right., \]

which we will refer to as the \textit{generalized chirality}, offers such possibility. In Fig. 1 \(\chi_0 = \frac{N_{\text{in}} - N_{\text{out}}}{N_{\text{in}} + N_{\text{out}}}\) is the ordinary chirality as defined in terms of the occupation \(N_{\pm}\) of each band, while \(k_{\text{in}}, k_{\text{out}}\) and \(k_{\pm}\) are geometrical parameters in momentum space characterizing the occupied regions (circles for the isotropic case) and are defined in Fig. 1. Depending on the relative occupation of the bands, \(\chi\) can acquire any value from zero to infinity and allows one to uniquely label the relevant set of many-particle states for fixed density \(n = N/L^2\). This must be contrasted with the ordinary chirality which satisfies the condition \(\chi_0 \leq 1\) and equals unity for all the states in which only one of the chiral bands is occupied.

Limiting for the time being our analysis to spatially homogeneous solutions, it is readily established that, because of the peculiar physics of the Rashba spin-orbit, the momentum space local orientation of the electron
only the lowest chiral band is occupied and the generalized spectrum. The plane of motion. The β particle plane wave states each characterized by its own \( \hat{\Psi} \). Accordingly our idea is to construct many-particle Fock states \( \hat{\Psi}[n_{\mathbf{k}\pm}, \hat{\mathbf{s}}_{\mathbf{k}}] \) with occupations \( n_{\mathbf{k}\pm} \) using single particle plane wave states each characterized by its own \( \hat{\mathbf{s}}_{\mathbf{k}} \). Our main task is therefore reduced to determine what, for a given density, is the most energetically favorable set of \( n_{\mathbf{k}\pm} \) and corresponding spin quantization axes \( \hat{\mathbf{s}}_{\mathbf{k}} \).

From a formal point of view this problem can be handled by making use of a standard Wick decoupling procedure. We find however more instructive and elegant to minimize the total energy as a functional of both \( n_{\mathbf{k}\pm} \) and \( \hat{\mathbf{s}}_{\mathbf{k}} \). It is a simple exercise to write down the expectation value of the full hamiltonian of the electron liquid taken over a generic single Slater determinant \( \hat{\Psi}[n_{\mathbf{k}\pm}, \hat{\mathbf{s}}_{\mathbf{k}}] \):

\[
E_{\Psi}[n_{\mathbf{k}\mu}, \hat{\mathbf{s}}_{\mathbf{k}}] = \sum_{\mathbf{k}, \mu=\pm} \left( \frac{\hbar^2 k^2}{2m} n_{\mathbf{k}\mu} - \hbar \alpha \mu \left( \hat{\mathbf{s}}_{\mathbf{k}} \cdot \mathbf{k} \right) n_{\mathbf{k}\mu} \right) - \frac{1}{4L^2} \sum_{\mathbf{k}, \mathbf{k}'; \mu, \mu' = \pm} v_{\mathbf{k}-\mathbf{k}'} \left( 1 + \mu \mu' \hat{\mathbf{s}}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}'} \right) n_{\mathbf{k}\mu} n_{\mathbf{k}'}\mu'.
\]

The corresponding, renormalized, single particle energies \( \epsilon_{\mathbf{k}\mu} \) can then be readily obtained by differentiation with respect to \( n_{\mathbf{k}\pm} \).

We begin our analysis of Eq. (5) by noting that, as one can show, for symmetric occupations, the case \( \gamma_{\mathbf{k}} = \phi_{\mathbf{k}} + \frac{\pi}{2} \) corresponds to an energy minimum. In this case by implementing the momentum rescaling

\[
\beta_{\mathbf{k}} = \tilde{\beta}(\frac{|\mathbf{k}|}{\sqrt{2\pi n}}),
\]

the functional \( E_{\Psi} \) can be expressed in Rydberg units as follows

\[
E_{\Psi}[n_{\mathbf{k}\mu}, \hat{\mathbf{s}}_{\mathbf{k}}] = \frac{\mathcal{K}(\chi)}{r_s^2} + \frac{\mathcal{R}[\chi; \tilde{\beta}]}{r_s} + E_{\mathcal{F}}[\chi; \tilde{\beta}],
\]

where we have also introduced the dimensionless parameters \( r_s^{-1} = \sqrt{n\alpha n} \) and \( \tilde{\alpha} = \frac{\alpha}{2} \). This formula is quite remarkable for it displays a simple explicit dependence on the spin-orbit coupling constant and an high degree of universality. Specifically \( \mathcal{K} \) is a simple function of \( \chi \):

\[
\mathcal{K}(\chi) = \theta(1-\chi)(1+\chi^2) + \theta(\chi-1)2\chi, \tag{8}
\]

while \( \mathcal{R} \) and \( E_{\mathcal{F}} \) are in addition universal functionals of the rescaled momentum dependent angle \( \tilde{\beta} \) whose expressions are reported elsewhere. For paramagnetic states the situation simplifies further since for this class of solutions \( \beta_{\mathbf{k}} = \frac{\pi}{2} \) and only the dependence on \( \chi \) survives. Figure 3 displays the typical dependence of \( \mathcal{R} \) and \( E_{\mathcal{F}} \) on \( \chi \) for actual solutions \( \beta \) of the problem for different values of \( \alpha \). As we show below, for a given value of the latter, the final values of \( \mathcal{R} \) and \( E_{\mathcal{F}} \) can be expressed as a function of \( \chi \) only. Notice the cuspy behavior about the critical value \( \chi = 1 \) which separates states for which one or two (renormalized) chiral bands are occupied.

At this point the mean field energy can be obtained by minimization with respect to both \( \chi \) and \( \beta_{\mathbf{k}} \):

\[
E_{MF}(\alpha, r_s) = \min_{\chi, \beta_{\mathbf{k}}} E_{\Psi}.
\]

For a fixed \( \chi \) minimization with respect to \( \beta_{\mathbf{k}} \) reduces to finding the lowest lying solutions of the corresponding mean field equation

\[
\tan \tilde{\beta}(\kappa) = \frac{\int_{1+\kappa}^{1-\kappa} d\kappa' \int_0^\pi \frac{\kappa' \sin \tilde{\beta}(\kappa') \cos \theta}{\sqrt{\kappa'^2 + \kappa'^4 - 2\kappa' \cos \theta}} d\theta + 4\pi\tilde{\alpha} \kappa}{\int_{1+\kappa}^{1-\kappa} d\kappa' \int_0^\pi \frac{\kappa' \cos \tilde{\beta}(\kappa') \cos \theta}{\sqrt{\kappa'^2 + \kappa'^4 - 2\kappa' \cos \theta}} d\theta}, \tag{10}
\]

here simplified to the relevant case \( \gamma_{\mathbf{k}} = \phi_{\mathbf{k}} + \frac{\pi}{2} \) corresponding to a vanishing in plane polarization. Remarkably this equation is devoid of any explicit dependence on \( r_s \), the solution \( \beta \) being only dependent on \( \alpha \) and \( \chi \). Notice that \( \beta = \frac{\pi}{2} \) is always a solution of Eq. (10). The latter has rather interesting symmetries. For instance
one can see that $\tilde{\beta}/\chi(\kappa) = \tilde{\beta}_\chi(\sqrt{\chi} \kappa)$. Eq. (11) makes it manifest how, for this class of solutions, the generalized chirality $\chi$ is the central parameter of the problem. As an illustration, typical solutions for the universal azimuthal angle $\tilde{\beta}(\kappa)$ are displayed in Fig. 4. There, solutions with $\tilde{\beta} \neq \pi/4$ correspond to polarized states in which the spin polarization points along the $z$-axis. Interestingly, these are constructed out of single particle states that are not solutions of the single particle hamiltonian (2) and display an intriguing spin texture in momentum space. This is shown in Fig. 5 where three possible cases are depicted.

Further minimization with respect to $\chi$ allows one to compare the energies of these homogeneous, symmetrically occupied states. This leads to the determination of the boundaries (lines of first order transitions) between the paramagnetic (PM) and the $z$-axis polarized phases (FZ, dotted area) in the relative phase diagram of Fig. 6. Within the ferromagnetic region the generalized chirality is constant and equals one. This phenomenon is due to the cuspidal behavior of $\mathcal{E}_x$ for this value of $\chi$. The fractional polarization is readily seen to be given by

$$p(\tilde{\alpha}, \chi) = \frac{2 \langle \hat{S}_z \rangle}{\hbar N} = \frac{2}{\sqrt{1+\chi}} \int \cos \tilde{\beta}(\kappa) d\kappa . \quad (11)$$

$p$ vanishes for unpolarized states ($\tilde{\beta} = \pi/4$) and acquires an $r_s$ independent value in the polarized phase for which $\tilde{\beta} \neq \pi/4$. In general the ferromagnetic polarization is less than one as it can be surmised from Fig. 4. On the other hand $p \to 1$ for vanishing $\alpha$ as one expects to recover the fully polarized Bloch ferromagnetic state of the two dimensional electron liquid in the absence of spin-orbit coupling. A most remarkable feature of this phase diagram is the reentrant paramagnetic phase at lower densities, something due to the density dependence of the Rashba term (see Eq. (7)).

We discuss next the possibility of inhomogeneous
states. It is clear that in the low density limit the system will form a Wigner crystal. On the other hand, we have found that, as in the absence of spin-orbit coupling, within the mean field approximation, homogeneous states are unstable to spin density wave type distortions. We have been able to construct a rigorous proof of this statement valid for all densities. The procedure is patterned after that of Ref. [3]. One assumes the following set of trial single particle wave functions:
\[ \psi_k(r) \simeq \varphi_{k,+}(r) + A_k \varphi_{k+Q,+}(r) + A_k - \varphi_{k-Q,+}(r), \] (12)
where we have chosen \( Q = 2k_F \hat{x} = \frac{2\hbar}{\varepsilon_F} \hat{x} \) as to connect states on opposite sides of the Fermi energy and suitable for the case of \( \varepsilon_F = 0 \) in Fig. 11. The corresponding leading change in the total mean field energy is a functional \( \Delta E_{MF}[\rho_{n\beta}] \) of the linear variations of the matrix elements of the single particle density matrix \( \rho_{n\beta} = \langle \Phi | \hat{a}_{n \alpha}^\dagger \hat{a}_{\beta} | \Phi \rangle \) whose expression can be found in Ref. [2]. At this point, after some algebra, one finds that the following judicious choice of the amplitudes
\[ A_{k\pm} = \begin{cases} \frac{bk_F}{\ln \frac{\varepsilon_F}{\Delta}} \sqrt{\frac{\sin^2 \varphi_{k+Q}^\prime}{\cos^2 \varphi_{k+Q}^\prime}} & |b_k| < 1, \\ 0 & \text{otherwise}, \end{cases} \] (13)
where \( b \) is an arbitrarily small positive number, leads to a negative \( \Delta E_{MF} \) even without allowing for momentum space repopulation.

An inspection of our procedure reveals that, within mean field theory, several of the effects of the interactions can be described in terms of the concept of effective magnetic field, a quantity defined as
\[ \frac{g \mu_B}{2} B_{eff} = -\hbar \alpha \hat{k} \phi_k - \frac{1}{2L^2} \sum_{k'} (n_{k'+} - n_{k'-}) \psi_{k'-} \hat{s}_{k'}, \] (14)
the last term being associated with the exchange energy. As it can be shown, this concept can be employed to write the mean field equation (10) at once.

We conclude by noticing that, as in the absence of spin-orbit, one should reasonably expect correlation effects to change the density range in which the various transitions occur. On the other hand the qualitative structure of the phase diagram should remain essentially unchanged. We also expect that the interplay of interactions and spin-orbit will lead to interesting novel phenomena not only in the transition region to the Wigner crystal, where the spin polarization of the states will play a major role, but also at intermediate densities where interesting in-plane spin structures could be stabilized by both exchange and correlations. The current analysis only offers a glimpse at the rich physical complexity of this problem.

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