Topological phase in 1D topological Kondo insulator: $Z_2$ topological insulator, Haldane-like phase and Kondo breakdown

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Abstract. We have simulated a half-filled 1D $p$-wave periodic Anderson model with numerically exact projector quantum Monte Carlo technique, and the system is indeed located in the Haldane-like state as detected in previous works on the $p$-wave Kondo lattice model, though the soluble non-interacting limit corresponds to the conventional $Z_2$ topological insulator. The site-resolved magnetization in an open boundary system and strange correlator for the periodic boundary have been used to identify the mentioned topological states. Interestingly, the edge magnetization in the Haldane-like state is not saturated to unit magnetic moment due to the intrinsic charge fluctuation in our periodic Anderson-like model, which is beyond the description of the Kondo lattice-like model in existing literature. The finding here underlies the correlation driven topological state in this prototypical interacting topological state of matter and naive use of non-interacting picture should be taken care. Moreover, no trace of the surface Kondo breakdown at zero temperature is observed and it is suspected that frustration-like interaction may be crucial in inducing such radical destruction of Kondo screening. The findings here may be relevant to our understanding of interacting topological materials like topological Kondo insulator candidate SmB$_6$.

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1 Introduction

Recently, the interest in the topological state of matter has been reignited since theoretical prediction and experimental realization of quantum spin Hall effect and 3D topological insulator.\cite{1,2,3,4,5,6,7,8,9} For most of real-life topological materials, for example time-reversal invariant $Z_2$ topological insulator in HgTe/CdTe quantum wells, Bi and Sb-series compounds,\cite{12} their basic properties can be readily understood in the framework of single-particle picture, e.g. topological band theory.\cite{4}

However, electron correlation effect in strongly interacting topological materials is still poorly understood, particularly for the well-known topological Kondo insulator candidate—Samarium Hexaboride (SmB$_6$).\cite{9} Although topological point of view provides appealing explanation to its mysterious low-temperature surface state,\cite{9,10} the light electron detected in such surface state hinders a satisfactory solution.\cite{11,12,13,14,15,16} Furthermore, recent high-field quantum oscillation measurement even gives rise to a possibility of a hidden three-dimensional Fermi surface in such bulk insulator.\cite{17}

In order to answer these serious problems, insightful ideas like surface Kondo breakdown, fractionalized Fermi liquid and Majorana Fermi sea are proposed in light of the wisdom that strong electron correlation may lead to radical reconstruction of low-energy physics and fractionalization of electrons is a fascinating option.\cite{18,19,20,21}

Unfortunately, in dimension larger than one, it is hard to verify these interesting ideas unbiasedly in terms of current analytical and numerical calculation tools, thus present studies mainly focus on a simplified one-dimensional topological Kondo insulator model, i.e. 1D $p$-wave Kondo lattice model invented by Alexandrov and Coleman,\cite{22} and further inspected by abelian bosonization and density matrix renormalization group (DMRG) techniques.\cite{23,24,25} The core finding in these works is that if quantum fluctuation effect is included, the paramagnetic end modes (usual fermion zero-energy mode) predicted in large-N mean-field theory are unstable toward a magnetic end state, which is a novel realization of the famous Haldane phase for spin-one antiferromagnetic chain.\cite{26,27,28}
Nevertheless, we recall that both the concept of topological Kondo insulator itself and its realistic material modeling start from the periodic Anderson-like model, which includes essential charge/valence fluctuation effect of f-electrons beyond the spin-only Kondo lattice-like model.\cite{10,20} For example, x-ray core-level spectroscopy measurement suggests the f level occupation of SmB$_6$ is approximated as 0.7,\cite{27} much smaller than unit as modeled in p-wave Kondo lattice model, thus it is not known whether the results found in such Kondo lattice-like model are applicable to the realistic mixed-valence compound like SmB$_6$.

Here, we directly study the 1D $p$-wave periodic Anderson model,\cite{23,28} (See Fig. 1) which is a natural extension of previous $p$-wave Kondo lattice model. In this model, the charge degree of freedom of f-electron is preserved and not only Kondo limit but also mixed-valence regime can be reliably explored by existing theoretical approaches. As a first step toward this interesting issue, we consider a half-filled system with particle-hole symmetry.\\ As we are only interested in insulating topological states, the model we have studied is the following 1D $p$-wave periodic Anderson model,\cite{10,24,28}

$$
H = \sum_{j \sigma} [t_{c} c_{j \sigma}^{\dagger} c_{j+1 \sigma} - t_{f} f_{j \sigma}^{\dagger} f_{j+1 \sigma} + \text{H.c.}] + \frac{V}{2} \sum_{j \sigma} [(c_{j+1 \sigma}^{\dagger} - c_{j-1 \sigma}^{\dagger}) f_{j \sigma} + f_{j \sigma}^{\dagger} (c_{j+1 \sigma} - c_{j-1 \sigma})] + E_{f} \sum_{j \sigma} f_{j \sigma}^{\dagger} f_{j \sigma} + U \sum_{j} f_{j \uparrow}^{\dagger} f_{j \uparrow} f_{j \downarrow}^{\dagger} f_{j \downarrow}.\\ (1)
$$

Here, $t_{c}$, $t_{f}$, and $U$ are the nearest-neighbor-hopping strengths, $E_{f}$ denotes the energy level of f-electron and local electron has also the conventional Hubbard on-site interaction ($U$-term). The $p$-wave hybridization between conduction and local electron is encoded by $V$ term, in which the coupling of conduction and local electron is non-local (due to non-trivial spin-orbit coupling between $d$-like conduction electron and $f$-like local electron) in contrast to the usual s-wave (on-site) hybridization in standard periodic Anderson model. (See also Fig. 1) As we will see below, such non-local hybridization leads to non-trivial topological phases and the main object of this article is to discuss their detailed features.

As we are only interested in insulating topological states in present work, the system is fixed to be half-filled, which means the total number of conduction and local electrons...
is equal to twice of lattice site number. Next, the hopping parameters $t_c$ and $t_f$ should have the same sign.\textsuperscript{20,39} i.e. $t_c t_f > 0$, otherwise even the non-interacting energy band will not be fully gapped and the topological argument will be meaningless. Furthermore, we choose $E_f = -U/2$, such that when interaction is turned on, it will exclude the fermion minus-sign problem for PQMC, which will be used to explore the effect of interaction.\textsuperscript{29}

In addition, in terms of a canonical transformation (i.e., a generalized Schrieffer-Wolff transformation), the model in Eq. 4 can lead to the 1D $p$-wave Kondo lattice model which was firstly proposed by Alexandrov and Coleman, and then further studied in Refs.\textsuperscript{22,23,24,25}.

(One finds $J_K = 4 t_f^2$ and $J_H = 2 V^2$ with our notation for $V_c$.)

### 2.1 Non-interacting limit: Bulk property

Firstly, we discuss an exactly soluble limit, where the Hubbard interaction is turned off ($U = 0$),

$$H_0 = \sum_k \psi^\dagger_k \left( \frac{\varepsilon_c(k) \hat{I} - iV \hat{S}_x \hat{S}_z}{-iV \hat{S}_x \hat{S}_z} + \varepsilon_f(k) \hat{I} \right) \psi_k = \sum_k \psi^\dagger_k \hat{H}(k) \psi_k.$$  

Here, the model has been transformed into momentum space via Fourier transformation and a four-component spinor $\psi_k$ has been introduced as $\psi_k = (c_k \xi, c_k \xi, f_k \xi, f_k \xi)^T$. $\hat{S}_x, \hat{S}_y, \hat{S}_z$ are the usual $2 \times 2$ Pauli matrices acting on orbital basis and $\hat{I}$ is the $2 \times 2$ unit matrix. The dispersion of conduction and $f$-electron is given by $\varepsilon_c(k) = 2t_c \cos k x$, and $\varepsilon_f(k) = -2t_f \cos k z$, respectively. Moreover, the $p$-wave hybridization is denoted by $V \hat{S}_x \hat{S}_z$ with form factor $s_z = \sin k_z$.

For this non-interacting model, its quasi-particle energy spectrum is easily found to be

$$E_{k \pm} = \frac{\varepsilon_c(k) + \varepsilon_f(k) \pm \sqrt{(\varepsilon_c(k) - \varepsilon_f(k))^2 + 4V^2 s_z^2}}{2} = \frac{(t_c - t_f) \cos k z \pm (t_c + t_f)^2 \cos^2 k z + V^2 \sin^2 k z}{2},$$

which has a two-fold spin degeneracy. When the system is half-filled, the lower band $E_{k -}$ is fully occupied and a gap exists for all quasi-particle excitations, thus we are truly considering a bulk insulator.

Following Ref.\textsuperscript{10}, the system $H_0$ is invariant under both time-reversal $\mathcal{T}$ and space-inversion $\mathcal{P}$ transformation since $\hat{H}(k)^T = \mathcal{T} \hat{H}(-k) \mathcal{T}^{-1}$ and $\hat{H}(k) = \mathcal{P} \hat{H}(-k) \mathcal{P}^{-1}$ with

$$\mathcal{T} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

So, the non-interacting Hamiltonian $H_0$ has time-reversal and inversion symmetry, and according to the Fu-Kane formula,\textsuperscript{31} the system can be a $Z_2$ topological insulator if the following $Z_2$ index $\nu = 1$:

$$(\nu)^{\nu} = \delta_T \delta_M,$$  

where $\delta_T, \delta_M$ are the parity at the high-symmetry points of 1D Brillouin zone. ($\Gamma = 0$ and $M = \pi$)

To find the parity at those two high-symmetry points, we rewrite $\hat{H}(k)$ as

$$\hat{H}(k) = (\varepsilon_c(k) + \varepsilon_f(k)) \begin{pmatrix} \hat{I} & 0 \\ 0 & -\hat{I} \end{pmatrix} + (\varepsilon_c(k) - \varepsilon_f(k)) \begin{pmatrix} \hat{I} & 0 \\ 0 & -\hat{I} \end{pmatrix} + iV \hat{S}_x \begin{pmatrix} 0 & \hat{\sigma}_y \\ -\hat{\sigma}_y & 0 \end{pmatrix}.$$  

Then, at high-symmetry points $\Gamma$ and $M$, the hybridization term vanishes since $s_z = \sin 0 = 0 = \sin \pi$ , which is a general result from time-reversal symmetry. Therefore, the parity is determined by relative position of $\varepsilon_c(k)$ and $\varepsilon_f(k)$, i.e.

$$\delta_T = \text{sign}(\varepsilon_c(0) - \varepsilon_f(0)) = \text{sign}[t_c + t_f]$$

$$\delta_M = \text{sign}(\varepsilon_c(\pi) - \varepsilon_f(\pi)) = -\text{sign}[t_c + t_f].$$

So, we find $\nu = 1$ ($(-1)^{nu} = \delta_T \delta_M = -1$) and the half-filled system is indeed a 1D $Z_2$ topological insulator. (In fact, if the $f$-electron level $E_f$ is reintroduced, we find the non-interacting system is still a $Z_2$ topological insulator when $-2|t_c + t_f| < E_f < 2|t_c + t_f|$, given the half-filling condition is satisfied and chemical potential is properly tuned.)

### 2.2 Non-interacting limit: Edge property

Alternatively, one may explore the topological property by inspecting the edge states of Hamiltonian $H_0$ in real space with open boundary condition:

$$H_0 = \sum_{\sigma} \sum_{j=1}^{L-1} \left[ t_c c^\dagger_j \sigma_c c_{j+1} \sigma - t_f f^\dagger_j \sigma_f f_{j+1} \sigma + H.c. \right]$$

$$+ \frac{V}{2} \sum_{\sigma} \left[ \epsilon_{c+1} \sigma_c f_{j+1} \sigma f_{j} \sigma + \epsilon_{c} \sigma_c f_{j} \sigma f_{j+1} \sigma + \epsilon_{c} \sigma_f f_{j} \sigma f_{j} \sigma + \epsilon_{c} \sigma_f f_{j+1} \sigma f_{j+1} \sigma \right]$$  

$$+ \frac{V}{2} \sum_{\sigma} \left[ \epsilon_{c} \sigma_c f_{1} \sigma f_{0} \sigma + \epsilon_{c} \sigma_c f_{0} \sigma f_{1} \sigma + \epsilon_{c} \sigma_f f_{L+1} \sigma f_{L} \sigma + \epsilon_{c} \sigma_f f_{L} \sigma f_{L+1} \sigma \right]$$

To elucidate the edge state, we consider a special case with $t_c = t_f = t$, such that

$$H_0(t) = (t + \frac{V}{2}) \sum_{\sigma} \sum_{j=1}^{L-1} \left[ b^\dagger_{j+1} \sigma a_{j+1} \sigma + a^\dagger_{j} \sigma b_{j+1} \sigma \right]$$

$$+ (t - \frac{V}{2}) \sum_{\sigma} \sum_{j=2}^{L} \left[ b^\dagger_{j-1} \sigma a_{j-1} \sigma + a^\dagger_{j} \sigma b_{j-1} \sigma \right].$$

We introduce new (bonding and anti-bonding) fermions $a_{j} \sigma = \frac{1}{\sqrt{2}} (f_{j} \sigma + c_{j} \sigma)$, and $b_{j} \sigma = \frac{1}{\sqrt{2}} (f_{j} \sigma - c_{j} \sigma)$. Furthermore, if $t = V/2$ (this is the so-called ‘Kitaev point’ and $t = -V/2$ case is similar), we have

$$H_0(t = V/2) = 2t \sum_{\sigma} \sum_{j=2}^{L} \left[ b^\dagger_{j-1} \sigma a_{j-1} \sigma + a^\dagger_{j} \sigma b_{j-1} \sigma \right],$$
which means zero energy fermion modes created by $a_1^\dagger_\sigma$ and $b_1^\dagger_\sigma$ are decoupled from Hamiltonian $H_0 (L = V/2)$. In other words, the expected edge states are actually formed by these fermion zero modes like $\langle \Psi_{\text{edge}} | \sim a_1^\dagger_\uparrow a_1^\dagger_\downarrow | 0 \rangle$, $a_1^\dagger_\uparrow b_1^\dagger_\downarrow | 0 \rangle$, $a_1^\dagger_\uparrow a_1^\dagger_\downarrow | 0 \rangle$, and $b_1^\dagger_\uparrow a_1^\dagger_\downarrow | 0 \rangle$, where one is able to obtain four-fold degenerated many-body ground-state wavefunction for this non-interacting case.

More generally, when $t_c \neq t_f \neq V/2$, these edge modes are still stable if no bulk gap is closed during evolution of Hamiltonian. (e.g. see Fig.3) In addition, we have checked that for all the cases with $t_c, t_f > 0$ and $V \neq 0$, the system shows fermion zero modes, which means the system itself is always in a topological state. This finding is consistent with the results of topological band theory (calculation of $Z_2$ index $\nu = 1$) seen in last subsection.

3 Turning on interaction: Brute-force quantum Monte Carlo simulation

From the analysis presented in the last section, we know that the non-interacting system is located in a $Z_2$ topological insulating phase with fermion edge mode.

When we turn on interaction $U$, a complicated situation may occur. For example, if adiabatic continuity works, then we expect the $U = 0$ topological phase to remain the same for not too large $U$. In contrast, particularly for 1D system, the effect of interaction is radical and even a small $U$ can lead the system into a new phase different from the non-interacting limit.

Here, we will use PQMC to simulate the 1D $p$-wave periodic Anderson model. Basically, in PQMC, one is able to calculate ground-state expectation value of observable $\mathcal{O}$ as

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi_g | \mathcal{O} | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle} = \lim_{\beta \to \infty} \frac{\langle \Psi_T | e^{-\beta H} \mathcal{O} e^{-\beta H} | \Psi_T \rangle}{\langle \Psi_T | e^{-\beta H} | \Psi_T \rangle} \quad (6)$$

where $| \Psi_g \rangle$ is the ground-state many-body wave-function of Eq. 1 obtained from an imaginary-time projection of trial wave-function $| \Psi_T \rangle$. This trial wave-function can be simply chosen as the ground-state of the non-interacting Hamiltonian, e.g. $H_0$ (Eq. 5), or a Hartree-Fock mean-field solution of the whole Hamiltonian. Moreover, the requirement $\langle \Psi_g | \Psi_T \rangle \neq 0$ should be fulfilled, otherwise the above projection method will not converge into the desirable interacting many-body ground-state. In realistic numerical calculation, the imaginary-time length $\beta$ is obviously finite but a large value of it is able to obtain a convergent result. (e.g. $\beta > L$ with $L$ being the size of the system)

Motivated by the previous study of 1D $p$-wave Kondo lattice, we will study this model by fixing hopping energy $t_c = t_f = 1$ such that a finite $U$ case may lead to visible Haldane state with insulating bulk and free local moments located on the boundary. Magnetization on each site and string order parameter may be used in order to find such phase however for the PQMC, the calculation of exponential of operators in string order is very challenging, thus we may calculate site-resolved magnetization to detect the possible edge local moment.

3.1 Benchmark: Non-interacting limit

Before discussing the interaction problem, we first show results in non-interacting limit ($U = 0$) with open boundary condition. From Fig. 3, we can see that the f-electron density $n_f (j) = \sum_\sigma \langle \Psi_f | f_j^\sigma | \Psi_f \rangle$ is uniform and the site-resolved magnetization $T_z (j) = \langle S_z^f (j) \rangle + \langle S_z^g (j) \rangle$ is zero for all sites. The double occupation number of f-electron $d_f (j) = \langle n_f^\dagger_\uparrow n_f^\dagger_\downarrow \rangle = (\langle f_f^\dagger f_f \rangle)^2 = 0.25$ for single occupation on each site. The $c-f$ hybridization $V_{cf} (j) = -\sum_{\sigma} \langle f_f^\dagger c_{j+1 \sigma} - c_{j-1 \sigma} \rangle$ is found to be weakened at boundary, where fewer conduction electron nearby reduces the hybridization. Moreover, the spin correlations $S_{yz} (j) = \langle S_z^f (L/2) S_y^g (j) \rangle$ and $S_{xy} (j) = \langle S_y^f (L/2) S_x^g (j) \rangle$ are all short-ranged. The typical correlation length in this case is about one or two sites. So, the system should be in a spin-disordered state while the $V = 0$ case with a much longer correlation length (5 to 10 sites) is a metallic state. The charge correlation (not shown here) is similar.

When we consider bulk system (with periodic boundary condition), the spin, charge and single-particle gap above the half-filled ground-state can be estimated as

$$\Delta_s = E(L+1, L-1) - E(L, L)$$
$$\Delta_c = E(L+1, L+1) - E(L, L)$$
$$\Delta_{sp} = 2(E(L+1, L) - E(L, L))$$

where $E(N_f, N_{\bar{f}})$ denotes the ground-state energy with $N_f$ referring to spin-up electron and $N_{\bar{f}}$ spin-down electron. For $L = 20$, $t_c = t_f = V = 1$, it is found that $\Delta_s = \Delta_c = \Delta_{sp} = 2$, which is consistent with direct calculation using Eq. 2. So, the bulk system is an insulator with both finite charge and spin gap. Now, we consider the open
chain with insulator discussed previously. Actually leads to an enhanced local moment in edge site. Such reduced double occupation possibility interaction since the non-interacting case shows uniform distribution. Such that, if we approximate the system as two coupled spin-1/2 chains, then the effective coupling between chains is ferromagnetic. Therefore, in the low-energy limit, a Haldane-like phase should form and the corresponding edge state has a free spin-1/2 magnetic moment, which agrees with the observation in the magnetization.

Now, we conclude that the interacting model shows the expected Haldane-like phase with free (spin-1/2) magnetic moment situated at the boundary, consistent with DMRG and bosonization,[22,23,24,25] but in contrast to the non-interacting case. So, we have seen that the adiabatic continuity breaks down in this model when interaction is added and the interaction effect is fundamental in 1D, where sophisticated techniques beyond mean-field theories should be used.

3.3 Strange correlator in 1D p-wave periodic Anderson model

Recently it has been proposed that the strange correlator is able to detect short-range entangled topological states and has been successful in identifying many topological states of matter including the Haldane phase in spin-one Heisenberg antiferromagnets, 1D and 2D AKLT states, quantum spin Hall state and bosonic symmetry-protected topological state.[32,33,34,35] The virtue of strange correlator is that no bipartition of a system is involved and the finite-size effect from the open boundary calculation is heavily reduced.

For our cases, we use PQMC to sample the target ground-state wave-function from the imaginary evolution of a trial wave-function $|\Psi_0\rangle$ while a trivial state $|\Omega\rangle$ is chosen to be a state with $E_\Omega = 10$. Thus, the following strange correlator calculated:

$$\langle U_{s} \bar{D} \rangle$$
Strange correlator $C(k)$ in 1D p-wave periodic Anderson model, $U = 0$ versus $U = 2$. The divergent point is at $k_x = 0$ while the finite-size cutoff is also seen.

\[
C(k) = \frac{1}{L^2} \sum_{j,l} e^{i(j-l)k} C_{jl} = \frac{1}{L^2} \sum_{j,l} \frac{\langle \Omega | c_j \sigma c_l^{\dagger} | \Psi \rangle}{\langle \Omega | \Psi \rangle} \tag{7}
\]

In Fig. 6 we see that both the non-interacting case ($U = 0$) and interacting case ($U = 2$) show divergent-like behavior in their strange correlators, which means they are all non-trivial topological states, although the divergence is cut off by finite-size effect. Interestingly, the interacting system has stronger divergence than the non-interacting one, which may indicate that the Haldane-like phase may be more entangled than its non-interacting counterpart, the $Z_2$ topological insulating state. The results here supplement the observation in site-resolved magnetization and agree with each other.

4 Edge magnetization under different interaction $U$ and hybridization $V$

In the last section, we have seen that a Haldane-like phase is found in our 1D p-wave periodic Anderson model, whose essential feature is the existence of free magnetic moment at the boundary of an open chain system and is detected by non-vanished magnetization of both conduction and local electron.

In this section, we proceed to see the evolution of edge magnetization under different interaction strength $U$ and hybridization $V$. This may encode how edge magnetic moment is free from the ones in a bulk system.

4.1 Effect of Hubbard interaction $U$ on the edge magnetization

First, we change the strength of Hubbard interaction $U$ while keeping other parameters intact. ($t_c = t_f = V = 1$)

In Fig. 7 we find that the edge magnetization increases from zero to unit when interaction $U$ is gradually enhanced. (When $U = 0$, magnetization is vanished as seen in Fig. 4) It is noted that the case with $U = 0.5$ has inverted magnetization in comparison to other cases and the reason is that in all numerical simulations performed in this work, we consider a total spin-singlet system but since edge magnetization is able to build at two equivalent direction (e.g. spin-up and spin down direction), it inevitably leads to two degenerated ground-states. However, for PQMC, it only randomly selects one of ground-states and this explains the observed distinction.

4.2 Effect of hybridization strength $V$

Next, tuning different values of hybridization strength $V$ leads to the results shown in Fig. 8. Here, we have observed that larger $V$ results in the smaller edge magnetization,
which is due to the enhanced Kondo screening and charge fluctuation for larger $V$. Specifically, the system with $V = 1.5$ has boundary magnetization $T_z \approx 0.7$ compared to $T_z \approx 1.0$ for $V = 1.0$ case. Furthermore, when $V$ is as small as 0.5 for fixed other parameters, magnetization at boundary sites (see red dots for $j = 1$ and $j = 20$ in Fig. [3]) actually exceeds unit.

4.3 Why edge magnetization is not unit

After all, we find that these results show that with generic parameters chosen for our model, the edge magnetization is deviated from unit as in pure spin-one antiferromagnetic chain, where decoupled (fractionalized) spin-half objects appear at the boundary.

In our present model, charge fluctuation of local electron always exists due to the hybridization $V$ between local and conduction electron unlike the previously studied p-wave Kondo lattice model, where charge fluctuation is completely excluded by canonical transformation with assumption of $V/U << 1$. For a strong hybridization (e.g. $V \gg U$), empty, spin-up, spin-down and double occupation are all allowed and it is not reasonable to expect a frozen unit magnetization at boundary when its particle occupation is rapidly changed among these four states. Instead, in this condition, due to the mentioned charge fluctuation, we expect a reduced magnetization at edge sites. In the opposite limit, $V$ is smaller than $U$ and Hubbard interaction is able to stabilize local moment, thus a large magnetization at boundary is possible in this case. Moreover, as has been discussed in Sec.3.2, we may think that the on-site conduction and local electron have ferromagnetic coupling, thus the total edge magnetization may exceed unit since two kinds of electron can contribute.

In addition, we may imagine that a putative spin-1/2 object at boundary will fluctuate into a spin-one composite or a zero-spin one, thus the effective magnetic moment at edge is not unit but changed by its surrounding electron configuration. It is noted that similar results have been found in doped three-legged Hubbard ladder, where the insulating phase is always the Haldane phase regardless of the suppression from unity of spin.[36]

5 Discussions

5.1 Why magnetic end states appear in interacting system

Here, we provide a qualitative argument on why magnetic end states appear in interacting system. Firstly, we know that when $t_c = t_f = V/2$ (Kitaev point), the non-interacting ground-state under open boundary condition can be approximated as a superposition of four zero-modes $a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle$, $a_{1\uparrow}^\dagger b_{1\uparrow}^\dagger |0\rangle$, $a_{1\downarrow}^\dagger b_{1\downarrow}^\dagger |0\rangle$, $b_{1\uparrow}^\dagger b_{1\downarrow}^\dagger |0\rangle$. In this case, the contribution of these four degenerated states is equal and the magnetization is obviously zero and no magnetic end state exists.

However, when Hubbard-$U$ interaction is turned on, the double-occupation on local electron site is suppressed, thus states like $a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle$ and $b_{1\uparrow}^\dagger b_{1\downarrow}^\dagger |0\rangle$ have small contribution to the system and the remaining ones are $a_{1\uparrow}^\dagger b_{1\uparrow}^\dagger |0\rangle$ and $a_{1\downarrow}^\dagger b_{1\downarrow}^\dagger |0\rangle$. Clearly, these two survivals are degenerated, but for numerical simulation like PQMC performed in this work, one is only able to obtain one of these two states at a time. In other words, in one simulation, we may obtain $a_{1\uparrow}^\dagger b_{1\uparrow}^\dagger |0\rangle$ as our ground-state while in other simulation, $a_{1\downarrow}^\dagger b_{1\downarrow}^\dagger |0\rangle$ may be observed. (See e.g. Fig. [4]) Therefore, for each of state, we can observe the magnetic end mode. More generally, since the topological feature is not changed under (smooth) continuous mapping of Hamiltonian, we expect the argument at special point $t_c = t_f = V/2$ is still valid at least qualitatively for generic conditions. In some sense, the interaction in our p-wave periodic Anderson model reduces the four-fold degeneracy of non-interacting ground-state into double degeneracy for interacting ground-state, which is similar to the findings in Su-Schrieffer-Heeger-Hubbard model and symmetry-protected one-dimensional fermionic superconducting phases.[37][38]

5.2 How about surface Kondo breakdown

In Refs. [18][19][20][22], authors have proposed that for topological Kondo insulator, whose $c-f$ hybridization is non-local in nature, Kondo screening at boundary may be weakened or even not developed due to smaller number of nearly electrons. In Sec. [19] we have seen that the effective $c-f$ hybridization $V_{c-f}$ is indeed weakened at boundary sites but its value is larger than 0.1. (recall $V > 1$ in these cases) Thus, no breakdown of Kondo screening is found in this uniform $V$ case.

A careful reader may note that a more conventional quantity to measure the strength of Kondo screening is spin-singlet correlator, i.e. $c-f$ spin correlation function like $\langle S_i^z S_j^z \rangle$. (see e.g. Ref. [30]) We have checked that the results of our simplified definition of $V_{c-f}$ are physically consistent with the more conventional spin-singlet correlator.

Now, following the suggestion in Refs. [18][22], in order to see possible Kondo breakdown at boundary, one may decrease the bare $c-f$ hybridization $V_{c-f}$ at edge site while keeping bulk $V$ intact. In Fig. [4] we have chosen $V_{c-f} = 2, 1, 0.4, 0.2, 0.1, 0.05$ (bulk $V$ is fixed to unit) and it is found that the $c-f$ hybridization $V_{c-f}$ is indeed reduced but still finite even though the edge hybridization $V_{c-f}$ is much smaller than the bulk hybridization $V$. Therefore, no surface Kondo breakdown is found in our numerical simulation at zero temperature.

However, it is important to emphasize that we do not conclude that the surface Kondo breakdown would not take place in realistic 3D materials like SmB$_6$. Our study here is just a simplified 1D lattice model, and is obviously not invented for the real-life materials. The only thing we have obtained here is that at least for this simplified 1D
TKI model at zero $T$, the Kondo breakdown is not observed in our numerical calculation. Although we do not find clue of Kondo breakdown in our present work, we expect a well devised 3D TKI model (but beyond our present numerical technique because both 2D and 3D TKI models in literature have severe fermion minus-sign problem) may support Kondo breakdown even at $T = 0$.

5.3 Spin-only model

In the main text, we have studied the $p$-wave periodic Anderson model, where both charge and spin degree of freedom of electrons are included. Here, it is interesting to think whether a spin-only model may capture the topological phases found in Kondo lattice and periodic Anderson-like models. In literature, 1D Kondo necklace model might be the desirable one and we propose its $p$-wave version as follows[10-11]

$$H_{p-KN} = -t \sum_j (\tau^x_j \tau^x_{j+1} + \tau^y_j \tau^y_{j+1}) + J \sum_j (\tau_{j+1} - \tau_{j-1}) \cdot S_j$$

where $\tau^x, \tau^y$ represents the spin degrees of freedom coming from original conduction electron and $S_j$ denotes local moment of f-electron. The $J$-term denotes the $p$-wave-like ‘Kondo’ coupling and it has staggered features, which may lead to effective ferromagnetic coupling between these two chains and we expect a Haldane-like phase can form in this model.[12] However, we should remind the reader that the Kondo necklace model cannot be derived from the original Kondo lattice model at half-filling but can only be considered as a phenomenological model devised for studying the low-lying spin excitations.

5.4 Realization in cold-atom setup

As proposed in Ref. [23], the $p$-wave periodic Anderson model may be realized by $p$-band optical lattices with a balanced mixture of two-component Fermi atoms (e.g. $^6\text{Li}$ or $^{40}\text{K}$). On the other hand, one may use ultracold alkaline earth-like atoms, e.g. $^{173}\text{Yb}$, to simulate our calculated model via suitable laser excitations.[33-44] However, it should be emphasized that the reachable temperature in current optical lattice experiments is still too high to observe the low-temperature Kondo (lattice) physics and the corresponding topological phases. Thus, preliminary exploration on finite temperature regime for our model will be more useful for future experiments on this interesting topic.

6 Conclusion and direction for future work

In conclusion, we have studied the $p$-wave periodic Anderson model (Eq. 1) in terms of the unbiased PQMC simulation. The ground-state is the expected Haldane-like phase with magnetic end mode driven by electron correlation effect beyond effective non-interacting single-particle picture. In addition, we have not found any evidence of the surface Kondo breakdown proposed in the literature at least for zero temperature, so it is suspected that frustration-like interaction, e.g. ring-exchange interaction among nearest sites, may be crucial in inducing such radical destruction of Kondo screening in the lattice fermion model.

Alternatively, one may investigate the finite temperature effect on the stability of Haldane-like phase. Physically, the topological state will still be protected by the bulk gap unless the thermal fluctuation overwhelms such gap. At the same time, the elevated temperature has the potential to destroy Kondo screening and it is expected that we can detect the breakdown of the surface Kondo effect with the help of finite-temperature determinant quantum Monte Carlo algorithm widely used in the simulation of correlated electron problems.[18-45] Future work in this direction will be of great help in clarifying the possibility of the temperature-driven surface Kondo breakdown mechanism.

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8 Contribution statement

Y. Zhong suggested the issue and carried out the calculation. All of authors wrote and revised this article.
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