SCIENCE CHINA
Physics, Mechanics & Astronomy

• Letter to the Editor •

February 2020 Vol. 63 No. 2: 227422
https://doi.org/10.1007/s11433-019-1439-3

Attractive electron-electron interaction induced by geometric phase in a Bloch band

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Received July 12, 2019; accepted September 2, 2019; published online September 27, 2019

Citation: J. R. Shi, and Q. Niu, Attractive electron-electron interaction induced by geometric phase in a Bloch band, Sci. China-Phys. Mech. Astron. **63**, 227422 (2020), https://doi.org/10.1007/s11433-019-1439-3

Attractive interaction between electrons (or neutral fermions) is responsible for superconductivity (or superfluidity). In condensed matter systems, attractive interaction is usually induced by the boson-exchange mechanism [1]. Indeed, in the celebrated Bardeen-Cooper-Schreiffer (BCS) theory, electrons develop attractive interaction by exchanging phonons [2]. Subsequent studies show that other collective excitations such as charge density waves [3] and spin fluctuations [4] can also induce attractive interaction. The boson-exchange mechanism, together with the concept of Cooper-pair, is considered to be the cornerstone of the modern theory of superconductivity.

In this Letter, we show a new possibility for the occurrence of attractive electron-electron (e-e) interaction in ferromagnetic metals with spin-orbit coupling. We take the ferromagnetic state as given, and focus on the effect of the Berry curvature field which exists ubiquitously in such materials [5,6]. Our question is relevant because superconductivity has been found within ferromagnetic phase, such as in UGe_2 [7] and URhGe [8]. The Berry curvature effect on electron motion is analogous to a magnetic field in the reciprocal space [9,10], and has been invoked to successfully explain the anomalous Hall effect in ferromagnets [11-13]. On the other hand, unlike a magnetic field in real space, monopole sources for the Berry curvature field can occur in the reciprocal space at band degeneracy points. In the vicinity of the monopoles, the Berry curvature becomes very strong.

Our theory is formulated within an effective one band model, where ferromagnetism and spin-orbit coupling has already been taken into account, such as one calculated self-consistently from a spin-density functional theory. Figure 1(a) shows the origin of the Berry curvature field: an electron evolving adiabatically in the reciprocal space will accumulate a geometric (Berry) phase $\phi_{\mathrm{B}} = \int_\gamma \langle u_{\mathbf{k}} | \mathrm{i}\partial_{\mathbf{k}} u_{\mathbf{k}} \rangle \cdot \mathrm{d}\mathbf{k}$ associating with the adiabatic change of the quasi-momentum $\mathbf{k}$ [14], in analogy to the Aharanov-Bohm phase acquired by electron moving in the real space in the presence of a magnetic field. It suggests a fictitious "magnetic field" in the reciprocal space with the "vector potential" $\mathcal{A}(\mathbf{k}) = \langle u_{\mathbf{k}} | \mathrm{i}\partial_{\mathbf{k}} u_{\mathbf{k}} \rangle$ and the corresponding "physical field" (Berry curvature field) $\mathbf{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}(\mathbf{k})$, where $u_{\mathbf{k}}$ is the periodic part of the Bloch wave function for the electron band concerned.

The central result of this work is that attractive interactions in the p-wave channel may be produced with the help of the Berry curvature field. We show that the presence of a sufficiently strong Berry curvature field on the Fermi surface can transform a repulsive e-e interaction into an attractive one in the p-wave channel. There is also a topological effect analogous to the Aharanov-Bohm phase. This is for a situation where the Berry curvature field vanishes or is negligible on the Fermi surface but not so inside of it. A Berry phase around the Fermi surface can still result from the flux

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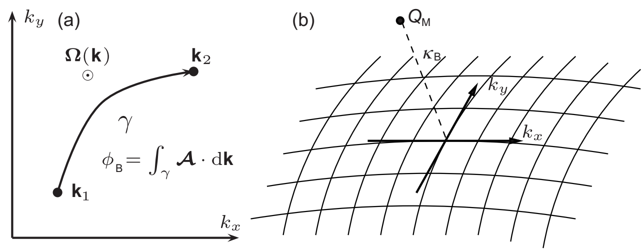

Figure 1 (a) Electron moving adiabatically in the reciprocal space acquires a Berry phase; (b) Berry curvature field in the vicinity of a band degeneracy split by magnetization and spin-orbit coupling can be modeled as a "magnetic field" in the reciprocal space generated by a "monopole" out of the 2D Brillouin manifold.

within. We show that an originally attractive interaction in the s-wave channel can be turned into one in the p-wave channel.

To be specific, we investigate the following effective one-band many-body Hamiltonian:

$$\hat{H} = \sum_i \epsilon(\hat{\mathbf{k}}_i) + \sum_{i<j} V(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j), \tag{1}$$

where $\epsilon(\hat{\mathbf{k}})$ is the quasi-particle dispersion operator, and $V(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)$ is the two-body e-e interaction. $\hat{\mathbf{k}}$ ($\hat{\mathbf{r}}$) is the quasi-momentum (position) operator, and the indexes i, j denote the particle number.

Our study is motivated by the understanding that in the presence of the Berry curvature field, the different components of the position operator $\hat{\mathbf{r}}$ do not commute [12, 15, 16]:

$$[\hat{r}_\mu, \hat{r}_\nu] = \mathrm{i}\epsilon_{\mu\nu\gamma}\Omega_\gamma, \tag{2}$$

where $\mu, \nu = x, y, z$ denote the different components of the position operator. It is then interesting to see how the change of the electron dynamics dictated by the non-commutative position operator affects the electron correlations in our system (1).

To proceed, we introduce the canonical coordinates $\hat{\mathbf{R}}$ which satisfy the usual commutation relations $[\hat{R}_\mu, \hat{R}_\nu] = 0$ and $[\hat{R}_\mu, \hat{k}_\nu] = \mathrm{i}\delta_{\mu\nu}$, which can be realized if we define

$$\hat{\mathbf{R}} = \hat{\mathbf{r}} - \mathcal{A}(\hat{\mathbf{k}}), \tag{3}$$

where $\mathcal{A}(\mathbf{k}) = \langle u_{\mathbf{k}} | \mathrm{i}\partial_{\mathbf{k}} u_{\mathbf{k}} \rangle$ is the "vector potential" corresponding to the Berry curvature field $\mathbf{\Omega}$. We can then second-quantize the many-body Hamiltonian eq. (1). We first re-express the interaction potential in terms of the canonical coordinates $\hat{\mathbf{R}}$. This can be done by making use of the Fourier expansion $V(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j) = (2\pi)^{-d} \int \mathrm{d}\mathbf{q} v(\mathbf{q}) \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\hat{\mathbf{r}}_i} \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\hat{\mathbf{r}}_j}$ and the relation $\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\hat{\mathbf{r}}} = \mathrm{e}^{\mathrm{i}\chi(\mathbf{q},\hat{\mathbf{k}})} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\hat{\mathbf{R}}} \mathrm{e}^{-\mathrm{i}\chi(\mathbf{q},\hat{\mathbf{k}})}$, where χ is defined by the equation $\mathbf{q} \cdot \nabla_{\mathbf{k}} \chi(\mathbf{q}, \mathbf{k}) = \mathbf{q} \cdot \mathcal{A}(\mathbf{k})$. The interaction potential can then be expressed in the plane wave basis $\psi_{\mathbf{k}}(\mathbf{R}) = \mathbf{1}/\sqrt{\mathcal{V}} \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{R})$, from which its second-quantized form can be easily read out, yielding finally

$$\hat{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{K}} u(\mathbf{k}, \mathbf{k}'; \mathbf{K}) c^\dagger_{\frac{\mathbf{K}}{2}+\mathbf{k}'} c^\dagger_{\frac{\mathbf{K}}{2}-\mathbf{k}'} c_{\frac{\mathbf{K}}{2}-\mathbf{k}} c_{\frac{\mathbf{K}}{2}+\mathbf{k}}, \tag{4}$$

where $\mathcal{V}$ is the total volume of the system, $c^\dagger$ (c) is the quasi-particle creation (annihilation) operator, and

$$u(\mathbf{k}, \mathbf{k}'; \mathbf{K}) = v(\mathbf{k}' - \mathbf{k}) \mathrm{e}^{\mathrm{i}\phi_B\left(\frac{\mathbf{K}}{2}+\mathbf{k}', \frac{\mathbf{K}}{2}+\mathbf{k}\right) + \mathrm{i}\phi_B\left(\frac{\mathbf{K}}{2}-\mathbf{k}', \frac{\mathbf{K}}{2}-\mathbf{k}\right)}, \tag{5}$$

i.e., the interaction is modified by a geometric phase defined as $\phi_B(\mathbf{k}, \mathbf{k}') = \int_{\mathbf{k}}^{\mathbf{k}'} \mathcal{A}(\mathbf{k}) \cdot \mathrm{d}\mathbf{k}$ with the integral along the straight line connecting $\mathbf{k}$ and $\mathbf{k}'$ in the reciprocal space. ϕ_B is exactly the Berry phase acquired by an electron scattered from $\mathbf{k}$ to $\mathbf{k}'$. In eq. (4), we omit the spin index, and focus on ferromagnetic systems in which the spin degrees of freedom are fully quenched due to the strong magnetization and spin-orbit coupling.

In the following, we investigate how the geometric phase modifies the e-e interaction. We notice that the distribution of the Berry curvature field in a Brillouin zone is governed by the $\mathbf{k}$-points of band degeneracies, which in mathematics are equivalent to "magnetic monopoles" in the reciprocal space [12,14,17]. We thus focus on one of such "monopoles" and see how the geometric phase in its vicinity modifies e-e interaction. To identify the essential physics without being obscured by complexities in mathematics, we limit our study on a two dimensional (2D) ferromagnetic system. In such a system, there is usually no band degeneracy [14]. However, one can usually find band near-degeneracies at high symmetry points of the Brillouin zone which are only split by the presence of magnetization and spin-orbit coupling. In the vicinity of these points, the Berry curvature field can be modeled as a "magnetic field" in the reciprocal space generated by a "monopole" out of the 2D Brillouin manifold, as shown in Figure 1(b). We thus have: $\mathbf{\Omega}(\mathbf{k}) = (Q_M/2)\kappa_B/(k^2 + \kappa_B^2)^{3/2}\hat{k}_z$ and

$$\mathcal{A}(\mathbf{k}) = \frac{Q_M}{2k^2}\left(1 - \frac{\kappa_B}{\sqrt{k^2 + \kappa_B^2}}\right)\mathbf{k} \times \hat{k}_z, \tag{6}$$

where we assume that the "monopole" is located at $(0, 0, \kappa_B)$. $Q_M = \pm 1$ is the charge of the "monopole". κ_B measures how close the 2D system is to the band degeneracy. It is related to the magnitude of the band gap induced by the magnetization and spin-orbit coupling: the larger band gap, the larger κ_B (for instance, see ref. [18]).

Attractive e-e interaction induced by the Berry curvature field: First, we demonstrate that the strong Berry curvature field in the vicinity of a reciprocal space "magnetic monopole" could transform a repulsive e-e interaction to an attractive one in p-wave channel. The e-e interaction in a typical metal can be modeled as $V(\mathbf{r}) = V_0 \exp[-\kappa_{TF}(\sqrt{r^2 + a^2} - a)]/\sqrt{(r/a)^2 + 1}$, which is screened at large distances for $r \gg 1/\kappa_{\mathrm{TF}}$ and saturates at small distances for $r \ll a$, where

$\kappa_{\rm TF}$ is the Thomas-Fermi screening wave vector [19]. Its Fourier transformation reads,

$$v(\mathbf{q}) = v_0 \frac{\exp\left[-a\left(\sqrt{q^2+\kappa_{\rm TF}^2}-\kappa_{\rm TF}\right)\right]}{\sqrt{(q/\kappa_{\rm TF})^2+1}}, \tag{7}$$

with $v_0 = 2\pi V_0 a/\kappa_{\rm TF}$. Eq. (7) should be considered as the renormalized interaction between "dressed" electrons resulting from a complete treatment of a bare many-body Hamiltonian [20].

For the isotropic model considered here, the effective interaction between a pair of electrons with the opposite momentum ($\mathbf{K} = 0$) can be classified by their relative angular momentum $L_z = m\hbar$. For channel m, the effective potential is [20]

$$u_m(k,k') = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta v(\mathbf{k}'-\mathbf{k})\mathrm{e}^{2\mathrm{i}\phi_{\rm B}(\mathbf{k}',\mathbf{k})}\mathrm{e}^{\mathrm{i}m\theta}, \tag{8}$$

where θ is the angle from $\mathbf{k}$ to $\mathbf{k}'$ and we have made use of the relation $\phi_{\rm B}(-\mathbf{k}',-\mathbf{k}) = \phi_{\rm B}(\mathbf{k}',\mathbf{k})$.

Figure 2(a) shows the the effective interaction for different channels for a given set of parameters. Attractive interaction (i.e., $u_m(k,k) < 0$) is evident for channel $m = 1$ (p-wave) and $m = 3$ (f-wave). Unlike the conventional attractive interaction due to boson exchange which is always present in a thin shell near the Fermi surface [1], the effective interaction due to the geometric phase is attractive only in the vicinity of the "monopole" (i.e., $\mathbf{k} = 0$). Figure 2(b) and (c) show the dependence of the effective interaction (k-position where the effective interaction is the most attractive, and its magnitude, respectively) on the parameters ($\kappa_{\rm B}$, $\kappa_{\rm TF}$, a) for the p-wave channel ($m = 1$). We note that the attractive interaction only

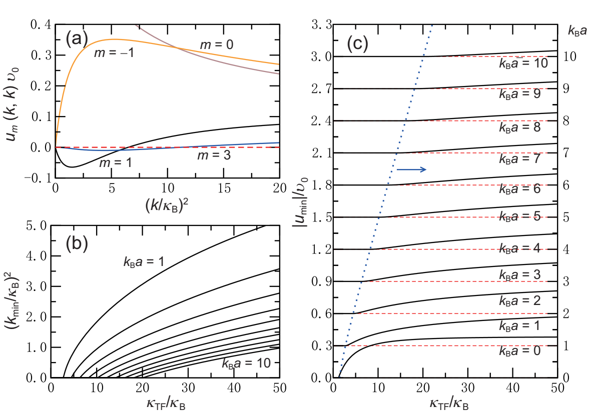

Figure 2 (Color online) Effective e-e interaction u_m. (a) Typical behavior of $u_m(k,k)$ for different m. Parameters: $\kappa_{\rm B}a = 0.2$ and $\kappa_{\rm TF}/\kappa_{\rm B} = 2.6$; (b) k-position of the $u_{m=1}(k,k)$ minimum as a function of $\kappa_{\rm TF}/\kappa_{\rm B}$ for different values of $\kappa_{\rm B}a$ from 1 to 10; (c) The minimum (most attractive) value of the effective potential for p-wave channel ($m = 1$) as a function of $\kappa_{\rm TF}/\kappa_{\rm B}$ for different values of $\kappa_{\rm B}a$. The different curves are offset vertically for clarity, with red dashed lines indicating respective baselines. The dotted line shows the boundary determined from eq. (11) for the onset of attractive interaction. $Q_{\rm M} = 1$.

occurs in a certain regime of the parameter space.

The condition for the onset of attractive effective interaction can be determined by examining the limit of $k,k' \ll \kappa_{\rm B},\kappa_{\rm TF}$, where $v(\mathbf{q}) \approx v_0\exp\left[-q^2/2\kappa_u^2\right]$ with $\kappa_u \equiv \kappa_{\rm TF}/\sqrt{1+\kappa_{\rm TF}a}$ and the Berry curvature field can be considered as a constant $\Omega_z(\mathbf{k}) \approx \Omega_0 \equiv Q_{\rm M}/2\kappa_{\rm B}^2$, with the corresponding geometric phase:

$$\phi_{\rm B}(\mathbf{k},\mathbf{k}') = \frac{1}{2}\Omega_0 kk'\sin\theta. \tag{9}$$

Then it follows that

$$\begin{aligned} u_m(k,k') \approx & v_0\left|\frac{1-\phi_\Omega}{1+\phi_\Omega}\right|^{m/2}\exp\left[-\frac{k^2+k'^2}{2\kappa_u^2}\right] \\ & \times\begin{cases} I_m\left(\dfrac{kk'}{\kappa_u^2}\sqrt{1-\phi_\Omega^2}\right), & |\phi_\Omega| \le 1, \\ (-1)^m J_m\left(\dfrac{kk'}{\kappa_u^2}\mathrm{sgn}(\phi_\Omega)\sqrt{\phi_\Omega^2-1}\right), & |\phi_\Omega| > 1, \end{cases} \end{aligned} \tag{10}$$

where $\phi_\Omega \equiv \Omega_0\kappa_u^2$. J_m (I_m) is the (modified) Bessel function of the first kind. The attractive interaction (i.e., $u_m(k,k) < 0$) arises in the channels with odd positive (negative) m for $\Omega_0 > 0$ ($\Omega_0 < 0$) if

$$|\Omega_0|\kappa_u^2 > 1\,. \tag{11}$$

The boundary determined from the condition is shown as the dotted line in Figure 2(c), which coincides well with the boundary directly determined from the numerical result.

We apply the BCS gap equation in ref. [20] to investigate the superconducting phase induced by the attractive interaction. The result is summarized in Figure 3. The superconducting state has p-wave symmetry with $\Delta(\mathbf{k}) = \Delta(k)(\hat{k}_x \pm \mathrm{i}\hat{k}_y)$ (for $Q_{\rm M} = \pm 1$). The magnitude of the superconducting gap strongly depends on the position of the Fermi surface, which is a direct result of the strong k-dependence of the effective potential.

The superconductivity we predict is closely associated with ferromagnetism, which breaks the time-reversal symmetry, and together with spin-orbit coupling, gives rise to the Berry curvature field in the vicinity of the high symmetry $\mathbf{k}$-points. In this picture, the superconducting phase naturally coexists with ferromagnetism and disappears when the ferromagnetism is suppressed. This behavior makes it a plausible alternative theory for the recently discovered ferromagnetic superconductors $\mathrm{UGe_2}$ [7] and URhGe [8]. In the traditional picture, enhanced spin fluctuations near a quantum critical point are responsible for the pairing of electrons. It predicts the superconducting phase on both sides of the ferromagnetic-paramagnetic transition point [21], which contradicts the experimental finding that the superconducting phase only exists in the ferromagnetic side. On the other hand, we note that the conditions for the onset of superconductivity with the mechanism (i.e., eq. (11) and the Fermi

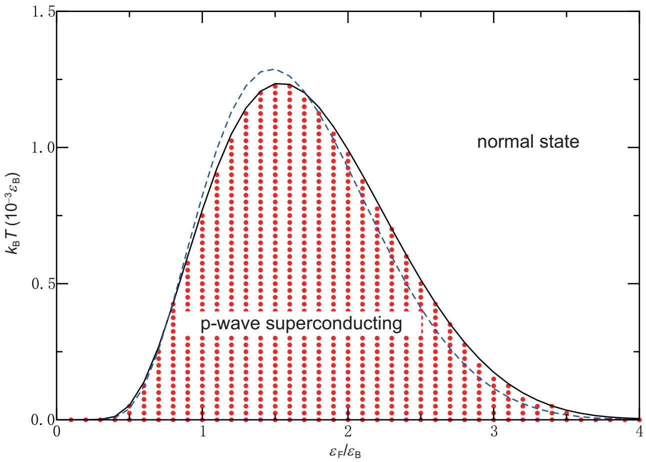

Figure 3 (Color online) Phase diagram in ϵ_F (Fermi energy)-T (Temperature) plane. $\epsilon_B \equiv \epsilon(\kappa_B)$. Filled dots indicate the region occupied by the superconducting phase. Solid line shows the superconducting gap $\Delta_F(0)$ at the Fermi surface and at the zero temperature, scaled by a factor $1/1.76$. The good correspondence between the phase boundary and the solid line suggests the usual BCS relation $\Delta_F(0)/kT_c \approx 1.76$. The dashed line shows an empirical fitting $\Delta_F(0) \approx a\epsilon_B \exp[-1/\rho_F|u_m(k_F, k_F)|]$, where ρ_F is the density of states at Fermi surface and $a \approx 5$. The reasonably good fitting suggests the correlation between the magnitude of the superconducting gap and the strength of the attractive interaction at the Fermi surface. Parameters: $\kappa_B a = 0.2$, $\kappa_{TF}/\kappa_B = 2.6$, and $\rho_F v_0 = 2$. The electron dispersion is assumed to be the simple parabolic form. $Q_M = 1$.

surface must reside in the vicinity of the "monopole") are rather stringent . Further investigations is required for establishing the definite connection between the theory and real systems.

Unconventional pairing symmetry of the topological origin: Second, we consider the case that the Fermi-surface (-circle) is far from the "monopole", i.e., $k_F \gg \kappa_B$. While there is no strong presence of the Berry curvature field on Fermi-circle in this case, the "monopole" still presents a reciprocal space "magnetic flux" threading through the Fermi-disc with a total flux $\Phi_B = \pi Q_M$. The corresponding geometric phase in the vicinity of the Fermi-circle reads:

$$\phi_B(\mathbf{k}, \mathbf{k}') \approx \frac{Q_M}{2}\theta. \tag{12}$$

Using eq. (8), the effective e-e interaction in channel m is

$$u_m(k, k') \approx v_{m+Q_M}(k, k'), \tag{13}$$

where v_m is the Fourier component of the bare e-e interaction at channel m. For an originally attractive interaction in s-wave channel (i.e., $v_{m=0} < 0$), the effective interaction u_m is attractive in channel $m = -Q_M = \mp 1$, giving rise the p-wave pairing symmetry. The unconventional pairing symmetry has a topological origin, i.e., the "monopole" (band degeneracy) buried deep inside the Fermi-sea. Were the "magnetic monopole" not present, the bare interaction would favor the s-wave pairing symmetry.

So far, our discussion is built upon the Berry curvature field associating with the adiabatic evolution of quasi-electrons in reciprocal space. It is valid only when the interaction potential varies slowly over the atomic length scale. When the potential is not slowly varying, we have to work with the matrix elements between the Bloch states, $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{\mathbf{k}}(\mathbf{r})\rangle$. In this case, the effective interaction matrix element has the form (for $\mathbf{K} = 0$)

$$u(\mathbf{k}, \mathbf{k}'; \mathbf{K} = 0) = v(\mathbf{k}' - \mathbf{k})\langle u_{\mathbf{k}'}|u_{\mathbf{k}}\rangle\langle u_{-\mathbf{k}'}|u_{-\mathbf{k}}\rangle. \tag{14}$$

The extra phases are now the Pancharatnam geometric phases [22]. For smooth potentials, only forward scattering with small $\mathbf{k}' - \mathbf{k}$ is important, the Pancharatnam phases reduce to the Berry phases [23].

Notes added: The paper was originally posted as arXiv:cond-mat/0601531 in 2006. We are grateful that it finds applications in later developments [24-26]. Thanks to Prof. Zhenyu Zhang's recommendation, we submit it for publication after minor revisions.

JunRen Shi was supported by the Program of "One Hundred Talented People" of Chinese Academy of Sciences, and the National Natural Science Foundation of China (Grant No. 10604063). Qian Niu was supported by the Welch Foundation (Grant No. F-1255).

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