On the two dimensional electron liquid in the presence of spin-orbit coupling

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A spin-orbit coupling of the Rashba type has profound effects on the spin degrees of freedom of a two dimensional electron liquid. In this system a prominent role is played by the local electron spin quantization axis in momentum space. We find that a useful device for the classification of the corresponding many-electron determinantal states is provided by the concept of generalized chirality. This allows us to systematically study the Hartree-Fock scenario for homogeneous, isotropic states. The ensuing relative phase diagram contains both chiral unpolarized and chiral spin polarized states which are characterized by peculiar distributions of the local electron spin quantization axis in momentum space.

1. Introduction

Great advances in electronic spin control have lately been achieved by taking advantage of the spin-orbit interaction of the Rashba [1, 2] or Dresselhaus [3] type experienced by the carriers in suitably prepared low dimensional electronic systems. Recent examples include spin current injection by magnetic focusing [4] and elastic reflection from a sharp boundary [5]. It is our aim to present here a number of results of a study of the effects of the interplay between the electron-electron interaction and the Rashba spin-orbit in a two dimensional electron liquid [6], a system believed to provide an accurate model for the description of the physics at hand. This problem is still far from having been properly explored and understood. A more detailed analysis can be found in reference [7].

2. The generalized chirality

We begin by considering the non interacting hamiltonian [1, 2]:

$$\hat{H}_0 \;=\; \hat{K}_0 + \hat{R}_0 \;=\; \frac{\hat{\mathbf{p}}^2}{2m} + \alpha\,(\hat{\sigma}_x \hat{p}_y - \hat{\sigma}_y \hat{p}_x)\;, \tag{2.1}$$

where the electronic motion is limited to the (x,y) plane and, by definition, the spin-orbit coupling constant α is assumed positive. This model hamiltonian is designed to describe the spin-orbit interaction induced under appropriate conditions by the confining potential.

It is readily found that the eigenstates of $\hat{H}_0$ are plane waves with spin oriented in the plane of motion in a direction perpendicular to the wave vector $\mathbf{k}$, i.e.

$$\varphi_{\mathbf{k},\pm}(\mathbf{r}) \;=\; \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{2L^2}} \begin{pmatrix} \pm 1 \\ i e^{i\phi_{\mathbf{k}}} \end{pmatrix} , \tag{2.2}$$

where the $\pm$ sub index on the left hand side labels positive or negative *chiral states*. The corresponding eigenvalues are

$$\epsilon_{\mathbf{k}\pm} = \frac{\hbar^2 \mathbf{k}^2}{2m} \mp \hbar\alpha\, k \; . \tag{2.3}$$

Non interacting many electron states of the system consist of single Slater determinants made out of the states of Eq. (2.2). Two topologically different yet compact possible ways of occupying such states are shown in Figure 1. The top panel represents a low density situation in which only one energy branch is compactly occupied, while the bottom panel depicts a high density regime in which both energy branches are compactly occupied. These states are completely determined by the geometrical parameters k_{in}, k_{out}, k_- and k_+ which are defined in Figure 1. We will refer to these two types of occupations as the basic compact occupation schemes. While it is clear that giving the electron density n (as for instance expressed in terms of the parameter $r_s = 1/\sqrt{\pi a_B^2 n}$) completely determines the state of lowest energy, the excited states of compact occupation necessitate in general two independent parameters for their classification. The physical significance of the second parameter is determined next. We notice first that all the states are characterized by a chiral polarization (or chirality) defined as

$$\chi_0 = \frac{n_+ - n_-}{n_+ + n_-} \; , \tag{2.4}$$

where $n_\pm$ is the number density of right handed and left handed electrons with $n = n_+ + n_-$. It is then clear that while all the high density states of this type can be uniquely classified by means of the value of their chirality $\chi_0 = \frac{k_+^2 - k_-^2}{k_+^2 + k_-^2} \leq 1$, the corresponding low density states are not amenable to such a classification since for all of them $\chi_0 = 1$. We find that, for a

given density, an elegant way to classify all the different basic compact occupations is provided by the generalized chirality χ defined as:

$$\chi = \begin{cases} \chi_0 & \text{for } 0 < \chi_0 < 1 \,, \\ \dfrac{k_{out}^2 + k_{in}^2}{k_{out}^2 - k_{in}^2} & \text{for } \chi_0 = 1 \,. \end{cases} \tag{2.5}$$

Once the density and the generalized chirality are given the geometrical parameters characterizing the basic compact occupation schemes are immediately determined by the relations

$$k_{\pm} = \sqrt{2\pi n(1 \pm \chi)} \qquad \text{for } 0 < \chi < 1 \tag{2.6}$$

$$k_{out(in)} = \sqrt{2\pi n(\chi \pm 1)} \qquad \text{for } \chi \geq 1 \,. \tag{2.7}$$

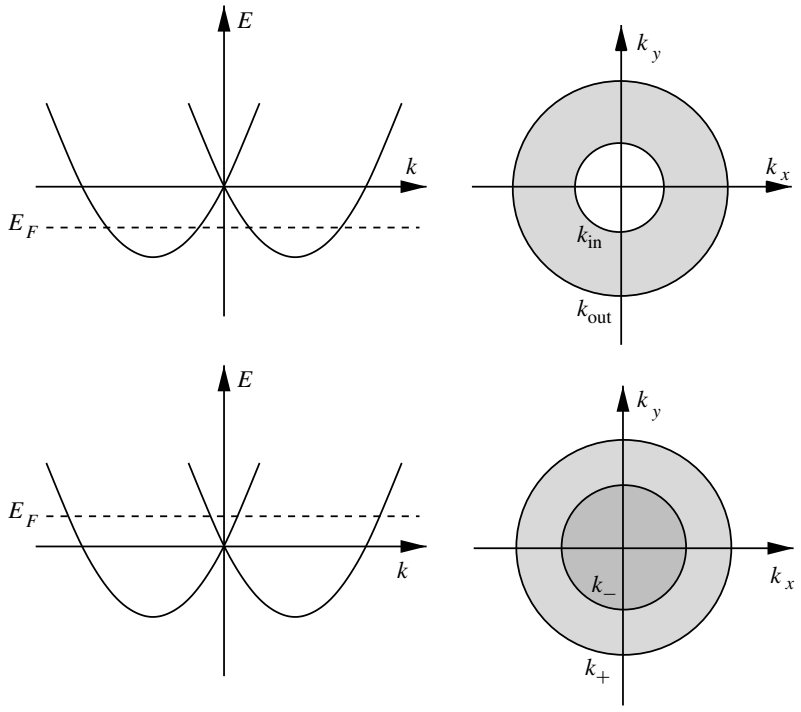

Figure 1. Two different ways of occupying non interacting chiral states in **k** space.

3. Interacting system: Mean field theory

The fully interacting problem is described by the many-body hamiltonian

$$\hat{H} = \sum_i \hat{H}_{0i} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} + \hat{H}_B \,, \tag{3.8}$$

where the last term represents the contributions stemming from the existence of a homogeneous neutralizing background. A number of properties of this system have been studied in reference [8] within a limited approach based on a first order perturbative expansion in terms of an *ad hoc* static screened interaction.

Limiting our study to the case of homogeneous, isotropic solutions, an interesting class of mean field states is represented by the Slater determinants formed occupying the single particle states obtained as the result of the following Bogolubov transformation:

$$\begin{pmatrix} \hat{b}^\dagger_{\mathbf{k}+} \\ \hat{b}^\dagger_{\mathbf{k}-} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta_\mathbf{k}}{2} & e^{i\gamma_\mathbf{k}}\sin\frac{\beta_\mathbf{k}}{2} \\ e^{-i\gamma_\mathbf{k}}\sin\frac{\beta_\mathbf{k}}{2} & -\cos\frac{\beta_\mathbf{k}}{2} \end{pmatrix} \begin{pmatrix} \hat{a}^\dagger_{\mathbf{k}\uparrow} \\ \hat{a}^\dagger_{\mathbf{k}\downarrow} \end{pmatrix} , \tag{3.9}$$

where the initial operators $\hat{a}_{\mathbf{k}\sigma}$ correspond to the standard plane wave spinors with spin quantization axis taken along the direction $\hat{z}$ perpendicular to the plane of motion. For a given $\mathbf{k}$, this transformation simply affects a rotation of the spin quantization axis from $\hat{z}$ to an arbitrary orientation $\hat{s}_\mathbf{k}$. The geometry of this rotation as well as the definition of the corresponding polar and azimuthal angles $\gamma_\mathbf{k}$ and $\beta_\mathbf{k}$ are provided in Figure 2. Notice that the choice $\gamma_\mathbf{k} = \phi_\mathbf{k} + \frac{\pi}{2}$ ($\phi_\mathbf{k}$ being the angle between $\mathbf{k}$ and the x-axis) and $\beta_\mathbf{k} = \frac{\pi}{2}$ leads to the eigenstates of $\hat{H}_0$ of Eq. (2.2).

At this point we evaluate the expectation value of the exact hamiltonian $\hat{H}$ over any of these determinantal states obtaining the following expression:

$$E_{HF}[n_{\mathbf{k}\pm}, \hat{s}_\mathbf{k}] = \sum_{\mathbf{k},\,\mu} \frac{\hbar^2\mathbf{k}^2}{2m}\, n_{\mathbf{k}\,\mu} - \hbar\alpha \sum_{\mathbf{k},\,\mu} \mu\, k\, \hat{\phi}_\mathbf{k}\cdot\hat{s}_\mathbf{k}\, n_{\mathbf{k}\,\mu} + \tag{3.10}$$

$$-\frac{1}{2L^2}\sum_{\mathbf{k},\mathbf{k}',\,\mu,\mu'} v_{\mathbf{k}-\mathbf{k}'}\, \frac{1+\mu\mu'\,\hat{s}_\mathbf{k}\cdot\hat{s}_{\mathbf{k}'}}{2}\, n_{\mathbf{k}\,\mu} n_{\mathbf{k}'\mu'} \,,$$

where the indices μ and μ' are summed over the values $\pm$. Clearly E_{HF} represents the (total) Hartree-Fock (HF) energy of this particular class of states and is a functional of the occupation numbers $n_{\mathbf{k}\pm}$ and of the orientation of the (wave vector space) local spin quantization axis unit

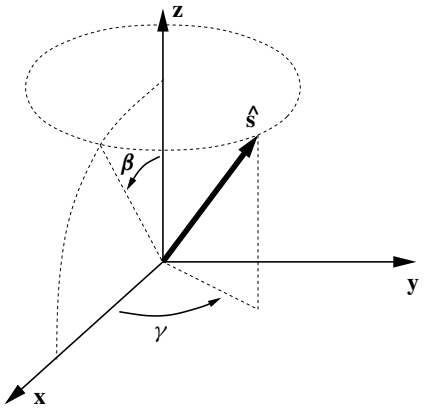

Figure 2. Geometry of the Bogolubov transformation.

vector $\hat{s}_{\mathbf{k}}$. It is still to be assessed which of these states correspond to actual solutions of the HF problem [9]. This we do by means of a standard Wick theorem based decoupling and diagonalization of the hamiltonian $\hat{H}$ expressed in terms of the operators $\hat{b}_{\mathbf{k}\pm}$.

As it turns out, the analysis is greatly simplified by setting $\gamma_{\mathbf{k}} = \phi_{\mathbf{k}} + \frac{\pi}{2}$ [10]. The resulting self-consistent equation involving the remaining functions $\beta_{\mathbf{k}}$ and $n_{\mathbf{k}\pm}$ reads:

$$\tan\beta_{\mathbf{k}} = \frac{\frac{1}{2L^2}\sum_{\mathbf{k}',\,\mu'} n_{\mathbf{k}'\mu'} v_{\mathbf{k}-\mathbf{k}'}\ \mu'\ \sin\beta_{\mathbf{k}'}\cos\left(\phi_{\mathbf{k}} - \phi_{\mathbf{k}'}\right) + \hbar\alpha k}{\frac{1}{2L^2}\sum_{\mathbf{k}',\,\mu'} n_{\mathbf{k}'\mu'} v_{\mathbf{k}-\mathbf{k}'}\ \mu'\ \cos\beta_{\mathbf{k}'}} \,. \quad (3.11)$$

Although many possible solutions for the functions $n_{\mathbf{k}\pm}$ and $\beta_{\mathbf{k}}$ can in principle be found, it must be kept in mind that not all of them correspond to minima of the HF energy. Even restricting our analysis to wave vector space occupations of the basic compact types (and therefore to spatially isotropic states), solving the HF problem is not trivial. In this situation a simplifying feature is represented by the fact that, when the wave vector dependence of the function β is properly rescaled, the solutions of Eq. (3.11) have the form $\beta_{\mathbf{k}} = \bar{\beta}(\frac{|\mathbf{k}|}{\sqrt{2\pi n}})$, with $\bar{\beta}$ independent of the electron density, being completely determined by the generalized chirality χ. We find that given the coupling constant α, the problem always admits at least the solution $\beta_{\mathbf{k}} = \frac{\pi}{2}$ corresponding to a paramagnetic state constructed out of the eigenfunctions of the non interacting problem posed by $\hat{H}_0$. Moreover, for certain values of χ, a second (polarized) solution also exists for which $\beta_{\mathbf{k}} \neq \frac{\pi}{2}$. This will be discussed below.

Once a set of HF solutions has been established, the putative ground state can be found by minimization of the energy E_{HF} over the set.

Within our approach, the lowest energy state must be accordingly found optimizing the value of χ, i.e.

$$\mathcal{E}_{HF}(\bar{\alpha}, r_s) \;=\; \min_{\chi}[\mathcal{E}(\bar{\alpha}, r_s, \chi)]\,, \tag{3.12}$$

where we have introduced the dimensionless parameter $\bar{\alpha} = \frac{\hbar\alpha}{e^2}$ and have used the notation $\mathcal{E}_{HF}$ to represent an HF energy per particle in Ry units.

Finally, for each HF state, the corresponding single particle energies can be calculated from the expression

$$\begin{aligned}\epsilon_{\mu}(\mathbf{k}) = \quad & \frac{\hbar\mathbf{k}^2}{2m} - \frac{1}{2L^2}\sum_{\mathbf{k}',\,\mu'} v_{\mathbf{k}-\mathbf{k}'} n_{\mathbf{k}'\mu'} \\ & -\mu\hbar\alpha k\,\hat{\phi}_{\mathbf{k}}\cdot\hat{s}_{\mathbf{k}} - \frac{\mu}{2L^2}\sum_{\mathbf{k}',\mu'}\mu' n_{\mathbf{k}'\mu'} v_{\mathbf{k}-\mathbf{k}'}\hat{s}_{\mathbf{k}'}\cdot\hat{s}_{\mathbf{k}}\,,\end{aligned} \tag{3.13}$$

which is easily derived from Eq. (3.10).

As already noted, a possible set of unpolarized HF solutions have $\beta_{\mathbf{k}} = \frac{\pi}{2}$ and are simply obtained by any circularly symmetric occupation of the states (2.2) of the non interacting hamiltonian. Following the general procedure outlined above, the total energy is readily calculated and can be expressed in the interesting following form:

$$\begin{aligned}\mathcal{E}^{(\mathrm{unpol})}(\bar{\alpha}, r_s, \chi) \;&=\; \mathcal{K}(r_s, \chi) + \mathcal{R}^{(\mathrm{unpol})}(\bar{\alpha}, r_s, \chi) + \mathcal{E}_x^{(\mathrm{unpol})}(r_s, \chi) \\ &=\; \frac{\tilde{\mathcal{K}}(\chi)}{r_s^2} + \frac{\bar{\alpha}\,\tilde{\mathcal{R}}^{(\mathrm{unpol})}(\chi)}{r_s} + \frac{\tilde{\mathcal{E}}_x^{(\mathrm{unpol})}(\chi)}{r_s}\,,\end{aligned} \tag{3.14}$$

where $\tilde{\mathcal{K}}^{(\mathrm{unpol})}(\chi)$ and $\tilde{\mathcal{R}}^{(\mathrm{unpol})}(\chi)$ have simple closed form expressions [7]. The dependence of the exchange energy product $\tilde{\mathcal{E}}_x^{(\mathrm{unpol})}(\chi) = r_s\mathcal{E}_x^{(\mathrm{unpol})}(r_s, \chi)$, on the other hand, can be obtained from a simple quadrature. A plot of this function is provided in Figure 3. It displays an interesting minimum for $\chi \simeq 0.9147$ and behaves like $\tilde{\mathcal{E}}_x(\chi) \simeq -\frac{\sqrt{2}\log\chi}{\pi\sqrt{\chi}}$ for large χ.

Since the spin axis orientation $\hat{s}_{\mathbf{k}}$ of the non interacting state and that of the HF unpolarized states of this type do coincide, the only difference is due to momentum space repopulation. This is exemplified by the fact that, for a given density, the value of $\chi_{\min}$ corresponding to the lowest energy differs in the two cases. This situation is displayed in Figure 6. As one would expect, the deviation is larger at lower density.

Polarized states are obtained as nontrivial solutions of Eq. (3.11). Typical results for the function $\bar{\beta}$ are plotted versus $y = \frac{|\mathbf{k}|}{\sqrt{2\pi n}}$ in Figure 4.

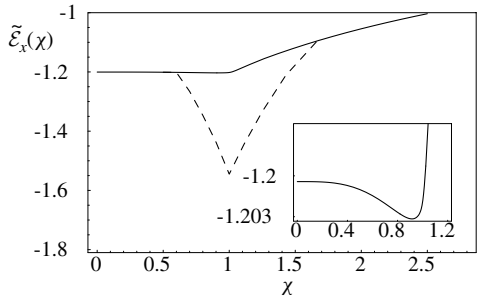

Figure 3. Dependence of $\tilde{\mathcal{E}}_x^{(\mathrm{unpol})}(\chi)$ (see Eq. (3.14) in the text) and of $\tilde{\mathcal{E}}_x^{(\mathrm{pol})}(\bar{\alpha}, \chi)$ (see Eq. (3.16)) on the generalized chirality χ. For the polarized case $\bar{\alpha} = 0.2$. In the inset, a particular of $\tilde{\mathcal{E}}_x^{(\mathrm{unpol})}(\chi)$ is shown.

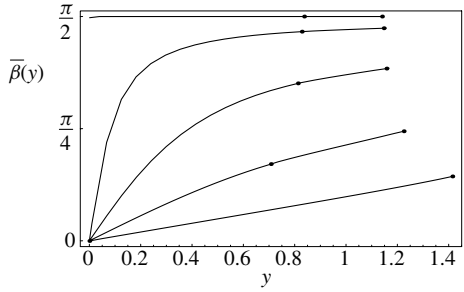

Figure 4. Plot of the complete $\bar{\beta}(y)$ (where $y = \frac{|\mathbf{k}|}{\sqrt{2\pi n}}$) for $\bar{\alpha} = 0.1$. The values of the generalized chirality are (from the top) $\chi = 0.3,\ 0.315,\ 0.34,\ 0.5,\ 1$. The dots mark the $[\sqrt{1-\chi}, \sqrt{1+\chi}]$ intervals.

Notice that as χ decreases towards an $\bar{\alpha}$ dependent critical value, the curves converge to the unpolarized solution. This corresponds to the fact that polarized solutions of Eq. (3.11) only exist for χ in a finite range of values.

Since $\beta_{\mathbf{k}}$ differs from $\frac{\pi}{2}$, these states have spin quantization axes $\hat{s}_{\mathbf{k}}$ lying outside of the plane of motion and therefore not only display an intriguing momentum space spin texture but also have a net fractional spin polarization that can be calculated from the relation:

$$p\,(\bar{\alpha}, \chi) = \frac{2\,\langle S_z \rangle}{\hbar\, N} = \int_{\sqrt{|1-\chi|}}^{\sqrt{|1+\chi|}} y\, \cos\bar{\beta}(y)\, \mathrm{d}y\ . \tag{3.15}$$

Note that in this case the fractional spin polarization does not coincide with the fraction of electrons with unpaired spin, as it is the case when spin-orbit is absent.

The energy per particle in Ry units can be calculated also in this case and can be cast in the following form:

$$\begin{aligned}\mathcal{E}^{(\mathrm{pol})}(\bar{\alpha}, r_s, \chi) &= \mathcal{K}(r_s, \chi) + \mathcal{R}^{(\mathrm{pol})}(\bar{\alpha}, r_s, \chi) + \mathcal{E}_x^{(\mathrm{pol})}(\bar{\alpha}, r_s, \chi) \\ &= \frac{\tilde{\mathcal{K}}(\chi)}{r_s^2} + \frac{\tilde{\mathcal{R}}^{(\mathrm{pol})}(\bar{\alpha}, \chi)}{r_s} + \frac{\tilde{\mathcal{E}}_x^{(\mathrm{pol})}(\bar{\alpha}, \chi)}{r_s}\,, \qquad (3.16)\end{aligned}$$

where $\tilde{\mathcal{R}}^{(\mathrm{pol})}(\bar{\alpha}, \chi)$ and $\tilde{\mathcal{E}}_x^{(\mathrm{pol})}(\bar{\alpha}, \chi)$ are expressed in terms of integrals involving $\bar{\beta}(y)$ [7]. A plot of $\tilde{\mathcal{E}}_x^{(\mathrm{pol})}(\bar{\alpha}, \chi)$ is provided in Figure 3 where it can be compared to the corresponding unpolarized result of Eq. (3.14). Again, for each density and spin-orbit strength, the ground state energy $\mathcal{E}_{HF}^{(\mathrm{pol})}(\bar{\alpha}, r_s)$ is determined by minimization with respect to χ. From numerical evaluations we find that, similarly to the $\alpha = 0$ case, the polarized ground state is obtained when $\chi_{\min} = 1$.

4. Relative phase diagram

A relative phase diagram within the space of the homogeneous, isotropic compactly occupied states described in the previous Sections can be obtained by comparing the lowest energy in the various phases. The dependence of $\mathcal{E}_{HF}(\bar{\alpha}, r_s)$ and $\chi_{\min}$ on the density at particular values of $\bar{\alpha}$ is plotted in Figures 5 and 6. The ensuing scenario is as follows: the gas is unpolarized both at reasonably low and at high values of the density while a spin polarized state exists in a finite range of r_s. While the high density transition is the analog of the Bloch transition that occurs in absence of

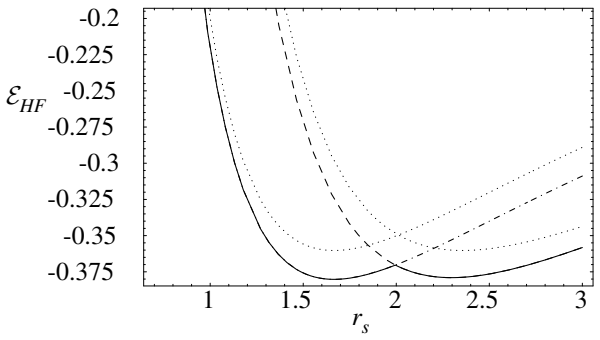

Figure 5. Plot of the total energy per particle in Ry units as function of the density parameter r_s ($\bar{\alpha} = 0.1$). Dot-dashed curve: unpolarized ground state; dashed curve: maximally polarized ($\chi = 1$) ground state; dotted curves: corresponding results for the familiar $\bar{\alpha} = 0$ case.

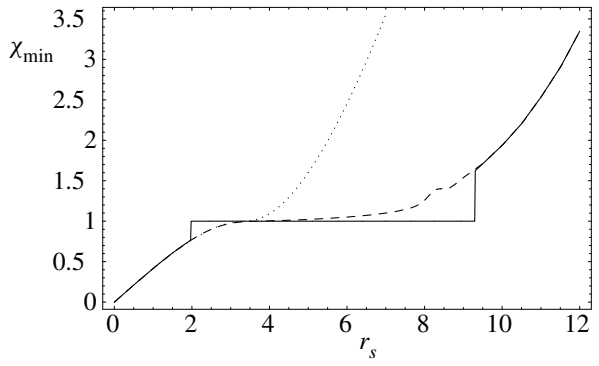

Figure 6. Value of the chirality $\chi_{\min}$ of the homogeneous, isotropic HF state of lowest energy as function of r_s (solid line). The flat region with $\chi = 1$ corresponds to the polarized state while outside of this density range the system is unpolarized. The dashed and dotted lines respectively represent the values appropriate to the unpolarized state and the non interacting one in the region where the polarized state lies lowest. For illustration purposes we have here chosen $\bar{\alpha} = 0.3$.

spin-orbit [9], the low density transition has no analog in absence of spin-orbit interaction. This simple phase diagram is also shown in Figure 7 in the $(r_s, \bar{\alpha})$ plane. One expects that as the density is further lowered, the system will make a transition into a Wigner crystal like state. It must be however noticed that the actual sequence of the transitions depends on the value of $\bar{\alpha}$. It is in fact possible, when $\bar{\alpha}$ is very small, for Wigner crystallization to preempt the reentrant unpolarized state transition [11].

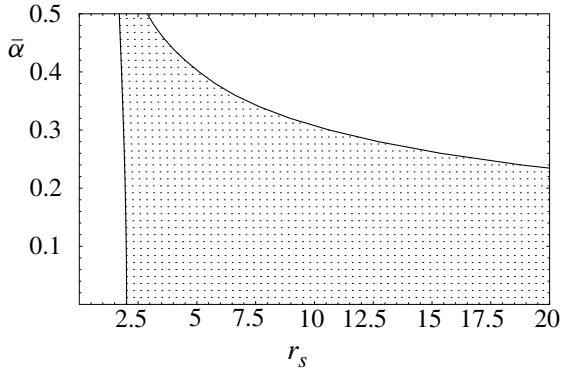

Figure 7. Phase diagram in the $(r_s, \bar{\alpha})$ plane. In the shaded region the gas is polarized.

Finally, Figure 8 shows the fractional polarization $p(\bar{\alpha}, 1)$, calculated from Eq. (3.15). This quantity is independent of r_s. Notice that, even if the state is maximally polarized (having $\chi = 1$), the fractional spin polarization drops to zero for large values of the spin-orbit coupling $\bar{\alpha}$.

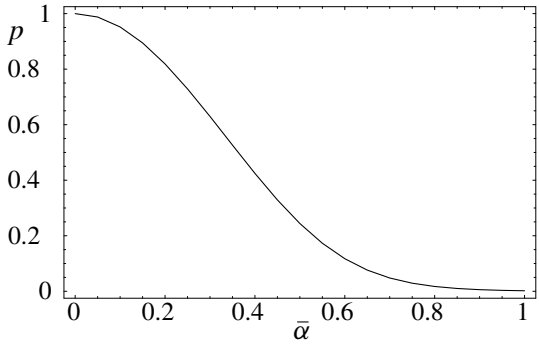

Figure 8. Plot of the polarization $p\,(\bar{\alpha}, 1)$ as function of $\bar{\alpha}$.

5. Conclusions

The concept of generalized chirality allows one to classify a vast class of compactly occupied determinantal states of a two dimensional electron liquid in the presence of Rashba spin-orbit. This enormously facilitates the study of the homogeneous, isotropic HF solutions for the problem. Our results show that within the HF theory the system admits both unpolarized and polarized states. The latter present a non trivial spin texture in momentum space. While the high density relative phase diagrams for these states closely patterns that, well known, of the same system in the absence of spin-orbit coupling, for suitably large values of the Rashba coupling constant $\bar{\alpha}$ a reentrant transition to the unpolarized state appears. The interplay of this transition and the phenomenon of Wigner crystallization still presents an untackled challenge.

While understanding the physical aspects of these spatially homogeneous states can be expected to prove reasonably useful, similarly to the standard electron liquid case, one can show that a class of inhomogeneous HF solutions of lower energy of the charge- and spin-density-wave type exists [12]. Ultimately the whole physical picture must be analyzed allowing for correlation effects beyond HF. While such a program is rather formidable we would like to conclude our contribution by stating that a possible avenue for the inclusion of correlations is suggested by a classical analogue of the problem that can be constructed starting from a direct inspection of the fundamental Eq. (3.10). This developments must await future consideration.

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References

[1] E. I. RASHBA, Sov. Phys.-Solid State **2** (1960), 1109.
[2] Y. A. BYCHKOV and E. I. RASHBA, JETP Lett. **39** (1984), 78; J. Phys. C **17** (1984), 6039.
[3] G. DRESSELHAUS, Phys. Rev. **100** (1955), 580.
[4] L. P. ROKHINSON, V. LARKINA, Y. B. LYANDA-GELLER, L. N. PFEIFFER and K. W. WEST, Phys. Rev. Lett. **93** (2004), 146601.
[5] H. CHEN, J. J. HEREMANS, J. A. PETERS, A. O. GOVOROV, N. GOEL, S. J. CHUNG and M. B. SANTOS, Appl. Phys. Lett. **86** (2005), 032113.
[6] By a trivial spin rotation, the present analysis can be applied also to the case in which the spin-orbit interaction is of the Dresselhaus type.
[7] S. CHESI and G. F. GIULIANI, to be published.
[8] G.-H. CHEN and M. E. RAIKH, Phys. Rev. B **59** (1999), 5090; Phys. Rev. B **60** (1999), 4826.
[9] G. F. GIULIANI and G. VIGNALE, "Quantum Theory of the Electron Liquid", Cambridge University Press, Cambridge, 2005.
[10] It is possible to prove that this choice of the polar angle $\gamma_{\mathbf{k}}$ minimizes the total energy.
[11] The effects of the spin-orbit interaction on the Wigner crystallization (which in absence of spin-orbit coupling occurs for $r_s \geq 34$) are to date unexplored. The fact that the spin-orbit energy scales with r_s in the same way as the Coulomb interaction does present an intriguing problem.
[12] G. SIMION and G. F. GIULIANI, to be published.