Staggered spin-orbit coupling order: A new paradigm of broken symmetry phases of matter

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Abstract

We propose a novel spin-orbit coupling density wave order which can arise in variety of material classes. In systems where the non-interacting wavefunctions are defined by exotic quantum number such as total angular momentum, pseudospin or helical quantum number owing to spin-orbit coupling of various natures, interaction can induce emergent spin-orbit coupling density wave even when time-reversal symmetry is intact. This density wave order is different from standard time-reversal breaking spin- or orbital density wave. We apply this idea to explain the enigmatic 'hidden order' phase in heavy fermion URu_2Si_2 as well as an unknown gapped quasiparticle state observed in two-dimensional electron gases, such as surface state of $BiAg_2$.

Introduction

The formation of order parameter, due to either 'spontaneous' broken symmetry or symmetry invariant, leads to new phases of matter. In a broken symmetry state, the emerging order parameter relies incipiently on the good quantum number that defines the 'parent Hamiltonian' or the Hamiltonian of the non-ordered state. Among the mostly studied broken symmetry states, we have spin-density wave, charge density wave, orbital density wave, superconductivity in which the broken symmetries are spin, charge, orbital of the electrons, or gauge symmetry, respectively.[1] Recently, it is realized both theoretically and experimentally that the symmetry properties of the

crystal and electronic wave functions can conspire in such a way that novel topological order can emerges in condensed matter systems. For symmetry invariant orders, we have the quantum Hall states of various types,[2] and the recently discovered topological insulators[3] which are defined by the topological Chern number obtained by wave function properties. In the latter cases spin-orbit coupling (SOC) often plays an important role.

SOC in condensed matter has many origins, and thus has characteristic implications on the ground state of the system. In heavy elements, the interplay between Hund's coupling (J_H) (governed by the Pauli's exclusion principle and Coulomb interaction) and SOC (λ) gives rise to either $\boldsymbol{L.S}$ coupling or $\boldsymbol{j}$-$\boldsymbol{j}$ coupling. In systems having $J_H > \lambda$, total spin $\boldsymbol{S} = \Sigma_i \boldsymbol{s}_i$ and angular momentum $\boldsymbol{L} = \Sigma_i \boldsymbol{l}_i$ (where $\boldsymbol{s}_i$, and $\boldsymbol{l}_i$ are the spin and angular momentum for the i^{th} electron) are formed prior to the inclusion of SOC. With turning on of SOC, the dipole term $H_{SOC} = \lambda \boldsymbol{L.S}$ appears. On the other hand, for systems such as actinide *f*-electron materials,[4] in which SOC is larger than the effective Coulomb interaction, it is instructive to write down the Hamiltonian in the $\boldsymbol{j}$-$\boldsymbol{j}$ coupling scheme. In this case, the eigenstates are defined by the total angular momentum $\boldsymbol{j}_i = \boldsymbol{l}_i + \boldsymbol{s}_i$, owing to the SOC. We explore below that when the Coulomb interaction is included to the $\boldsymbol{j}$-$\boldsymbol{j}$ coupled states, various emergent order parameters may develop in the SOC channel which break symmetries in various ways.

Furthermore, in systems with inversion asymmetry in the bulk or in the structure, one can obtain SOC in which the spin of electron becomes locked to their motion (defined by band velocity $\boldsymbol{v}$ or wave vector $\boldsymbol{k}$) via relativistic effect. As Dresselhaus[5] pointed out that in zinc-blende-like crystal structure, such as GaAs, the electric field generated

by the lack of inversion symmetry appears as magnetic field in the reference frame of the moving electron. Similarly, in quasi-two-dimensional (2D) semiconductor structures such as quantum wells (QWs), surface states, or in heterostructures, the absence of inversion symmetry along the *z*-axis gives rise a similar relativistic magnetic field effect experienced by the moving electrons on the 2D plane. This is known as Rashba SOC coupling.[6] Finally, in three dimensional (3D) bulk topological insulator, an effective magnetic field appears on the 2D surface state owing to the presence of inversion symmetry and time-reversal symmetry.[7] The effective magnetic field experienced in the moving reference frame of the moving electron can be represented as

$$\begin{aligned} \boldsymbol{B}_{eff} &= (\alpha/g\mu_B)\,(k_y \boldsymbol{i} - k_x \boldsymbol{j}), \quad \text{Rashba SOC on 2D electron gas, heterostructure etc.} \\ &= (\beta/g\mu_B)\,(k_y \boldsymbol{i} + k_x \boldsymbol{j}), \quad \text{Dressenhaus SOC on zinc-blende-like structure} \\ &= (\gamma/g\mu_B)\,(k_x \boldsymbol{i} + k_y \boldsymbol{j}), \quad \text{SOC on 2D surface of topological insulator.} \end{aligned} \tag{1}$$

Here α, β, γ are the SOC constants and g, μ_B are the electron's g factor and Bohr magneton, respectively. This effective magnetic field couples to the electron spin (defined in terms of Pauli matrices $\boldsymbol{\sigma}$ here) via a Zeeman term $H_{SOC} = \boldsymbol{B}_{eff} \,.\, \boldsymbol{\sigma}$. In such cases, the spin degeneracy of the non-interacting electronic dispersion is lifted and the electronic state (defined by the quantum number $\boldsymbol{k}$ in translational invariant system) are assigned with a specific spin-orientation which is called helicity quantum number $v = \pm$.

Here we will study the situations where the translational symmetry (or more generally any other symmetry such as four-fold symmetry) is broken due to Fermi surface (FS) nesting or by other means in the parent helical system. We demonstrate that in these cases a novel order parameter in the SOC channel develops which we will be calling

SOC density wave or staggered SOC. We will focus mainly on two situations as ***j-j*** type and Rashba-type SOC coupling, however the theory can be easily generalized to other SOCs. The SOC density wave order parameter within ***j-j*** will be shown in details to be responsible for the mysterious 'hidden order' state of heavy fermion metal URu_2Si_2.[4] Finally, the Rashba SOC density wave will be shown to develop in the surface state of $BiAg_2$ heterostructure[8,9].

SOC density wave as 'hidden-order' state in URu_2Si_2

The actinide heavy fermion metal URu_2Si_2 offers an unique opportunity to study many emergent phenomena of condensed matter physics because it naturally hosts diverse quantum mechanical phases including Kondo physics, antiferromagnetism, exotic 'hidden-order' state, and superconductivity.[10] Most interestingly, the 'hidden order' parameter responsible for a second-order phase transition at T_h = 17.5 K has remained a long-standing mystery despite three decades of monumental efforts.[4] The conventional spin-, charge, orbital density wave models have failed to explain the salient experimental signatures of this phase.

Owing to strong SOC coupling dominating over the Coulomb interaction, the ***j-j*** SOC commences in these systems which renders into Γ_6 atomic states in the low-energy states as labelled by m_J = ±5/2, ±3/2, and ±1/2 where m_J is the *z*-component of the total angular momentum $\boldsymbol{J}$. [Here σ = ± is the pseudospin index which is equivalent to the helicity index v = ± defined above for other forms of SOC.] Furthermore, we have demonstrated earlier by first-principle band structure calculation [11] that, among these three doublets, m_J = ±3/2 and m_J = ±1/2 states show a remarkable FS nesting with the wave vector $\boldsymbol{Q}_h$ = (1±0.4,0,0). This nesting vector has been observed

by inelastic neutron scattering measurements (INSs),[12] quasiparticle interference (QPI) pattern as measured by scanning tunnelling microscopy/ spectroscopy (STM/S)[13] in this system. We desire to show that due to this FS instability via translational symmetry breaking with wave vector $\boldsymbol{Q}_h$, a SOC order parameter appears in the hidden order state of this system.

We start with the two orbital non-interacting Hamiltonian in the pseudospinor field $\Psi^{\dagger}_{\boldsymbol{k}} = (f_{\boldsymbol{k},3/2,+}, f_{\boldsymbol{k},1/2,+}, f_{\boldsymbol{k},3/2,-}, f_{\boldsymbol{k},1/2,-})^{\dagger}$, where $f_{\boldsymbol{k},\tau,\sigma,}$ is the annihilation operator for an electron in the orbital τ = ½ (+), 3/2 (-) with momentum $\boldsymbol{k}$ and `pseudospin' σ. In this basis the 2×2 orbital block of the Hamiltonian can be written in terms of the Pauli matrices $\boldsymbol{\tau}$ for the orbital as $h_{\tau\tau'}(\boldsymbol{k}) = \xi_{\tau\tau'}(\boldsymbol{k}).\boldsymbol{\tau}^0 + d_{\tau\tau'}(\boldsymbol{k}).\boldsymbol{\tau}$, where $\boldsymbol{\tau}^0$ is the 2×2 unitary matrix. The single-particle hopping terms are represented in the Slater-Koster formalism which gives $[\xi(\boldsymbol{k}), d^x, d^y, d^z]_{11} = [-2t(\cos k_x + \cos k_y) - \mu, -2t_1 \sin k_x, 2t_1 \sin k_y, -2t_2(\cos k_x - \cos k_y)]$, and $[\xi(\boldsymbol{k}), d^x, d^y, d^z]_{12} = [0, 0, 0, -4t_z \cos(k_x/2)\cos(k_y/2)\cos(k_z/2)]$. The time-reversal invariance implies that $h_{11}(\boldsymbol{k}) = h_{22}^{*}(-\boldsymbol{k})$ and $h_{12}(\boldsymbol{k}) = h_{21}^{*}(-\boldsymbol{k})$. The energy spectrum can be derived as $E^{\tau\sigma}(\boldsymbol{k}) = \xi(\boldsymbol{k}) + \tau\sqrt{(\sum_i |d^i{}_{12}(\boldsymbol{k})|^2)} + \sigma\sqrt{(\sum_i |d^i{}_{11}(\boldsymbol{k})|^2)}$.

SOC density wave: Now we include the interaction via incorporating the FS nesting at Q_h. In this case, the pseudospinor is doubled as $\Psi^{\dagger}_{\boldsymbol{k}} = (\Psi_{\boldsymbol{k}}, \Psi_{\boldsymbol{k}+\boldsymbol{Q}h})^{\dagger}$. In this notation, the modulated SOC interaction term can be written in general as $H_{\mathrm{SODW}} = g \sum_{\boldsymbol{k}} [\Psi_{\boldsymbol{k}} \boldsymbol{\tau}^y (\times) \boldsymbol{\sigma}^z \Psi_{\boldsymbol{k}+\boldsymbol{Q}h}]^2$, where $(\times)$ represent the tensor product and g is the contact interaction strength. We fix the pseudospin orientation along z direction and the orbital part is taken to be $\boldsymbol{\tau}^y$, which allows the product to be time-reversal invariant. We have shown earlier [11] that this is the only term, among 16 different possible terms, which open a gap. Constrained by the point ground symmetry, which belongs to E_g for the body

centered crystal structure of URu_2Si_2, we define an itinerant gap vector as $\boldsymbol{b}^y(\boldsymbol{k})=2ig\Delta\sin(k_x)\boldsymbol{\tau}^y$ and $\boldsymbol{b}^y(\boldsymbol{k})=2ig\Delta\sin(k_y)\boldsymbol{\tau}^y$ for the nestings $\boldsymbol{Q}^x{}_h=(1\pm0.4,0,0)$ and $\boldsymbol{Q}^y{}_h=(0,1\pm0.4,0)$, respectively. Substituting the anisotropic gap function, and employing the standard mean-field decomposition to the interaction Hamiltonian defined above, we obtain the hidden order parameter as $M^y = <\sum_{\tau\tau'\sigma\sigma'} f_{\boldsymbol{k},\tau,\sigma}[\boldsymbol{b}^y(\boldsymbol{k})(\times)\boldsymbol{\sigma}^z]$ $f_{\boldsymbol{k}+\boldsymbol{Q}h,\tau',\sigma'}>$.

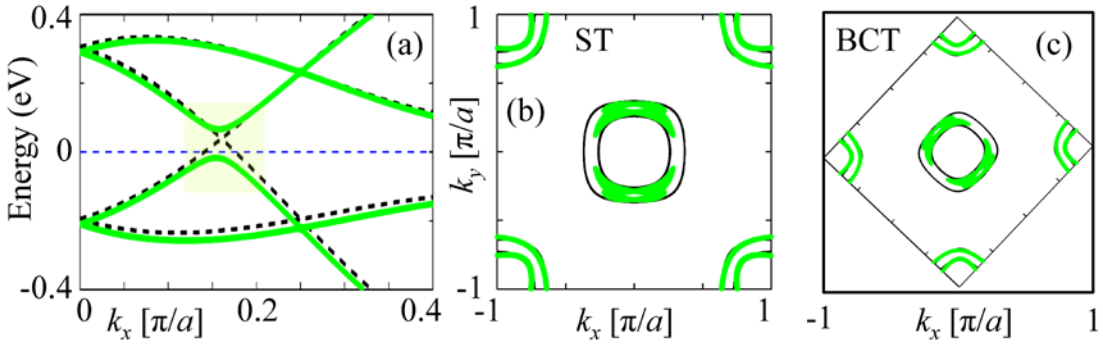

Figure 1 - Quasiparticle state in the presence of *j-j* SOC density wave in URu_2Si_2. (a) Dispersion spectrum for non-interacting case (black dashed line) and with SOC density wave (green solid line) along (100) direction. (b) Corresponding FS evolution for the unidirectional nesting $\boldsymbol{Q}^x{}_h$ = (1±0.4,0,0). The Brillouin zone is chosen here to be simple tetragonal (ST) while the actual Brillouin zone of this system is body centered tetragonal (BCT). (c) The FS is rotated by 45^o to mimic the BCT unit cell.

In Fig. 1, we show how the quasiparticle gap opening occurs due to the turning on of this SOC density wave order. The band-crossings of the electronic states before the hidden order is marked by four-fold degeneracy (two orbitals and two spins). One such degenerate Dirac point is shown in Fig.1(a) along (1,0,0) direction, which becomes gapped in the hidden order state. The corresponding FS is demonstrated in Fig. 1(b).

We postpone a detailed calculation of other aspects of the SOC density wave for this system for future study. However, here we comment on some of the proposed

research. (1) Since the SOC gapping occurs in the particle-hole channel, we can define a SOC susceptibility, in analogy with the spin susceptibility. Within random-phase approximation, we expect to observe a resonance mode at or slightly below the quasiparticle gap energy. However, this mode is time-reversal invariant, and thus one requires to perform a polarized neutron scattering measurement to detect it. (2) Muon spin-resonance (μSR), nuclear magnetic resonance (NMR) can also be able to detect the SOC density wave, in which one requires to pay attention to the Lande '*g*' value to be able to distinguish a SOC mode from a spin mode. Because g=2 for spin, and g~0.8 for J=5/2 state of the present *f*-electron system. (3) Most interesting aspect of the SOC density order is that it is time-reversal invariant. Therefore, any time-reversal invariant perturbation such as pressure will not be able to destroy it. On the other hand, time-reversal breaking perturbation such as magnetic field will destroy this order. This fact is very much similar to the situation of topologically protected state. Since the quasiparticle states are gapped by this order parameter, thermodynamically one requires a finite value of magnetic field determined by $\Delta=\chi B^2$, where χ is the SOC susceptibility, to destroy the order. In what follows, we expect a quantum critical point (QCP) for the SOC density wave as a function of magnetic field. These properties as a function of pressure and magnetic field are in remarkable agreement with experimental phase diagram of URu_2Si_2.[14,15]

Rashba spin-orbit coupling density wave

Next we discuss the Rashba SOC density wave in 2DEG, based on a similar calculation. Formalism for Rashba spin-orbit spit electronic state is well-know and can be found for example in Ref. [6,16]. Here we generalize the equations to a lattice model. In this case, we start out with a single particle free-fermion state depicted as

$H_0 = \xi(\boldsymbol{k}) = 2t[\cos k_x + \cos k_y] - \mu$, where t is the nearest-neighbor hopping parameter and μ is the chemical potential. Writing the Rashba SOC introduced above in Eq. (1) within the lattice model we obtain $H_R = i\alpha(\sigma_x \sin k_y + \sigma_y \sin k_x)$. The Rashba SOC splits the bare dispersion in two spin-polarized state which are denoted by helical index $\nu=\pm$. Since our starting Hamiltonian is defined within more exotic quantum number, rather than typical spin and momentum quantum numbers, once the interaction is introduced the obtained order parameter should also be defined in this notation.

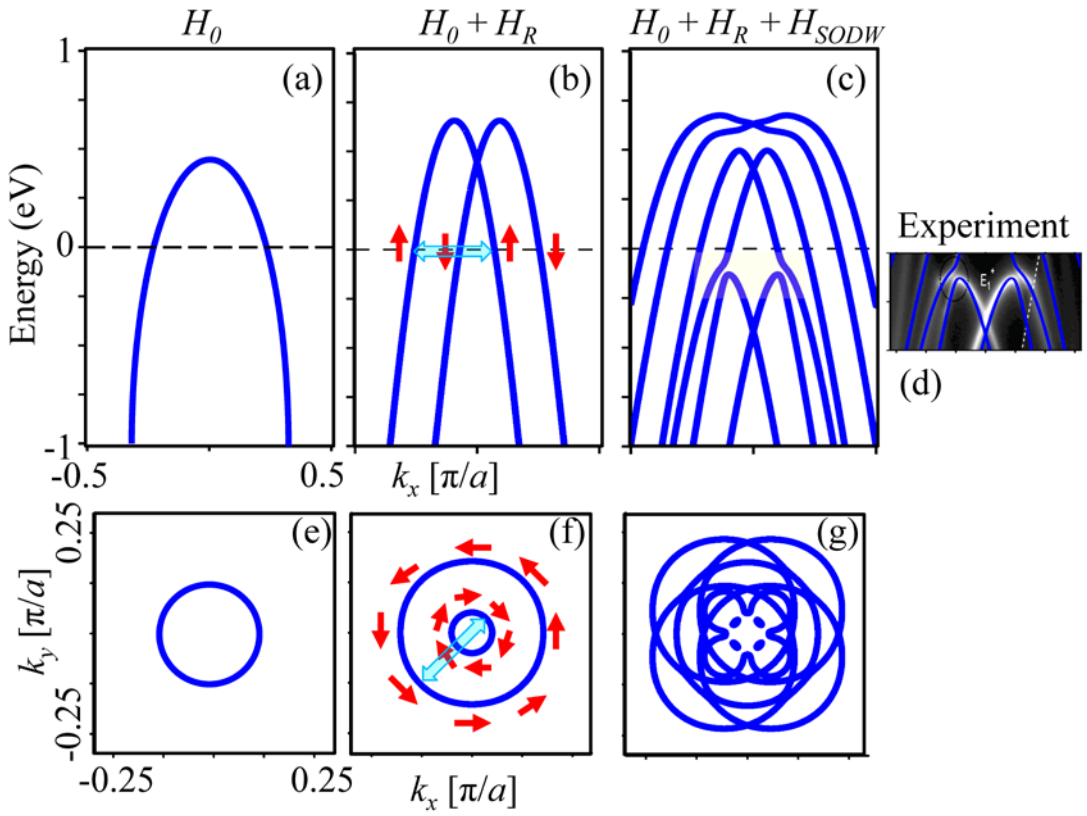

Figure 2 - Quasiparticle state in the presence of Rashba SOC density wave in $BiAg_2$ surface state. (a) Dispersion for non-interacting Hamiltonian without any SOC. (b) Corresponding dispersion with Rashba SOC. (c) The evolution of dispersion after including the Rashba SOC density wave order. (d) The theoretical results (blue lines) are compared with experimental data for BiAg2, plotted in black to white colormap.[8,9] (e)-(g) FS maps for the three cases discussed in their corresponding upper panels.

The obtained band-structure and FS are shown in Fig. 2(b) and 2(f), respectively. By calculating the susceptibility, we can immediately show that there exists a prominent

FS nesting between the two FS pieces at $\boldsymbol{Q}$=(0.115,115,0)π, as depicted by light blue arrow. Based on this nesting instability, we derive the mean-field expression for the Rashba SOC density wave order. The four-component Nambu-Gor'kov helical field for the translation breaking state is $\Psi^{\dagger}_{\boldsymbol{k}} = (\psi_{\boldsymbol{k},v}, \psi_{\boldsymbol{k},v'}, \psi_{\boldsymbol{k}+\boldsymbol{Q},v}, \psi_{\boldsymbol{k}+\boldsymbol{Q},v'})^{\dagger}$, where $v'=-v$**.** In this notation the two-body interaction in the singlet-channel can be characterized by a contact potential g, and the corresponding interaction Hamiltonian is $H_{SODW} = g\psi^{\dagger}_{\boldsymbol{k},v}\psi_{\boldsymbol{k},v'}\psi^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q},v}\psi_{\boldsymbol{k}+\boldsymbol{Q},v'}$. Finally, in order to reduce the above-derived action term into a ordered fermionic problem, we decouple the four-body interaction term by introducing the auxiliary SOC field $\Delta(\boldsymbol{k}) = g\psi^{\dagger}_{\boldsymbol{k},v}\psi_{\boldsymbol{k}+\boldsymbol{Q},v'}$.

The SOC order gaps out the quasiparticle states and the Fermi surface as demonstrated in Fig. 2(c), 2(d), and 2(g). It is important to note that despite the anisotropic gap features, the Kramers degenerate state at Γ-point remains intact, implying that the order parameter is not a standard spin-density wave, rather an exotic SOC density wave. Recently, such quasiparticle gapping is observed via angle-resolved photoemission spectroscopy on the surface state of $BiAg_2$,[8,9] and our results are in excellent agreement with the data, as shown in Fig. 2(g).

Conclusions

In this paper, we have introduced the general idea of SOC density wave that can appear due to electron-electron interaction on the systems whose ground state is defined by SOC wave numbers. We have demonstrated that in these systems where SOC renders exotic quantum number such as total angular momentum, pseudospin, or helical states, a typical spin-, or orbital density wave is unlikely unless time-reversal symmetry is broken. On the other hand, when time-reversal symmetry is intact, a

novel SOC density wave can arise. We have applied the model to heavy fermion URu_2Si_2[4,10,11] as well as to the 2DEG systems,[8,9] and tested our theory with their experimental data.

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