Quantized Berry phases of Kondo insulators

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Abstract. Quantized Berry phases proposed as local order parameters for gapped quantum liquids at zero temperature are studied to detect the Kondo singlet phase which is known as a theoretical prototype of the Kondo insulators. We deal with the Kondo lattice model and the periodic Anderson model as two basic models for heavy fermions. We show that the Berry phase is actually quantized as trivial or non-trivial value, i.e., 0 or $\pi$, and analytically obtained both in the strong coupling limit of the Kondo lattice model and in the weak coupling limit of the periodic Anderson model. In addition, the Heisenberg Kondo lattice model is studied numerically by the quantized Berry phase.

The topological feature which does not depend on the detail of systems has been attracting attention in the condensed matter physics. One of most remarkable examples is a quantum Hall effect, where a topological invariant known as the Chern number has been quantized and observed experimentally. In addition to the Chern numbers, the Berry phases can also be quantized. Quantized Berry phases have been used to classify quantum phases in gapped systems$^1$ and gapless systems$^2$. Especially, for gapped systems including integer quantum Hall systems, the topological quantities have the advantage that they are invariant against small perturbations such as randomness unless the gap closes. In other words, they are topologically protected due to the gap.

To classify phases, not only correlation functions corresponding to phases but also the string order parameter$^3$, entanglement entropy or concurrence$^4$, and Lieb-Schulz-Mattis twist operators$^5$ have been studied. The Berry phase is proposed as a new order parameter, which has the advantage that the value is quantized and topologically protected. Quantized Berry phases for gapped systems have been studied to characterize spin systems$^6$, spin ladder with ring exchange$^7$, surface states in semiconductors$^8$, and $t-J$ models$^9$. As a result, Berry phases are quantized to the following two values: a trivial value 0 or nontrivial value $\pi$. Since each Berry phase is defined by a local SU(2) twist, it has been used as a local order parameter. When a localized singlet or dimer is formed on a link, the non-trivial Berry phase is obtained on the corresponding link. When singlets can move in $t-J$ models, Berry phases defined by a multiplet below the spin gap give spatially uniform $\pi$ value, which corresponds to an itinerant singlet picture. Not only singlet but also plaquette singlet can be identified$^7$. However, the quantized Berry phase used as a local order parameter is not applied to the Kondo singlet phase.

The Kondo singlet phase or the spin liquid phase$^{10}$ is known as a theoretical prototype of the Kondo insulators. The singlet ground state is smoothly connected to the strong coupling limit where localized singlets are formed. A product state of the localized singlets captures...
essential physics of the insulating phase which has a charge gap and a spin gap.

In this paper, one of motivations is to detect a Kondo singlet with the quantized Berry phase. We deal with the Kondo lattice model (KLM) and the symmetric periodic Anderson model (PAM) as two basic models for heavy fermions. The Kondo singlet phase exists in both KLM and PAM. In the present study we will concentrate on the case of a half-filled conduction band. The orbitally non-degenerate PAM is given by

\[ H_{\text{KL}} = H_t + H_U, \]

where

\[ H_t = -t \sum_{(i,j)\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}), \]

\[ H_U = \sum_i \left[ v (c_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger c_{i\downarrow}) + U(f_{i\uparrow}^\dagger f_{i\uparrow} - 1/2)(f_{i\downarrow}^\dagger f_{i\downarrow} - 1/2) \right]. \]

After the Schrieffer and Wolff transformation[11], the KLM, where each \( f \) orbital is occupied by a single electron, is obtained as \( H_{\text{KL}} = H_t + H_J \), with \( H_J = J_K \sum_i s_i \cdot S_i \), where \( s_i = \frac{1}{2} \sum_{\sigma'\sigma} c_{i\sigma'}^\dagger \sigma \sigma' c_{i\sigma} \) are the spin-density operators of conduction electrons and \( S_i = \frac{1}{2} \sum_{\sigma'\sigma} \sigma \sigma' f_{i\sigma'}^\dagger f_{i\sigma} \) are localized spins. Here, \( \sigma \) is the vector form of the Pauli matrices. The parameters of the two models are related through \( J_K = 8v^2/U \).

Let us describe the definition of Berry phase for a parameter dependent Hamiltonian \( H(\theta) \) with the periodicity \( H(2\pi) = H(0) \). The following explanation is limited to Abelian Berry phase for degenerated ground states. The Berry phase \( \gamma \) means total phase which is gained through adiabatic modification from \( H(0) \) to \( H(2\pi) \). It is defined as \( \gamma = -i \int_0^{2\pi} A(\theta) d\theta (\text{mod}2\pi) \) with the Berry connection \( A(\theta) = \langle g_{\text{s.s.}}(\theta) | \partial_\theta | g_{\text{s.s.}}(\theta) \rangle \), where \( | g_{\text{s.s.}}(\theta) \rangle \) is the ground state of \( H(\theta) \). Discretizing the integral of \( \theta \) into \( M \) points[12] we obtain the Berry phase as \( \gamma = \lim_{M \to \infty} \gamma_M \) with \( \gamma_M = -\sum_{m=1}^M \arg \langle g_{\text{s.s.}}(\theta_m) | g_{\text{s.s.}}(\theta_{m+1}) \rangle (\text{mod}2\pi) \) and \( \theta_m = 2\pi m/M \). The periodicity \( | g_{\text{s.s.}}(\theta_{M+1}) \rangle = | g_{\text{s.s.}}(\theta_1) \rangle \) is imposed. The Berry phase is quantized due to an anti-unitary symmetry generally. The anti-unitary symmetry in the present case is the particle hole symmetry[1].

The quantized Berry phase depends on how the parameter \( \theta \) is introduced to \( H(\theta) \). It has been clarified that Berry phase can detect a spin singlet when \( \theta \) is introduced as a twisted spin exchange. The twisted spin exchange on a specified link \( i,j \) is introduced by replacing \( S_i^+ S_j^- + S_i^- S_j^+ \to e^{i\theta} S_i^+ S_j^- + e^{-i\theta} S_i^- S_j^+ \). Calculating the Berry phase on every link, we can obtain a texture pattern of the Berry phases, which reflects the property of the ground state. When we apply the Berry phase to the Kondo singlet phase, we should consider how twists are obtained a texture pattern of the Berry phases, which reflects the property of the ground state.

To detect the Kondo singlet in the KLM, we introduce the spin twist \( \theta \) into \( H_J \) at specified site \( i \) by replacing \( s_i^+ S_i^- + s_i^- S_i^+ \to e^{i\theta} s_i^+ S_i^- + e^{-i\theta} s_i^- S_i^+ \). We denote the twisted Hamiltonian as \( H_{\text{KL}}(\theta) \) and its Berry phase as \( \gamma_{s} \). Since \( H_{\text{KL}}(\theta) \) does not introduce any flux into the KLM, we can gauge out this spin twist \( \theta \), i.e., \( H_{\text{KL}}(\theta) = U(\theta)^\dagger H_{\text{KL}} U(\theta) \), with \( U(\theta) = e^{i\theta(S_i^2-1)/2} \). For the ground state \( | g_{\text{s.s.}}(\theta) \rangle = U(\theta)| g_{\text{s.s.}} \rangle \), the Berry phase is obtained as \( \gamma_{s} = \pi \) with using \( \partial_\theta | g_{\text{s.s.}}(\theta) \rangle = i(S_i^2 - 1/2)U(\theta)| g_{\text{s.s.}} \rangle \) and \( A(\theta) = i(g_{\text{s.s.}}(S_i^2 - 1/2)| g_{\text{s.s.}} \rangle = -i/2 \).

A spin twist at specified site \( i \) for \( H_{PA} \) corresponding that for \( H_{\text{KL}} \) can be introduced by replacing \( c_{i\sigma}^\dagger f_{i\sigma} + \text{h.c.} \to e^{i\theta} c_{i\sigma}^\dagger f_{i\sigma} + \text{h.c.} \). \( \theta_{s} \) is related to the spin twist \( \theta \) in \( H_{\text{KL}}(\theta) \) through the Schrieffer and Wolff transformation as \( \theta_{s} = \theta - \theta_{1} \). When we twist only spin-up electrons \( \theta = \theta_{1} \) with fixing \( \theta_{1} = 0 \), the twisted Hamiltonian \( H_{PA}(\theta) \) is obtained. We can also gauge out the spin twist: \( H_{PA}(\theta) = U'(\theta)^\dagger H_{PA} U'(\theta) \) with \( U'(\theta) = e^{i\theta} f_{i\uparrow}^\dagger f_{i\uparrow} \). For the ground state \( | g_{\text{s.s.}}(\theta) \rangle = U'(\theta)| g_{\text{s.s.}} \rangle \), the Berry phase is obtained as \( \gamma_{s} = \pi \) with using \( \partial_\theta | g_{\text{s.s.}}(\theta) \rangle = f_{i\uparrow}^\dagger f_{i\uparrow} U'(\theta)| g_{\text{s.s.}} \rangle \) and \( A(\theta) = i(g_{\text{s.s.}}| f_{i\uparrow}^\dagger f_{i\uparrow} | g_{\text{s.s.}} \rangle = 1/2 \). Here, we suppose the gapped ground state is fulfilled and unique as is in the PAM. It should be noted that the periodicities \( U'(2\pi) = U'(0) \) and \( | g_{\text{s.s.}}(2\pi) \rangle = | g_{\text{s.s.}}(0) \rangle \) are broken if we introduce a twist as \( U'(\theta) = e^{i\theta/2}(f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\uparrow}^\dagger f_{i\uparrow} - 1) \), which is a natural extension of \( U(\theta) = e^{i\theta(S_i^2-1)/2} \).
In addition to $\gamma_s$, we can introduce the twist on a link $i, j$ in $H_t$ by replacing $c^\dag_{i\uparrow}c_{j\uparrow} + c^\dag_{j\downarrow}c_{i\downarrow}$ with $e^{i\theta}c^\dag_{i\uparrow}c_{j\uparrow} + e^{-i\theta}c^\dag_{j\downarrow}c_{i\downarrow}$. We denote its Berry phase as $\gamma_t$. Although we can introduce $\theta$ in the hopping of down-spin electrons, the result is the same when we consider the singlet ground state. We can not gauge out this twist and the result is not trivial.

The meaning of the Berry phase becomes clear when we consider decoupled models in the strong coupling limit $t/J \to 0$, i.e., $H_{KL}|_{t=0} = H_J$ for the KLM. Its ground state is a direct product state of local singlets exactly, $|gs\rangle = \prod_j \left[ \frac{f_{i,j}^\dagger c_{i\uparrow} - f_{i,j}^\dagger c_{i\downarrow}}{\sqrt{2}} \right]|0\rangle$. It is trivial that $\gamma_t = 0$ and $\gamma_s = \pi$. The latter result is trivial due to the gauge transformation and is directly calculated by $|gs(\theta)\rangle = e^{-i\theta}f_{i,j}^\dagger c_{i\uparrow} - f_{i,j}^\dagger c_{i\downarrow} \prod_j \left[ \frac{f_{i,j}^\dagger c_{i\uparrow} - f_{i,j}^\dagger c_{i\downarrow}}{\sqrt{2}} \right]|0\rangle$ as that is calculated by the singlet ground state in a two-site Heisenberg model [1]. When we consider the perturbation $t/J$ from the strong coupling limit, it is naively expected that the Berry phases remain the same. In other words, the response to the local twist of the ground state is expected to be identical to that of the direct product state of singlets. In this sense, the Berry phases classify the property of the phase.

An alternative limit is the weak coupling limit of the PAM, i.e., $U \to 0$. For the case of $U = 0$, the PAM is a non-interacting two-band model with a hybridization gap. At half filling, the ground state is easily obtained as $|gs\rangle = \prod_{k\sigma} a^\dagger_{k\sigma} |0\rangle$, with $a^\dagger_{k\sigma} = u_k c^\dagger_{k\uparrow} + v_k f^\dagger_{k\sigma}$, $a^\dagger_{k\sigma-} = -u_k c^\dagger_{k\downarrow} + v_k f^\dagger_{k\sigma}$. Here, parameters $u_k$, $v_k$ satisfy $|u_k|^2 + |v_k|^2 = 1$. The one-particle energy spectrum consists of the lower and upper hybridization bands, $E_{k\pm} = \frac{1}{2} \left( \epsilon_k \pm \sqrt{\epsilon_k^2 + 4v^2} \right)$. To obtain $\gamma_t$, we consider an adiabatic transformation to a decoupled model at $U = 0$, $t = 0$. Note that the hybridization gap always open in the adiabatic transformation due to nonzero $v$. In the decoupled model $H_{PA}|_{U=0,t=0}$, the hybridization gap is given by $2|v|$. $\gamma_t$ is zero because there is no hopping term, and the ground state becomes the direct product state of dimers $|gs\rangle = \prod_{\sigma} \left[ \frac{c_{i\uparrow} - f_{i\sigma}^\dagger}{\sqrt{2}} \right]|0\rangle$. If the gap does not close in the adiabatic transformation to the decoupled model, the Berry phase $\gamma_t$ remains the same, i.e., zero. When we introduce the twist $\theta$ which corresponds to $\gamma_t$, $\theta$ can be considered as a flux in the system of spin-up electrons and the one-particle energy spectrum of spin-up electrons becomes $E_{k\pm}(\theta) = E_{k\mp} + \theta L\pm$. If the system size $L$ is large enough, $\theta$ dependence of the hybridization gap is negligible. Then, the gap does not close in the adiabatic transformation and $\gamma_t = 0$ for nonzero $v$. On the other hand, $\gamma_s$ is $\pi$ due to the gauge transformation. That is, both Berry phases $\gamma_t$ and $\gamma_s$ in the non-interacting limit of the PAM are the same as those in the strong coupling limit $H_{KL}|_{t=0}$. It should be noted that two decoupled models $H_{KL}|_{t=0}$ and $H_{PA}|_{U=0,t=0}$ are connected a direct path $H_{PA}|_{t=0}$. The quantized Berry phases have the advantage that they are topologically protected against small perturbations if there is no gap-closing. Although it is trivial that the KLM and PAM give $\gamma_s = \pi$ due to the gauge transformation, it is not trivial that the Berry phase remains the same when we add small Heisenberg interaction between local spins to $H_{KL}$ or small hopping terms between $f$ electrons to $H_{PA}$, where the spin twist can not be gauged out. To check the advantage numerically, we shall consider a one-dimensional Hamiltonian $H_{HKL} = H_{KL} + H_h$, with $H_h = J_h \sum_{\langle i,j \rangle} S_i \cdot S_j$. Here, it is not a trivial problem to obtain $\gamma_s$ by introducing the corresponding spin twist to $H_{HKL}$ as shown in 1. Figure 2 shows energy diagram as a function of the spin twist $\theta$. Since the spin twist can not be gauged out, the ground state energy depends on $\theta$. For small $J_h$, the Berry phases $\gamma_s = \pi$ and $\gamma_t = 0$ are obtained numerically. The excitation gap has a minimum value at $\theta = \pi$ and becomes small as $J_h$ increases. If the gap closes at large $J_h$, there can be a transition of the Berry phase. However, the gap-closing is not observed at the system size $L = 4$. It is preliminary investigation but is interesting when we compare $H_{HKL}$ with the spin ladder[7] which has the transition from the rung-singlet phase, which corresponds to the Kondo singlet phase.
In conclusion, the quantized Berry phase used as a local order parameter has been applied to the KLM and the PAM. It characterized the Kondo singlet phase successfully as $\gamma_s = \pi$ and $\gamma_t = 0$. It means that the quantized Berry phase identifies a Kondo singlet locally, while a non-trivial $\pi$ Berry phase has identified a localized singlet or dimer on the corresponding link in the previous study. Here, the Kondo singlet detected by the Berry phases is the spin singlet in the strong coupling limit of the KLM and the dimer in the weak coupling limit of the PAM. The results in the two limits are applicable to higher dimensions. However, there is the transition from the Kondo singlet phase to the antiferromagnetically ordered phase in higher dimensions in the weak coupling region of the KLM or the strong coupling region of the PAM. Finally, the advantage that the quantized Berry phases are topologically protected against small perturbations has been numerically shown. This method will be useful even for frustrated electron systems.

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