Dynamic generation of spin orbit coupling

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Spin-orbit coupling plays an important role in determining the properties of solids, and is crucial for spintronics device applications. Conventional spin-orbit coupling arises microscopically from relativistic effects described by the Dirac equation, and is described as a single particle band effect. In this work, we propose a new mechanism in which spin-orbit coupling can be generated dynamically in strongly correlated, non-relativistic systems as the result of fermi surface instabilities in higher angular momentum channels. Various spin-orbit couplings can emerge in these new phases, and their magnitudes can be continuously tuned by temperature or other quantum parameters.

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Most microscopic interactions in condensed matter physics can be accurately described by non-relativistic physics. However, spin-orbit (SP) coupling is a notable exception, which arises from the relativistic Dirac equation of the electrons [1]. The emerging science of spintronics makes crucial use of the S-P coupling to manipulate electron spins by purely electric means. The proposed Datta-Das device [2] modulates the current flow through the spin procession caused by the SP coupling. More recently, Murakami, Nagaosa and Zhang [3, 4] proposed a method of generating the dissipationless spin current by applying an electric field in the p-doped semiconductors. This effect and the similar proposal for the n-doped semiconductors [5] both make crucial use of the SP coupling. In contrast to the generation of the spin current by coupling to the ferromagnetic moment, purely electric manipulation has an intrinsic advantage. However, unlike the ferromagnetic moment, which can be spontaneously generated through the strong correlation of spins, the conventional wisdom states that the SP coupling is a non-interacting one-body effect, whose microscopic magnitude is fixed by the underlying relativistic physics.

On the other hand, recent interests are revived on the Landau-Pomeranchuk (L-P) [6] fermi surface instabilities, largely in connection with electronic liquid crystal states with spontaneously broken rotational symmetry [6, 7, 8, 9], and in connections with hidden orders in heavy fermion systems [10, 11, 12]. Varma’s recent work showed that the L-P instability could lead to the opening of an anisotropic gap at the fermi surface [12]. In this paper, we show that the SP coupling can be generated dynamically in a non-relativistic system through strong correlation effects as the L-P instability in the spin channel with higher orbital angular momentum. It emerges collectively after a phase transition, which is continuously tunable either by temperature or by a quantum parameter at zero temperature. Unlike the ferromagnet, our ordered phase keeps time reversal symmetry. Also in contrast to the L-P instabilities considered by the majority of previous theories, most translationally invariant liquid phases in our model do not break rotational symmetry, and some of them preserve time reversal and parity symmetries as well. Most correlated phases in condensed matter physics are characterized by their broken symmetries [16]. Solids break translational symmetry, liquid crystals break rotational symmetry, superfluids and superconductors break gauge symmetry and ferromagnets break time reversal symmetry and rotational symmetry. As far as we are aware, the new phase reported in this work is the only one besides the fermi liquid which does not break any of the above symmetries. It is distinguished from the fermi liquid by only breaking the “relative spin orbit symmetry”, a concept first introduced in the context of the 3He liquid [17].

We first discuss the dynamic generation of SP coupling from the L-P instability within the Landau-Fermi liquid theory triggered by the negative Landau parameter $F^{\mu}_1$, and then present its exact definition. This instability lies in particle-hole channel with total spin one and relative angular momentum one. Operators in matrix forms are defined as $Q^{\mu\nu}(r) = \psi_1^\dagger(r)\sigma^\mu_{\alpha\beta}(-i\nabla^\alpha)\psi_\beta(r)$, where Greek indices denote the direction in the spin space, Latin indices denote the direction in the orbital space, and the operation of $\nabla^\alpha$ on the plane wave is defined as $\nabla^\alpha e^{i\vec{k}\cdot\vec{r}} = (\nabla^\alpha/|\vec{k}|)e^{i\vec{k}\cdot\vec{r}} = \vec{k}_\alpha e^{i\vec{k}\cdot\vec{r}}$. $Q^{\mu\nu}(r)$ is essentially the spin-current operator up to a constant factor. We use a Hamiltonian similar to that of Ref. [8], but in the $F^\nu_1$ channel:

$$
H = \int d^3\vec{r} \psi_\alpha^\dagger(\vec{r})\left(\epsilon(\vec{\nabla}) - \mu\right)\psi_\alpha(\vec{r}) + h_{\mu\alpha}Q^{\mu\alpha}(\vec{r}) + \frac{1}{2}\int d^3\vec{r}d^3\vec{r}' f_1^\dagger(\vec{r} - \vec{r}') Q^{\mu\alpha}(\vec{r})Q^{\beta\alpha}(\vec{r}'),
$$

(1)

where $\mu$ is the chemical potential and the small $h_{\mu\alpha}$ is dubbed as the “spin-orbit field”, which plays a role similar to the external magnetic field. For later convenience [8], we keep both the linear and the cubic terms in the expansion of the single particle dispersion relation around the fermi wavevector $k_f$, $\epsilon(\vec{k}) = v_f\Delta k[1 + k^2/(\Delta k/k_f)^2]$, with $\Delta k = k - k_f$. We assume that the Fourier components of $f_1^\dagger(\vec{r})$ take the form $f_1^\dagger(\vec{q}) = \int d\vec{r} e^{i\vec{q}\cdot\vec{r}} f_1^\dagger(\vec{r}) = f_1^\dagger/(1 + k|\vec{f}_1|^2)$ and define the dimensionless Landau parameter $F^{\nu}_1 = N_f f_1^\dagger$, where $N_f$ is the density of states at fermi energy. The symmetry of the Hamiltonian [9] is a direct product $SO(3)_L \otimes SO(3)_S$ in the orbital and spin channels.
We define the spin-orbit susceptibility as $\chi_{\mu a,\nu b} = \langle Q^{\mu a}\rangle / h_{\nu b}$ in the limit $h_{\nu b} \to 0$, which is diagonal, i.e., $\chi_{\mu a,\nu b} = \delta_{\mu a}\delta_{\nu b}$, in the normal fermi liquid phase. The fermi liquid correction to $\chi$ is given by

$$\chi_{FL} = \chi_0 \frac{m^*}{m} \frac{1}{1 + F_1^3/3},$$

(2)

with $m^*/m$ the ratio between the effective and bare masses. The spin-orbital susceptibility is enhanced for $F_1^3 < 0$ and divergent as the critical point $F_1^3 = -3$ is reached.

In the mean-field (MF) analysis, the p-h channel triplet order parameter is defined as $n^{\mu a}(r) = -\int d^3 r' f_0^n(r - r') (Q^{\mu a}(r'))$, and the external spin-orbit field $\hbar\mu$ is set to zero. Using the uniform ansatz $n^{\mu a}(r) = n^{\mu a}$, Eq. 1 is decoupled into $H_{MF} = \int d^3 r' \psi^\dagger(r') (\epsilon(r) - n^{\mu a} \sigma^\mu (i\nabla - \mu) \psi(r) + V n^{\mu a} n^{\mu a}/(2 f_1^3))$, with $V$ the space volume. The self-consistent equation for the order parameters reads

$$n^{\mu a} = |f_1^3| \int \frac{d^3 k}{(2\pi)^3} \langle \psi(k) | \sigma^\mu k^a \psi(k) \rangle,$$

(3)

which is valid when the interaction range $r_0 = \sqrt{\kappa |f_1^3|}$ is much larger than the distance between particles $1/k_f$, i.e., the dimensionless parameter $\eta = k_f \sqrt{|f_1^3|} \gg 1$.

The phase structures can be determined from the Ginzburg-Landau (G-L) free energy, which is similar to the triplet pairing order parameter in the $^3$He system \[12, 13\]. Under the independent SO(3) rotations in the orbital and spin spaces $R_L$ and $R_S$, $n^{\mu a}$ transforms as $n^{\mu a} \to R_{L,\mu a} n^{\mu b} R_{S,\alpha b}^{-1}$. Furthermore, $n^{\mu a}$ is even under the time-reversal but odd under the parity transformation. With these symmetry requirements, the G-L free energy can be constructed up to the quartic order as

$$F(n) = A \text{tr}[n^T n] + B_1 (\text{tr}[n^T n]^2) + B_2 \text{tr}[(n^T n)^2].$$

(4)

Compared with the complex order parameter in the superfluid $^3$He case, the reality of the $n_{\mu a}$ restricts the free energy to contain only two quartic terms. Explicitly, $\text{tr}[n^T n] = n^{\mu a} n^{\mu a} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$, and $\text{tr}[(n^T n)^2] = n^{\mu a} n^{\mu b} n^{\nu a} n^{\nu b} = \lambda_1^4 + \lambda_2^4 + \lambda_3^4$, where $\lambda_{1,2,3}$ are eigenvalues of $n^T n$. For $B_2 < 0$ or $B_2 > 0$, Eq. 1 favors the structures of $\lambda_1^2$, $\lambda_2^2$, $\lambda_3^2$ to be proportional to $(1,0,0)$ or $(1,1,1)$, respectively. We name them as $\alpha$ or $\beta$-phases whose general order parameter matrix structures are given by

$$n^{\mu a} = \begin{cases} \bar{n} \hat{d}_a \hat{\epsilon}_a & \text{\alpha-phase, for } B_2 < 0 \\ \bar{n} D_{\mu a} & \text{\beta-phase, for } B_2 > 0 \end{cases},$$

(5)

where $\hat{d}$ and $\hat{\epsilon}$ are two arbitrary unit vectors in the spin and orbital space respectively, $D_{\mu a}$ is any SO(3) rotation matrix, and $\bar{n}$ is a real number. In other words, the correlation functions of operators $Q^{\mu a}$ acquire a long range part in the ordered states

$$\langle Q^{\mu a}(r) Q^{\nu b}(r') \rangle \to \delta_{\mu a} \delta_{\nu b} \frac{\eta^2}{|f_1^3|^2} \times \begin{cases} \bar{n} \hat{d}_a \hat{\epsilon}_a & \text{\alpha-phase} \\ D_{\mu a} & \text{\beta-phase} \end{cases}$$

(6)

as $|r - r'| \to \infty$. This correlation function gives the rigorous definition for the new phases, independent of the approximate Fermi liquid theory used here.

The $\alpha$-phase is a straightforward generalization of the nematic fermi liquid $\bar{S}$ to the triplet channel as shown in Fig. 1 where the spin and orbital degrees of freedom remain decoupled, and the rotational symmetry is broken. Taking a special case $n^{\mu a} = \bar{n} \delta_{\mu a} \delta_\alpha$, the dispersion relations for spin up and down branches are $\xi^\alpha(k) = \epsilon(k) - \mu \mp \bar{n} \cos \theta$, where $\theta$ is the angle between $k$ and $\hat{z}$-axis. The fermi surfaces for the two spin components are distorted in an opposite way as $\Delta k_{f1,2}(\theta)/k_f = \pm x \cos \theta (1 - bx^2 \cos^2 \theta) - 1/3 x^2$, with the dimensionless parameter $x = \bar{n}/(v_f k_f)$. The chemical potential $\mu$ is shifted to ensure the particle number conservation as $\delta \mu/(v_f k_f) = -x^2/3$. The remaining symmetry is $SO(2)_L \otimes SO(2)_S$ with the Goldstone manifold $S_1^2 \otimes S_2^2$. Two Goldstone modes are the oscillations of the distorted fermi surfaces, and the other two are the oscillations of the spin directions.

In the $\beta$-phase, the rotational symmetry is preserved with the dynamic generation of spin-orbit coupling as shown in Fig. 1. For example, with the ansatz $n^{\mu a} = \bar{n} \delta_{\mu a}$, the MF Hamiltonian is reduced to

$$H_{MF} = \sum_k \psi^\dagger(k) (\epsilon(k) - \mu - \bar{n} \hat{\sigma} \cdot \hat{k}) \psi(k).$$

(7)

The single particle states can be classified according to the eigenvalues $\pm 1$ of the helicity operator $\hat{\sigma} \cdot \hat{k}$, with dispersion relations $\xi^\beta(k)_{1,2} = \epsilon(k) - \mu \pm \bar{n}$. The fermi surface distortions of two helicity bands are $\Delta k_{f1,2}/k_f = \pm x(1 - bx^2) - x^2$ and the chemical potential shift $\delta \mu/(v_f k_f) = -x^2$. Similar to the superfluid $^3$He-B phase, the $\beta$-phase is essentially isotropic. The orbital $\hat{L}$ and the spin $\hat{S}$ angular momenta are no longer separately conserved, but the total angular momentum $\vec{J} = \vec{L} + \vec{S} = 0$ remains conserved. The Goldstone manifold is $[SO(3)_L \otimes SO(3)_S] / [SO(3)_L \otimes SO(3)_S]$ with three
branches of Goldstone modes. For the general case of $n_{\mu a} = \hat{n}D_{\mu a}$, it is equivalent to a redefinition of spin operators as $S'_\mu = S_\mu D_{\mu a} \delta_{\mu a}$, thus fermi surface distortions remain isotropic and $\hat{J} = \hat{L} + \hat{S}$ is conserved. A similar symmetry breaking pattern also appears in the quantum chromodynamics where the two-flavor chiral symmetry $SU(2)_L \times SU(2)_R$ is broken into the diagonal $SU(2)_{L+R}$ [19]. In that case, both $SU(2)_{L,R}$ are internal symmetries, and thus there is no flavor-orbit coupling.

The coefficients of the G-L free energy Eq. 4 can be microscopically derived from the MF theory as

$$A = \frac{1}{2} \frac{1}{|f|^2} \frac{N_f}{3}, \quad B_1 = \frac{N_f}{20v_f^2k_f^2(1 + \frac{b}{3})},$$
$$B_2 = \frac{N_f}{30v_f^2k_f^2} (-\frac{1}{3} + b),$$

(8)

where $b$ describes the cubic part of the dispersion $\epsilon(k)$, as explained earlier. With the definition of $\delta = 1/|f|^2 - 1/3$, the L-P instability takes place at $\delta < 0$, i.e., $F^a_2 < -3$. For $b < 1/3$, i.e., $B_2 < 0$, the $\alpha$-phase appears with $|\vec{n}|^2 = \frac{|A|^2}{2(1 + B_2)}$. For $b > 1/3$, i.e., $B_2 > 0$, the $\beta$-phase is stabilized at with $|\vec{n}|^2 = \frac{|A|^2}{2(1 + B_2)}$. The largest fermi surface distortion $\Delta k_{f,max}/k_f$ in the $\alpha$-phase is larger than the uniform one $\Delta k_{f}/k_f$ in the $\beta$-phase, thus a large positive $b$ is helpful to the $\beta$-phase. However, we emphasize that this is only one of the options to change the sign of $B_2$.

To apply the $\alpha$ and $\beta$ phases in the lattice system, we only need replace the $SO(3)_L$ symmetry with the lattice point group. For example, for the simple cubic lattice, we define $Q^{\mu a} = i\epsilon^{\mu}(\vec{x})\sigma^\mu \epsilon(\vec{x} + \hat{e}_a) - h.c.$ with $\hat{e}_a$ the base vector in the $a$-direction. The unbroken symmetry is $O_L \otimes SO(3)_S$ where $O_L$ is the orbit lattice octahedral group. The mean field Hamiltonian for the $\beta$ phase reads

$$H_{MF} = \sum_k \psi_k^\dagger (\epsilon_k - \mu - \hat{n}\sigma_{\mu} \sin \hat{k}_{\mu a}) \psi_k,$$

(9)

with lattice momentum $\hat{k}$ restricted in the first Brillouin zone. The helicity structure for each $\hat{k}$ is aligned along the direction of $(\sin k_x, \sin k_y, \sin k_z)$, which breaks the symmetry down to the combined octahedral rotation in the orbit and spin space $O_{L+S}$. As a real space analogy, the hexagonal non-colinear anti-ferromagnet YMnO$_3$ [20, 21] has the spin order pattern inside the unit cell which is also invariant under the combined spin-orbit point group rotations. The difference is that the spin order in the $\beta$ phase lies in the momentum space and no spatial spin order exists each lattice site. The lattice $\alpha$-phase was originally studied under the name of “spin-split state” by Hirsch [22] to explain the phase transition at $T_N = 311 K$ in the Chromium system.

By reducing the space dimension to 2, the mean field Hamiltonian for the $\beta$-phase reduce to the familiar Rashba [22] and Dresselhaus Hamiltonians [24] in the 2D semiconductor heterostructures. The order parameter $n_{\mu a}$ is a 3 × 2 matrix with $\mu = x, y, z$ and $a = x, y$. Its third row of $\mu = z$ can be transformed to zero by performing suitable $SO(3)$ rotation on the index $\mu$, thus we take $n_{\mu a}$ as a 2 × 2 matrix. The G-L free energy is also the same as in Eq. 4 but with the new coefficients

$$A = \frac{1}{2} \left( \frac{1}{|f|^2} - \frac{N_f}{2} \right), \quad B_1 = \frac{N_f}{32v_f^2k_f^2}, \quad B_2 = \frac{bN_f}{8v_f^2k_f^2}$$

(10)

and the L-P instability occurs at $F^a_2 < -2$. The $\alpha$ and $\beta$-phase structures are similar as before in Eq. 4. However, there are two options in the $\beta$-phase with $n_{\mu a} = \hat{n}D_{\mu a}$, where $D_{\mu a}$ is a $O(2)$ matrix. If det $D = 1$, then $J_z = L_z + S_z$ is conserved. With the MF ansatz $n_{\mu a} = \hat{n}\epsilon_{\mu a}$, we arrive at the Rashba-like Hamiltonian

$$H_R = \int d^2\vec{r} \psi^\dagger \left\{ \left( \nabla \right) - \hat{n}\epsilon \sigma_{\mu a} \sigma^\mu \left[ -i \nabla a \right] \right\} \psi.$$  

(11)

If det $D = -1$, $J_z$ is not conserved while the energy spectrum and fermi surface distortions are still the same as the case of det $D = 1$. With the MF ansatz $n_{\mu a} = \hat{n} \text{diag}\{1, -1\}$, we arrive at the 2D Dresselhaus-like Hamiltonian as

$$H_D = \int d^2\vec{r} \psi^\dagger \left\{ \epsilon(x) \nabla - \hat{n}\epsilon \sigma_{\mu a} \sigma^\mu \left[ -i \nabla a \right] \right\} \psi.$$  

(12)

If we generalize the mechanism of dynamical generation of the spin-orbit coupling to the spin 3/2 fermionic system, an interesting phase can be obtained which preserves all familiar symmetries including the parity symmetry, breaking only the relative spin orbit symmetry. It has been recently shown that any generic model of spin 3/2 with local interactions has an exact SO(5) symmetry in the spin space [25]. The four spin components form the spinor representation of the SO(5) group. Using the Dirac $\Gamma$ matrix defined there, the spin 3/2 Landau interaction functions are classified into the SO(5)’s scalar, vector and tensor channels [25]:

$$f_{\alpha\beta,\gamma\delta}(\vec{p},\vec{p}') = f^+\left(\vec{p},\vec{p}'\right) + f^-(\vec{p},\vec{p}') \left(\Gamma^a/2\right)_{\alpha\beta} \left(\Gamma^a/2\right)_{\gamma\delta},$$

(13)

We further pick out its $L = 2$ part of the orbital angular momentum in the spin 2 vector channel denoted as the $F^a_2$ channel. We define operators $Q^{\mu a}(\vec{r}) = \psi_{\alpha}^\dagger(\vec{r}) \Gamma^a_{\alpha\beta} d^\mu(\nabla) \psi_{\beta}(\vec{r}) \left(1 \leq \mu, \alpha, a \leq 5\right)$, where $d^\mu(\nabla) = \left[\sqrt{3} \nabla_x \nabla_y, -\sqrt{3} \nabla_x \nabla_z, \sqrt{3} \nabla_y \nabla_z, -\frac{1}{2}(3\nabla_x^2 - \nabla_y^2), \frac{1}{2}(3\nabla_x^2 - \nabla_y^2)\right]$. The model Hamiltonian is constructed as follows:

$$H = \int d^3\vec{r} \psi^\dagger(\vec{r}) \left( \epsilon(\vec{r}) - \mu \right) \psi(\vec{r}) + \frac{1}{2} \int d^3\vec{r} d^3\vec{r}' f_{2}^a(\vec{r} - \vec{r}') Q^{\mu a}(\vec{r}) Q^{\mu a}(\vec{r}'),$$

(14)

with the symmetry of $SO(3)_L \otimes SO(5)_S$. The order parameter is defined as before $n_{\mu a}(\vec{r}) = -\int d^3\vec{r} f_{2}^a(\vec{r} - \vec{r}')\left(\Gamma^{\mu a}(\vec{r}')\right)$ and the L-P instability occurs when $F^a_2 = N f_{2}^a(q = 0) < -5$. 


The ordered phases after the L-P instability can also be classified into two categories as before: the α-phase with anisotropic fermi surface distortions and β-phase with spin-orbit coupling. The detail phase structures are much more complicated here. For example, the α-phase has two non-equivalent configurations because the \( L = 2 \) channel fermi surface distortions can be either uniaxial or biaxial. A comprehensive classification of all the possible phases is quite involved and is deferred to a future work. We focus here on the β-phase with the order parameter structure \( \nu^{\mu a} = \tilde{n}\delta_{\mu a} \). In this case, the MF Hamiltonian is reduced into \( H_{\text{MF}} = \int d^3 r \psi^\dagger(\vec{r}) \left\{ \psi(\nabla) - \mu - \tilde{n}\delta_{\mu a} \Gamma^\mu \nabla \psi(\vec{r}) \right\} \psi(\vec{r}) \). From the relation between the \( \Gamma^\mu \) matrices and the quadratic form of spin \( 3/2 \) matrices \( \bar{S} \), it can be easily recognized the Luttinger-like Hamiltonian [26]

\[
H_L = \int d^3 r \psi^\dagger(\vec{r}) \left\{ \psi(\nabla) - \mu - \tilde{n}(\vec{r}) \cdot \bar{S} \right\} \psi(\vec{r}),
\]

which is the standard model for the hole-doped III-V semiconductors. The original symmetry which is the standard model for the hole-doped III-Luttinger-like Hamiltonian [26]

\[
\int d^3 r \psi^\dagger(\vec{r}) \left\{ \psi(\nabla) - \mu - \tilde{n}\delta_{\mu a} \Gamma^\mu \nabla \psi(\vec{r}) \right\} \psi(\vec{r}) \].

Therefore, detecting the AHE signal turning on at a phase transition directly demonstrates that the phase transition breaks the relative spin-orbit symmetry. We propose to systematically search for these new phases in \(^{3}\text{He}\), ultracold atomic systems, semiconductors, heavy fermion materials and ruthenates, both in experiments and in microscopic numerical simulations. The new β phases can be experimentally detected through the standard predictions based on the spin-orbit coupling, but would have the remarkable and distinctive feature that these effects turn on and off near a phase transition. We conjecture that besides the familiar superfluid A and B-phases, \(^{3}\text{He}\) may contain the new phases proposed in this work. The Landau parameter \( F_3 \) in \(^{3}\text{He}\) was determined to be negative from various experiments [27, 28, 29, 30] such as the normal-state spin diffusion constant, spin-wave spectrum, and the temperature dependence of the specific heat etc. It varies from around \(-0.5\) to \(-1.2\) with increasing pressures to the melting point, reasonably close to the instability point \( F_3 = -3 \). Even though we presented mean field descriptions of the new phases with dynamically generated spin orbit coupling, the existence of these phase can obviously be studied by exact microscopic calculations of the correlation function Eq. [6] for realistic models.

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