Topological Change of the Fermi Surface in Low-Density Rashba Gases: Application to Superconductivity

E. Cappelluti,[1,2] C. Grimaldi,[3,4] and F. Marsiglio[4,5]

[1]SMC-INFM, CNR-INFM, via dei Taurini 19, 00185 Roma, Italy
[2]Dipartimento di Fisica, Università "La Sapienza," P.le A. Moro 2, 00185 Roma, Italy
[3]LPM, Ecole Polytechnique Fédérale de Lausanne, Station 17, CH-1015 Lausanne, Switzerland
[4]DPMC, Université de Genève, 24 Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland
[5]Department of Physics, University of Alberta, Edmonton, Alberta, Canada, T6G 2J1
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In this Letter we show how, for small values of the Fermi energy compared to the spin-orbit splitting of Rashba type, a topological change of the Fermi surface leads to an effective reduction of the dimensionality in the electronic density of states in the low charge density regime. We investigate its consequences on the onset of the superconducting instability. We show that the superconducting critical temperature is significantly tuned in this regime by the spin-orbit coupling. We suggest that materials with strong spin-orbit coupling are good candidates for enhanced superconductivity.

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Spin-orbit (SO) coupling arising from the lack of inversion symmetry plays a leading role in the field of spintronics [1]. One of the main goals in this field of research is the possibility of tuning the electron spin properties by means of electrical fields [2]. With this aim in mind, different features have been investigated, such as spin relaxation [3], magnetoconductance [4], spin-Hall currents [5], and the properties of a superconducting phase [6,7]. As a general rule, the SO coupling is assumed to be much smaller than other relevant energy scales, in particular, the electronic dispersion, so that the infinite bandwidth limit is often employed. However, this same assumption is becoming more suspect due to the steady report of materials with increasing SO coupling, like HgTe quantum wells [8], or the surface states of metals and semimetals [9,10]. This steady progress prompts us to wonder how the properties of SO systems are modified when the Rashba SO coupling E_0 (defined below) is no longer the smallest energy, in particular, when E_0 is the same order or larger than the Fermi energy E_F. Although not yet achieved, this limit can be probably reached in the near future, as suggested by the recent report of a E_0 as large as $E_0 \simeq 220$ meV in bismuth-silver surface alloys, where E_F can be tuned by Pb doping [11]. Other promising candidates from this perspective belong to the family of noncentrosymmetric superconductors $CePt_3Si$ [12,13], Li_2Pd_3B, Li_2Pt_3B [14,15], where $E_0 \simeq 30$–200 meV.

In spite of its clear interest, the possibility of having novel interesting features in low-density systems, defined by the condition $E_F \lesssim E_0$, has not been, in our opinion, sufficiently investigated to date, and only a few studies have been devoted to this problem. In Ref. [16], for instance, the vanishing of the spin-Hall current in the limit $E_F/E_0 \lesssim 1$ of Rashba disordered systems was shown not to be related to the vanishing of the vertex function but rather to the cancellation between on-Fermi surface and off-Fermi surface contributions. Another interesting effect was also pointed out in Ref. [17]: there the spin relaxation time τ_s for $E_F \ll E_0$ was shown to be proportional to the electron scattering time τ, in contrast with the standard Dyakonov-Perel behavior [18]. Interesting effects connected to the change of the Fermi surface topology for $E_F/E_0 \leq 1$ were also pointed out in Ref. [19] in relation to the disorder-induced localization.

The aim of this Letter is to explore in detail a fundamental feature arising from the topological change of the Fermi surface in low-density SO Rashba systems. We show that in this situation the enhanced phase space available for the electronic excitations gives rise to a SO-induced change of the electronic density of states (DOS) which can be described in terms of an effective reduced dimensionality. We discuss the consequences of this scenario on the superconducting instability criterion for both two- and three-dimensional Rashba systems. We show that, in contrast with the low SO coupling case $E_F/E_0 \gg 1$, the SO coupling in the $E_F/E_0 \lesssim 1$ regime systematically enhances the superconducting critical temperature, providing evidence that the lack of inversion symmetry can be remarkably beneficial for superconducting pairing.

We begin our analysis by considering the Rashba model [20], which describes the linear coupling of conduction electrons with a SO potential of the form $H_{SO} = \gamma(k_x\sigma_y - k_y\sigma_x)$, where σ_x, σ_y are Pauli matrices and γ is the Rashba coupling constant. For two-dimensional (2D) systems, a Rashba SO coupling arises from the asymmetric confining potential, while in bulk three-dimensional (3D) compounds it originates from the lack of the z-axis reflection symmetry, as in $CePt_3Si$. The SO coupling is reflected in an energy splitting of the two helicity bands. Assuming a parabolic band, the resulting electronic dispersion, for 2D and 3D cases, reduces to

$$E_{\pm}^{2D}(k) = \frac{\hbar^2}{2m^*}(k \pm k_0)^2, \tag{1}$$

$$E_{\pm}^{3D}(k) = \frac{\hbar^2}{2m^*}(k \pm k_0)^2 + \frac{\hbar^2 k_z^2}{2m^*}, \tag{2}$$

where $k = \sqrt{k_x^2 + k_y^2}$, k_z is the momentum along the z direction, m^* is the effective electron mass, and $k_0 = m^*\gamma/\hbar^2$ is the Rashba momentum. The dispersion for the 2D case is shown in Fig. 1(a), which can easily be generalized in the 3D case by taking into account the k_z dispersion. The two horizontal dashed lines correspond to the Fermi level for high-density and low-density regimes defined as $E_F > E_0$ and $E_F < E_0$, respectively, where $E_0 = \hbar^2 k_0^2/2m^*$ is the energy of the $k = 0$ point with respect to the bottom band edge at $k = k_0$ [see Fig. 1(a)].

Density of states.—Several studies in the literature have focused on the high-density regime, $E_F \gg E_0$, where the two Fermi surfaces belong to different helicity bands with corresponding Fermi vectors $k_{F,\pm} = \sqrt{2m^*/\hbar^2}(\sqrt{E_F} \mp \sqrt{E_0})$. In this case the electronic DOS at the Fermi level is given by

$$N^{2D}(E_F) = \sum_s \frac{1}{4\pi^2} \int_{S_{F,s}} \frac{dS_k}{\hbar|v_{k,s}|} = \sum_s \frac{1}{4\pi^2\hbar} \frac{S_{F,s}}{|v_{F,s}|}, \tag{3}$$

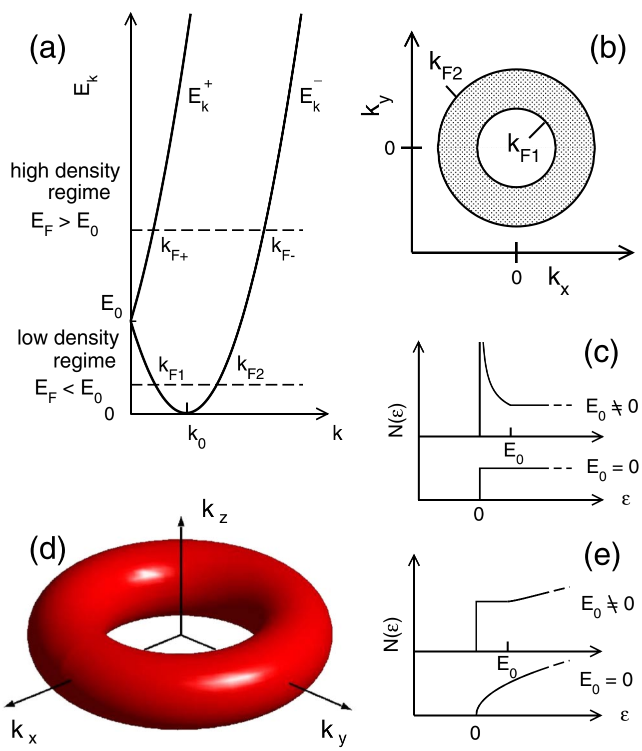

FIG. 1 (color online). (a) Electronic dispersion in the presence of SO coupling. For $E_F \geq E_0$ (high-density regime) the two Fermi surfaces belong to different helicity bands, while for $E_F \leq E_0$ (low-density regime) the Fermi surface exists only on the $E_{\mathbf{k}}^-$ band. (b),(c) Fermi surface and DOS, respectively, in the low-density regime for the 2D case. (d),(e) Fermi surface and DOS in the low-density regime for the 3D case.

where the Fermi velocity $|v_{F,\pm}| = \sqrt{2E_F/m^*}$ is independent of the helicity number $s = \pm$ and the Fermi surfaces are $S_{F,\pm} = 2\pi k_{F,\pm}$. Hence the total DOS in the $E_F > E_0$ regime $N^{2D}(E_F) = m^*/(\pi\hbar^2)$ is identical to the one in the absence of SO coupling. A similar result applies for the 3D case where, from Eq. (2), the corresponding DOS can be obtained as

$$N^{3D}(E_F) = \int \frac{dk_z}{2\pi} N^{2D}(E_F - \hbar^2 k_z^2/2m^*). \tag{4}$$

In the high-density regime $E_F \geq E_0$ we get $N^{3D}(E_F) = a\{\sqrt{E_F - E_0} + \sqrt{E_0}\arctan[\sqrt{E_0/(E_F - E_0)}]\}$, where $a = \sqrt{2}m^{*3/2}/(\pi^2\hbar^3)$, which reduces to $N^{3D}(E_F) \simeq a\sqrt{E_F}$ in the $E_F/E_0 \gg 1$ limit.

Let us now consider the $E_F \leq E_0$ regime. In this case the Fermi level intersects only the lower $E_-(k)$ band and the topology of the Fermi surfaces drastically changes. In the 2D case, for instance, only the annulus that lies between two Fermi circles of radii $k_{F,1}$ and $k_{F,2}$ with $k_{F,1(2)} = \sqrt{2m^*/\hbar^2}(\sqrt{E_0} \mp \sqrt{E_F})$ belonging to the same helicity band, is filled [Fig. 1(b)], and the inner Fermi surface is inwards oriented. We can still employ Eq. (3) by summing over the two Fermi surface indices $s = 1, 2$. Using $|v_{F,s}| = \sqrt{2E_F/m^*}$ and $S_{F,s} = 2\pi k_{F,s}$ we get

$$N^{2D}(E_F) = \frac{m^*}{\pi\hbar^2}\sqrt{\frac{E_0}{E_F}}, \tag{5}$$

which is valid as long as $E_F \leq E_0$ [Fig. 1(c)]. Most peculiar is the square-root divergence for $E_F \rightarrow 0$ that is reminiscent of one-dimensional behavior [11,17,19,21]. We relate such a feature to the nonvanishing in the low-density limit of the Fermi surface which remains finite, $S_{F,s} \propto \sqrt{E_0}$, while at the same time, the Fermi velocity vanishes as $\sqrt{E_F}$. The behavior of Eq. (5) has to be compared with the $\gamma = 0$ case where also the Fermi surface shrinks as $\sqrt{E_F}$ and the electron DOS has a nondivergent steplike behavior in the $E_F \rightarrow 0$ limit [22].

A similar reduction of effective dimensionality in the electron DOS appears also for the 3D systems in the $E_F \leq E_0$ regime. In this case the Fermi surface has a toruslike topology as shown in Fig. 1(d), with major radius $k_0 = \sqrt{2m^* E_0/\hbar^2}$ and minor radius $\sqrt{2m^* E_F/\hbar^2}$. Applying once more Eq. (4) we get for $E_F \leq E_0$:

$$N^{3D}(E_F) = \frac{\pi a}{2}\sqrt{E_0}. \tag{6}$$

Hence the SO coupling changes qualitatively the low-density behavior of the 3D DOS providing a finite steplike behavior [Fig. 1(e)] in contrast with a standard 3D electron gas whose DOS vanishes as $\sqrt{E_F}$.

Cooper instability.—The above described reduction of effective dimensionality sheds a new light on the possible existence of a superconducting phase in the low-density regime of SO systems. To illustrate this point let us consider the classical problem [23] of a Fermi surface instability toward the formation of a Cooper pair:

$$1 = V \int_0^{\omega_0} d\xi N(\xi) \frac{1}{2\xi + \Delta}, \tag{7}$$

where $\Delta > 0$ is the binding energy of the pair and where we introduce a standard BCS cutoff ω_0. V is the strength of the effective attractive interaction which we consider here for simplicity in the s-wave channel. Since the superconducting Cooper pairing is essentially a Fermi surface instability, the strength of the bound state and its very existence is intimately related to the phase space of the available electronic excitations. For instance, as is well known, in the low-density limit of 3D systems, where $N^{3D}(\xi) = a\sqrt{\xi}$, Eq. (7) predicts a finite critical coupling $V_c = 1/(a\sqrt{\omega_0})$ below which no bound state exists.

This result changes drastically for finite SO couplings where, as seen above, the electron DOS behaves now as an effective 2D system. Using Eq. (6) in Eq. (7) we get for $E_0 > \omega_0$ and weak coupling [24]:

$$\Delta_{3D} \simeq 2\omega_0 \exp\left(-\frac{4}{\pi a V \sqrt{E_0}}\right), \tag{8}$$

which explicitly shows that, contrary to the usual 3D case, the Cooper instability exists no matter how weak V is, with an exponential dependence on the SO coupling.

A similar change of the character of the Cooper instability occurs also in the 2D case. Indeed, in the absence of SO coupling, one would get the BCS-like result $\Delta = 2\omega_0 \exp(-2\pi\hbar^2/m^*V)$. On the other hand, due to the strong 1D-like divergence of the electron DOS, Eq. (5), the binding energy for finite SO coupling reads now

$$\Delta_{2D} = \frac{1}{2}\left(\frac{m^* V}{\hbar^2}\right)^2 E_0, \tag{9}$$

where the bosonic energy ω_0 is no longer present and the relevant energy scale is provided by E_0. Note also the quadratic dependence of Δ on V, and the absence of an isotope effect for the phonon-mediator case.

Superconducting critical temperature.—The above discussion of the single Cooper pair problem will be now a guide to the following investigation of the superconducting transition for finite (low) densities in fully interacting systems. In order to focus on the effects that the SO modulation of the DOS has on the superconducting critical temperature, we consider a Rashba-Holstein model where the SO coupled electrons interact with dispersionless bosons with energy ω_0 through an s-wave **k**-independent coupling with matrix element g [25]. It can be shown that in this case only the singlet symmetry appears, without mixed even or odd order parameter and singlet-triplet symmetry, which is instead expected for a generic **k**-dependent interaction in the lack of inversion symmetry [6,7]. Since the reduced dimensionality of the electron DOS is not peculiar to the s-wave singlet component but applies as well to the more complex anisotropic singlet-triplet case, this simplification is not expected to affect the general validity of our results. We evaluate thus the critical temperature T_c within the Eliashberg framework, which includes retardation effects, properly generalized in the presence of SO coupling.

In Figs. 2(a) and 2(c) we show the superconducting critical temperature T_c as a function of the Rashba energy E_0 for different electron densities n. In the figure the lower density values, $n = 10^{13}$ cm^{-2} and $n = 10^{20}$ cm^{-3}, correspond to Fermi energies $E_F \simeq 24$ meV and $E_F \simeq 46$ meV for the free electron gas in 2D and 3D, respectively. In addition, for a practical purpose one needs to introduce a finite bandwidth cutoff E_c, which is physically provided by the size of the Brillouin zone k_c. We set $E_c = 2000$ (430) meV which gives $k_c \simeq 0.72$ (0.33) Å^{-1} for the 2D (3D) case. We get thus an electronic DOS per unit cell which, for the density values reported above in the absence of SO coupling, is $N_{2D}(E_F = 24 \text{ meV}) \simeq 5 \times 10^{-4}$ meV^{-1} and $N_{3D}(E_F = 46 \text{ meV}) \simeq 12 \times 10^{-4}$ meV^{-1}. For all cases ω_0 has been fixed at $\omega_0 = 20$ meV and $g = 5\omega_0$. With these values we obtain dimensionless coupling constants $\lambda = 2g^2 N(E_F)/\omega_0$, respectively, $\lambda_{2D}(24 \text{ meV}) \simeq 0.5$ and $\lambda_{3D}(46 \text{ meV}) \simeq 0.6$. These small values of λ justify the use of the mean-field-like BCS and Eliashberg theories even for the highest values of the adiabatic ratio $\omega_0/E_F \sim 0.8$ considered here. Figures 2(a) and 2(c) show a significant increase of T_c as a function of E_0, in particular, for low densities where a small E_0 is sufficient to enter into the $E_F \lesssim E_0$ regime. This holds true for both 2D and 3D systems, and the

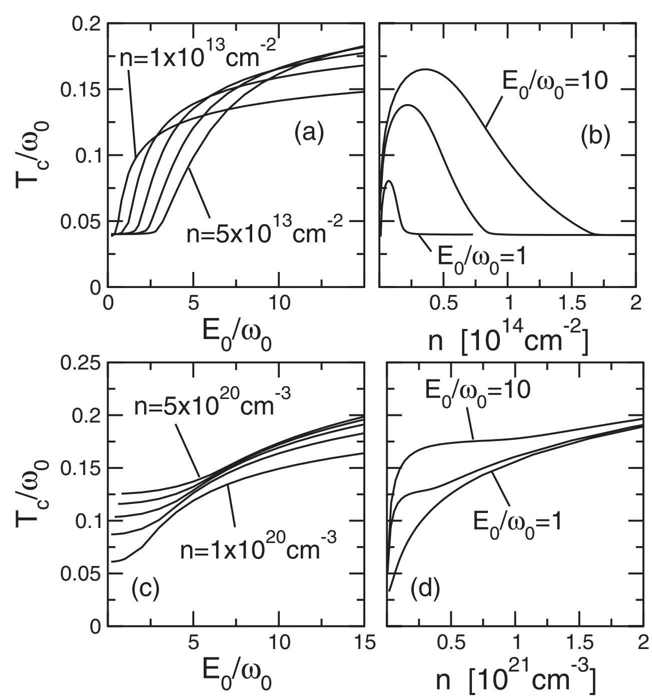

FIG. 2. (a),(b) Superconducting critical temperature T_c as a function of the Rashba energy E_0 and of the electron density n, respectively, for the 2D case. (c),(d) Same quantities for the 3D system.

enhancement of T_c can be as high as 300% with respect to the $E_0 \to 0$ limit. Assuming typical values $\omega_0 \approx 20$ meV and $E_0 \sim 30$–200 meV, we get $E_0/\omega_0 \sim 1$–10. Also interesting is the study of T_c as a function of the electron density n, as reported in Figs. 2(b) and 2(d), which show how the T_c vs n behavior reflects the effective reduced dimensionality of the underlying DOS. For the 2D case, for instance, the T_c vs n behavior presents strong peaks for $E_0 \neq 0$ which reflects the 1D-like singularity of the DOS. Note, however, that the retarded electron-boson interaction gives rise to dynamical one-particle renormalization effects which smear the singularity of the bare DOS.

Similarly, in the $E_0 \to 0$ limit of the 3D case T_c drops as the density n is reduced due to vanishing of $N_{3D}(E_F) \propto \sqrt{E_F}$. On the other hand, the 2D character of the DOS with $E_0 \neq 0$ gives rise to an almost flat dependence of T_c for sufficiently low n, with a critical temperature tuned by the Rashba energy E_0. Both the 2D and 3D cases thus show that the lack of inversion symmetry not only affects the character of the order parameter, as discussed in several works [6,7,13], but in principle can also lead to a substantial enhancement of the superconducting pairing in the low n regime.

Let us discuss now the relevance of our results in the context of real materials. Concerning the 2D case, for instance, surface states and low dimensional heterostructures could be natural candidates for the search of enhanced superconductivity. In particular, the issue of surface superconductivity [26] has recently been discussed in relation with systems like alkali-doped WO_3 [27] where evidence of superconductivity confined to the surface has been provided. Interesting perspectives are also given by the noncentrosymmetric superconductors. In the Li_2Pd_3B and Li_2Pt_3B compounds, in particular, a large SO coupling is accompanied by a strong electron-phonon interaction [28]. In this case, of course, as in the heavy fermion $CePt_3Si$ case, a proper generalization of the present results to the case of nonparabolic bands is needed. Before concluding, it is worth discussing the possibility of establishing an effective attraction even in the presence of a strong Coulomb repulsion. As is well known, in common superconductors this is achieved by the dynamical screening of the Coulomb repulsion which is related to the different electronic (E_F) and bosonic (ω_0) energy scales and which is operative in the range $\omega_0/E_F < 1$. This gives rise to a lower limit for E_F, which is, however, almost always fulfilled in systems of interest where E_0, $E_F \approx 10^2$ meV, and $\omega_0 \approx 10^1$ meV.

In summary, we have examined the impact of a strong Rashba SO interaction on the superconducting pairing in weakly coupled electron-boson systems. The primary result is an effective reduction in dimensionality of the low energy electronic DOS which increases significantly the phase space at the Fermi level. This allows binding in the zero density limit for arbitrarily weak interactions even for 3D systems. Full numerical calculations illustrate that the enhanced DOS has a remarkable impact on the superconducting critical temperature in a wide range of parameters. We suggest a search for higher T_c in materials with large SO coupling. In systems where electron density can be varied, one should be able to test some of the trends reported here.

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