Relationship between exceptional points and the Kondo effect in f-electron materials

Yoshihiro Michishita, 1 Tsuneya Yoshida, 2 and Robert Peters 1

1 Department of Physics, Kyoto University, Kyoto 606-8502, Japan
2 Department of Physics, Tsukuba University, Tsukuba, Japan

We study the impact of nonhermiticity due to strong correlations in f-electron materials. One of the most remarkable phenomena occurring in nonhermitian systems is the emergence of exceptional points at which the effective nonhermitian Hamiltonian becomes non-diagonalizable. We here demonstrate that Kondo temperature is related to the temperature at which exceptional points appear around the Fermi level.

For this purpose, we study the periodic Anderson model with local and nonlocal hybridization in the insulating and metallic regimes. By analyzing the effective nonhermitian Hamiltonian, which describes the single-particle spectral function, and the temperature dependence of the screening of the magnetic moment, from which the Kondo temperature can be found, we show that exceptional points appear at the temperature at which the magnetic moment is screened. These results suggest that the well-known crossover between localized and itinerant f electrons in f-electron materials is related to the emergent exceptional points in the single-particle spectral function.

I. INTRODUCTION

Recently, the phenomena described by an effective nonhermitian Hamiltonian are intensively studied especially in the context of artificial quantum systems.6,7,8,9,10 Effective nonhermitian Hamiltonian induces novel topological phases and the novel phenomena such as anomalous edge states9,11,12, unusual quantum critical phenomena13,14, unidirectional invisibility15,16, chiral transport17,18, and enhanced sensitivity19,20.

In open quantum systems, e.g. in cold atomic systems, it is possible to derive an effective nonhermitian Hamiltonian under certain conditions even though the Hamiltonian describing the total system is hermitian.21,22,23 However, certain conditions, such as the postselection or a $PT$-symmetric setup, which are necessary to obtain an effective nonhermitian Hamiltonian become more difficult as the system becomes larger. Thus, experiment about nonhermitian phenomena in the artificial quantum systems are especially done in one-dimensional or small systems. However, in two-dimensional (2D) or three-dimensional (3D) systems, it becomes much more difficult to implement these conditions because of technical problems and difficulty concerning postselection.

On the other hand, strongly correlated systems in equilibrium have not been considered to be related to nonhermitian systems until recently. Generally, the band structure of strongly correlated materials, which is given by the single-particle spectral function, is renormalized and broadened by the self-energy $\Sigma(\omega)$. The spectral function in equilibrium can always be written as $A(\omega) = -\frac{1}{\pi} \text{Im} \left\{ \text{tr} (\omega - H_{\text{eff}})^{-1} \right\}$, where $H_{\text{eff}} = H_0 + \Sigma$. $H_0$ is the non-interacting part of the Hamiltonian, and $\Sigma$ is the self-energy. The imaginary part of the self-energy can be related to the finite life time of quasi-particles in the strongly correlated material. Until recently, the effect of the imaginary part of the self-energy has been merely considered as a broadening of the spectral function. However, Kozii and Fu have shown that because of the imaginary part of the self-energy, the effective Hamiltonian describing the spectral function is nonhermitian, which can generate exotic phenomena3,24,25. For example, the effective nonhermitian Hamiltonian can be defective at an exceptional points (EP) in the Brillouin zone (BZ), where it cannot be diagonalized. At these EPs, a topological number can be defined. Moreover, different EPs in the BZ might be connected by bulk Fermi arcs which could be observed in ARPES spectroscopy. These nonhermitian phenomena which can be seen in the equilibrium state of strongly correlated materials are now studied vigorously. They also hold the potential to explain the pseudo-gap in cuprate superconductors or quantum oscillations in topological Kondo insulator SmB$_6$ and YbB$_{12}$.29,30,31

We note here that to obtain an effective nonhermitian Hamiltonian describing the spectral function, postselection or other difficult experimental setups are not necessary. Therefore, it seems reasonable that certain nonhermitian phenomena in bulk 2D or 3D systems can be observed more easily in strongly correlated materials than in artificial quantum systems.

It has been shown that a minimal model which can include exceptional points in the spectral function must consist of at least two hybridized bands which include different self-energy. A model exactly describing this situation is the periodic Anderson model (PAM), which consists of an uncorrelated band which is hybridized with a strongly correlated band. This model is generally used to describe f-electron materials, where the uncorrelated band describes conduction (c) electrons and the correlated band describes $f$-electrons. Because of the strong correlations, many remarkable phenomena can be observed in $f$-electron materials, such as magnetism, unconventional superconductivity, quantum criticality, and the Kondo effect.

In this work, we study nonhermitian phenomena induced by the self-energy in the Kondo regime of 2D $f$-electron materials by using the dynamical mean field the-
ory (DMFT) combined with the numerical renormalization group (NRG)\cite{35,37}. We elucidate the relationship between the appearance of exceptional points (or exceptional loops) in the spectral function and the transition from a metal at high temperatures to the Kondo insulator or the heavy fermion state at low temperature. Thus, the appearance of the exceptional points corresponds to the transition from localized f-electrons to itinerant f-electrons. We note that the emergence of a bulk Fermi arc has been reported for a Kondo lattice model\cite{31} and a periodic Anderson model which is a slightly different model\cite{38}.

The rest of this paper is organized as follows. In Sec II we introduce the models that we use in this work and we briefly explain about the exceptional points and their nonhermitian topological numbers in strongly correlated electron systems. In Sec III we show the numerical results by DMFT/NRG about the Kondo temperature and electron systems. In Sec IV, we conclude this paper.

II. MODELS AND NON-HERMITIAN PROPERTIES IN SCES

To analyze the exceptional points and the Kondo effect in f-electron materials, we use the periodic Anderson model,

\[
\mathcal{H} = \sum_{\mathbf{k}} \left( \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \epsilon_{f\mathbf{k}} f_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma} + (V_{i/f})_{\sigma\sigma'} (f_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma'} + h.c) \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}
\]

(1)

\[
\epsilon_{c/f} = -2t_{c/f}(\cos(kx) + \cos(ky)) + \mu_{c/f}
\]

(2)

\[
V_i = V \delta_{\sigma\sigma'}
\]

(3)

\[
V_p = V(\sigma \cdot \sin \mathbf{k}) \quad (\sin k = (\sin k_x, \sin k_y))
\]

(4)

where \(c_{\mathbf{k}\sigma}^\dagger, f_{\mathbf{k}\sigma}^\dagger\) are annihilation (creation) operators of the c- and f-electrons for momentum \(\mathbf{k}\) and spin-direction \(\sigma\). \(t_{c,f}\) are the inter-site hopping strengths for the c- and f-electrons. For simplicity we assume a two-dimensional square lattice.

\(\mu_{c/f}\) are the chemical potentials for the c- and f-orbitals. \(V_{i/f}\) describes a local and nonlocal hybridization between the c- and f-orbitals, respectively. Throughout this paper, we fix \(t_f = \pm 0.05t_c, \mu_c = 0, \mu_f = -1.0, U = 2.0\) and use \(t_c = 0.8\) as unit of the energy. Using this model, we analyze the relation between the Kondo effect and the emergence of exceptional points. We will focus on three different cases: \(t_f = -0.05t_c\) with a local hybridization, \(t_f = -0.05t_c\) with p-wave hybridization, and \(t_f = 0.05t_c\) with local hybridization.

In Figs. 1 and 2 we show the momentum resolved spectral functions and the Fermi surfaces of the different regimes. At high temperature, the f-electrons are localized and do not hybridize with the c-electrons as shown in Fig. 1(a) and Fig. 2(a). Below the Kondo temperature, f-electrons become itinerant and hybridize with the c-electrons, which results in strong changes in the spectral function. Figure 1(b) shows the spectral function of the Kondo insulator having a gap at the Fermi energy. Figure 1(c) shows the spectral function of the metallic regime with local hybridization, and Fig. 1(d) the spectral function of the p-wave hybridization case. Corresponding to these spectral functions, we show the spectral weight at the Fermi energy in Fig. 2. At high temperatures, Fig. 2(a), we only find the c electrons at

FIG. 1: (a)-(d) : The momentum resolved spectral functions for the Kondo insulator, the heavy-fermion state, and metallic state with p-wave hybridization for \(V=0.4\). Fig. 1(a) shows a high temperature spectral function, \(T=0.13\) of the Kondo insulator. Fig. 1(b)-(d) are spectral functions at low temperatures, for \(T=0.0005\), for the Kondo insulator, the heavy-fermion state, and the nonlocal hybridization cases, respectively.

FIG. 2: (a)-(d) : The momentum resolved spectral functions at \(\omega = 0\) corresponding to the spectral functions shown in Fig. 1. In (d), we have enhanced the visibility of the Fermi surface by changing the color.
the Fermi energy. At low temperatures, all three cases have very different Fermi surfaces. The Kondo insulating state, shown in Fig. 2(b), has no spectral weight at the Fermi energy. The heavy-Fermion state, Fig. 2(c), shows the Fermi surface corresponding to the metallic state. Finally, the metallic state for the $p$-wave hybridization has a point-like Fermi surface.

We employ the dynamical mean field theory (DMFT) combined with the numerical renormalization group (NRG) to calculate the physical properties in these models. DMFT takes local fluctuations fully into account by self-consistently solving the mean field equations. The lattice Hamiltonian is thereby mapped onto a quantum impurity model. DMFT neglects nonlocal fluctuations. Even though nonlocal fluctuations might not be small in 2D systems and even crucial for the magnetic state, they might be less important for the Kondo effect and the emergence of exceptional points. Furthermore, all shown results remain correct in three-dimensional systems, where nonlocal fluctuations are weaker compared to the 2D system. To solve the quantum impurity model, we use the NRG, which calculates low energy properties by iteratively discarding high-energy states. It has been shown that NRG is a very reliable tool at low temperature.

Before moving to the numerical results, we briefly introduce exceptional points in strongly correlated materials. As mentioned above, the periodic Anderson model is a minimum model for the emergence of the exceptional points. The effective nonhermitian Hamiltonian which describes the spectral function can be written by

$$H_{\text{eff}}(\omega) = \begin{pmatrix} \epsilon_c(k) & V(k) \\ V(k) & \epsilon_f(k) - \Sigma(\omega) \end{pmatrix}$$

$$= h_0 1 + h_1 \sigma^z - V(k) \sigma^x$$

$$h_0 = (\epsilon_c(k) + \epsilon_f(k) + \Sigma(\omega))/2$$

$$h_1 = (\epsilon_c(k) - \epsilon_f(k) - \Sigma(\omega))/2$$

$$E_{\pm} - h_0 = \pm \sqrt{h_1^2 + V^2(k)}$$

$$= \pm \left\{ \left( \frac{(\epsilon_c(k) - \epsilon_f(k) - \text{Re}\Sigma(\omega))^2}{4} + V^2(k) - \frac{(\text{Im}\Sigma(\omega))^2}{4} \right) \right. + \left. \frac{i}{2} \left( \text{Im}\Sigma(\omega) \left( \epsilon_c(k) - \epsilon_f(k) - \text{Re}\Sigma(\omega) \right) \right) \right\}^{\frac{1}{2}}$$

where $E_{\pm}$ are the eigenvalues of the effective Hamiltonian. This effective nonhermitian Hamiltonian becomes nondiagonalizable when the following conditions are satisfied:

$$\epsilon_c(k) - \epsilon_f(k) - \text{Re}\Sigma(\omega) = 0$$

$$\text{Im}\Sigma(\omega)/2 = V(k).$$

These points (sometimes loops) in the momentum space, for which the nonhermitian Hamiltonian cannot be diagonalized, are called exceptional points. Moreover, we can define a winding number on these points which reads

$$W = \oint_{\text{EP}} \frac{dk}{2\pi i} \cdot \nabla_k \log \det \mathcal{H}(k).$$

FIG. 3: (a)-(d): The temperature dependence of the imaginary and the real part of the self-energy calculated by DMFT/NRG. (a) and (b) shows $V=0.36$ and $t_f = -0.05t_c$ with the local hybridization. (c) and (d) shows $V=0.36$ and $t_f = -0.05t_c$ with the local hybridization. The black lines in (a) and (c) describe the condition $\text{Im}\Sigma(\omega)/2 = \max|V(k)|$ and the black lines in (b) and (d) describes the conditions of Eq. (10) and $\omega - \text{Re}(h_0) = 0$.

A $W \neq 0$ exceptional point is topologically stable because $W$ does not change unless the exceptional point is annihilated with another one.

We note that, in strongly correlated materials, the effective nonhermitian Hamiltonian is introduced for describing the spectral function. Therefore, when $h_0$ is not small, the spectral weight at the exceptional points is small and might only have a little effect on observable phenomena. We will thus distinguish the exceptional points with $\text{Re}(\omega - h_0) \simeq 0$ from the exceptional points when $|\text{Re}(\omega - h_0)|$ is large. In this paper, we call the former "exceptional points (EPs)" and the later "irrelevant exceptional point (iEP)." In short, iEPs have less spectral weight and therefore are less relevant to the physical phenomena than EPs.

In Fig. 3 we show an example of the temperature dependence of the self-energy calculated by DMFT/NRG. For the local hybridization case $V=0.36$, in Fig. 3(a)(b), the condition for the EPs is Eqs. (10) and (11). For the systems with local hybridization, Eq. (11) can be satisfies for all $k$ in BZ and therefore the iEPs can emerge at $\omega$ where the imaginary part of the self-energy crosses the black line. For the EPs, one more condition $\text{Re}(\omega - h_0) \simeq 0$ is needed and this is satisfied at the point where the black line $\epsilon_c(k)/4 + \epsilon_f(k) - \text{Re}\Sigma(\omega)$ crosses to the real part of the self-energy. In this case, only around $\omega = 0$, the EPs can emerge.
FIG. 4: (a)-(f): Comparison between the Kondo insulator, the heavy-fermion state, and the metallic state with p-wave hybridization for different strengths of $V$. (a)-(c) show the local susceptibility. The colors in (a)-(c) correspond to the different $V$. In (a) and (c), the green, skyblue, orange and red plot is respectively for $V = 0.36, 0.4, 0.44, 0.5$. In (b), the green, skyblue, orange and red plot is respectively for $V = 0.4, 0.44, 0.5, 0.55$. (d)-(f) show the temperature and the frequency dependence of the emergence of the iEPs and the EPs. The iEPs are drawn in black plots. In (d) and (f), the cross, point, triangle, and square dots are for $V = 0.36, 0.4, 0.44, 0.5$. In (e), the cross, point, triangle, and square dots are for $V = 0.4, 0.44, 0.5, 0.55$. The EPs are drawn in color plots. We use the same color plots as (a)-(c). In (e), there seem to be several EPs for each $V$. However, these stem from the numerical error and we think the EPs at the lowest temperature are the genuine ones. In (f), the EPs still exist under the $T_{EP}$ and therefore the red, orange, and the skyblue plots exist behind the other plots. (g)-(i) show momentum resolved spectral functions at the Fermi energy around for $T_{EP}$. (g) is for $V=0.36, T=0.0035$. (h) is for $V=0.4, T=0.0007$. (i) is for $V=0.36, T=0.0025$. The parameters are $U=2, t_c=0.8, t_f=-0.04, \mu_c=0, \mu_f=-1.0$. We draw the green line as the loop formed by the exceptional points in (g)(h). We also draw the red and blue plots as the EPs whose vorticity is $\pm 1/2$.

For nonlocal hybridization case $V=0.36$ in Fig. 3(c)(d), Eq. (11) can be satisfied at $\omega$ where the imaginary part of the self-energy is larger than the black line. Therefore, the iEPs and the EPs can appear more easily in this case as we will show in the next section. In the next section, we show that the temperature at which the EPs appear ($T_{EP}$) correspond with the Kondo temperature in $f$-electron materials by numerical calculation.

III. RELATION BETWEEN KONDO TEMPERATURE AND $T_{EP}$ IN $f$-ELECTRON MATERIALS

In Fig. 4(a)-(c), we show the magnetic moment of the $f$-electrons (contribution of the $f$-electron to the magnetic susceptibility, $T\chi^f(T)$). Around the Kondo temperature, the magnetic moment changes from 0.25 at high temperatures to 0 at low temperatures, which corresponds to the Kondo screening. The magnetic susceptibility in Fig. 3(a)-(c) is thereby calculated by applying a tiny magnetic field to the system and calculating the induced magnetic polarization of the $f$-electrons. There-
fore, we can estimate the Kondo temperature from Fig. 4 (a)-(c) for all three systems. Furthermore, we can use the self-energies obtained by DMFT/NRG, to analyze the emergence of EPs in the spectrum. We show these EPs in Fig. 4 (g)-(i), where we plot EPs with large eigenvalue \( \text{Re}(\omega - h_0) \) as black dots and EPs with \( \text{Re}(\omega - h_0) \approx 0 \) as colored dots corresponding to the colors of the hybridization in Fig. 4 (a)-(c). We see that EPs with \( \text{Re}(\omega - h_0) \approx 0 \) only appear at certain temperature for the local hybridization cases and appear below certain temperature for the nonlocal hybridization case. Finally, we show the Fermi surfaces of the models at the temperature in Fig. 4 (g)-(i).

Comparing the temperature at which EPs with \( \text{Re}(\omega - h_0) \approx 0 \) appear and the Kondo temperature, we see that both temperatures agree for all analyzed cases. In Fig. 4 (d)-(f), we can also see many iEPs with large \( \text{Re}(\omega - h_0) \), which appear at almost all temperatures. These iEPs are mainly related to the imaginary part of the self-energy away from the Fermi energy, particularly in the Hubbard bands, which are irrelevant to the Kondo effect. The Kondo effect in \( f \) electron materials occurs near the Fermi energy. The imaginary part in the Hubbard bands is nearly temperature independent. On the other hand, the self-energy at the Fermi energy strongly changes around the Kondo temperature, which is responsible for the emergence of EPs with \( \text{Re}(\omega - h_0) \approx 0 \) at the Fermi energy.

Fig. 4 (g)-(i) show the Fermi surfaces at \( T_{EP} \) for the local hybridization cases and at \( T < T_{EP} \) for the \( p \)-wave hybridization cases. For the local hybridization cases, the EPs appear only at \( T_{EP} \) and form a closed loop in the BZ. For the Fermi surface including the loop, we note that the vorticity is not well defined and that they are different from the symmetry-protected exceptional ring [10-12]. Therefore, this loop is considered to break down to the exceptional points and the bulk Fermi arc by considering the \( k \)-dependence of the self energy. For the \( p \)-wave hybridization cases, the EPs appear as single points in the spectrum and have nonzero vorticity. The exceptional points with different vorticity are connected by Fermi arcs. The momentum of these EPs changes satisfying Eq. (10) at different temperatures and at the zero temperature, they merge and disappear.

IV. CONCLUSION AND DISCUSSION

In summary, we have shown a relation between the Kondo temperature and the emergence of exceptional points for the Kondo insulator and the metallic state with a local hybridization, and the semimetallic state with a \( p \)-wave hybridization in the 2D periodic Anderson model by DMFT/NRG. Around the Kondo temperature, \( f \)-electrons changes from localized state to the itinerant state when lowering temperature. Thus, the emergence of EPs is a sign for the crossover between localized and itinerant \( f \)-electrons. For the local hybridization cases, EPs form an loop in BZ and appear only exactly at \( T_{EP} \) related to the Kondo temperature. For the \( p \)-wave hybridization, bulk Fermi arcs appear between the EPs with different vorticity below \( T_{EP} \). They are stable until they merge and disappear at zero temperature.

We can naturally expect that the relation between \( T_{EP} \) and the Kondo temperature hold for the three-dimensional systems because the DMFT results become more accurate for higher dimensions. The band structure of the three-dimensional systems can be understood by stacking the spectral function of two-dimensional systems, indicating that the presence of robust exceptional loops in three-dimensional BZ.

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