Gap structure and the effect of disorder on heavy fermions in an optical lattice

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Abstract – The understanding of the interplay between interaction and disorder in heavy fermions governed by the disordered Kondo lattice model is enhanced by demonstrating that the gap structure plays a crucial role in determining the effect of disorder on the heavy-fermion system. We show that in the insulating phases near the phase boundary the effect of disorder is strikingly reversed when the gap structure vanishes. For example, in the Kondo insulator phase near the phase boundary, the disorder-induced enhancement of the density fluctuation turns suppression when disorder destroys the hybridization gap, creating the poorly conducting phase at strong disorder.

Introduction. – Though Anderson localization describes the disordered noninteracting particles well [1], understanding the interplay between interaction and disorder in quantum many-body systems has still been a challenging topic for condensed matter physics community [2]. Unlike the solid-state systems, recent developments of ultracold gases in laser speckles or incommensurate optical lattices provide a new platform with both experimentally controlled interaction and disorder to reveal the physics of noninteracting and interacting particles in the disordered potentials [3–8]. Nowadays, though the task of mimicking disordered quantum magnetism has still been hindered by the required low temperature of spin ordering [9], the milestone realizations of the fermionic Mott insulator (MI) for alkali-metal or alkaline-earth-metal atoms (AEMAs) [10–13] have inspired the blossom of experimental and theoretical studies on disordered strongly correlated Fermi gases. For fundamental transport issues, the transition from a superfluid state to a poorly conducting state has been identified in disordered strongly interacting 6Li Feshbach molecules [14–16]. And very recently the disordered Fermi-Hubbard model (DFHM) has been probed with ultracold fermions in a disordered optical lattice, demonstrating that disorder disrupts the Hubbard gap by creating density fluctuations in the Mott insulator phase while the metallic phase is stabilized by interaction [16]. Theoretically, the three-dimensional expansion of a fermionic Mott wedding cake in the presence of disorder supports that disorder destabilizes the Mott insulator phase [17], and the effect of disorder on the compressibility property of the one-dimensional strongly correlated Fermi gases has also been reported, highlighted by a compressibility anomaly in the metallic phase at low density [18].

An intriguing many-body phenomenon in condensed matter physics is Kondo effect, which is of great importance in heavy-fermion materials, quantum magnetism and criticality [19–21]. Recently, it has been shown that fermionic AEMAs have unique properties that allows for reconstructing the Kondo lattice model (KLM) and investigating the physics of heavy-fermion system from different perspectives [22–24], which opens up avenues for the optical lattice simulation of the disordered Kondo lattice model (DKLM). To probe the DKLM with ultracold AEMAs, the atoms (for instance, 171Yb) with two clock states 1S0 (g) and 3P0 (e) are trapped in two independent optical
lattice potentials at the same periodicity \cite{23}, playing the roles of conduction electron and localized magnetic moment in heavy-fermion systems respectively \cite{22}. The $e$ atoms suffer lossy collision and are loaded into the lowest vibration band of the deep lattice to form a Mott insulator with the strong onsite $e-e$ interaction, while the $g$ atoms trapped in the swallow other lattice hop between adjacent sites with the negligible onsite $g-g$ interaction and interact with the $e$ atoms via the onsite antiferromagnetic Heisenberg-type exchange interaction \cite{23, 24}. An external laser speckle radiates the atoms and acts as the disordered potential experienced by the $g$ atoms, for the deeply trapped $e$ atoms are reasonably assumed to be unaffected by the laser speckle, but the state-dependent disorder is still preferable. The strength of the disorder is characterized by the average speckle potential energy at the focus of the lens and can be adjusted by tuning speckle laser power. However, to the best of our knowledge, the interplay between interaction and disorder at zero temperature of heavy fermions in disordered optical lattices has not been uncovered yet \cite{8}.

Motivated by this challenge, in this letter, we propose an exactly solvable model to capture the quantum phase transitions (QPTs) in the disordered heavy-fermion system and study the corresponding gap structure by the hybridization mean-field theory, and we demonstrate that the gap structure plays a crucial role in determining the effect of disorder on the heavy-fermion system. Subsequently, our demonstration is observed theoretically in the Kondo wedding cake by the experimentally accessible density profile and compressibility.

**Quantum phase transitions of heavy fermions in a disordered double-well potential.** Besides the sophisticated numerical recipes, such as density matrix renormalization group, the exactly solvable models are also nontrivial for understanding the interplay between interaction and disorder \cite{26}. Here, we propose the exactly solvable DKLM of heavy fermions in a disordered double-well (DW) potential, describing that the disordered $t_g$ itinerant $g$ atoms interact with a half-filling DW of localized $e$ atoms via the antiferromagnetic Kondo-exchange interaction $J_K$.

$$H_{DW} = -t_g \sum_{\sigma} \{c_{i\sigma}^\dagger c_{Rg\sigma} + h.c.\} + J_K \sum_{i} \vec{S}_{ig} \cdot \vec{S}_{ie} + \frac{\epsilon}{2} (n_{Lg} - n_{Rg}) - \mu_g (n_{Lg} + n_{Rg}), \quad (1)$$

where $c_{i\sigma}^\dagger (c_{i\sigma})$ creates (destroys) one atom in the lowest Wannier orbital of electronic state $\alpha \in \{e, g\}$ in site $i \in \{L, R\}$. $\vec{S}_{ia} = \frac{1}{2} \sum_{\sigma, \sigma', c_{ia\sigma}} \sigma \sigma' \sigma_{ia\sigma'}$, where $\sigma \in \{\uparrow, \downarrow\}$ denotes the spin state and $\vec{S}$ is the vector of Pauli matrices. And $\mu_g$ is the chemical potential of $g$ atoms. In the DW model, disorder is described by the random tilting $\epsilon$ between two subwells, choosing $P(\epsilon) = 1/(2\Delta)$, $\epsilon \in [-\Delta, \Delta]$, where $\Delta$ measures the disorder strength. For an arbitrary operator $O$, $\langle O \rangle_\epsilon$ is the ground state observation of $O$ at a fixed $\epsilon$, then straightforwardly in the disordered potential the ground state observation $\langle \langle O \rangle_\epsilon \rangle_\text{dis} = \int_{-\Delta}^{\Delta} d\epsilon P(\epsilon) \langle O \rangle_\epsilon$.

Considering the experimental accessibility, the requirement to reach the temperature smaller than the Kondo temperature $T_K \sim t_g e^{-t_g/J_K}$ can always be relaxed by choosing a larger $J_K$ in optical lattices \cite{24}. In this letter, we choose $J_K = 8 t_g$ and obtain $T_K \sim t_g$, so only a temperature smaller than the tunneling energy is needed to realize the artificial DKLM. Moreover, in this chosen parameter regime, the Kondo physics overpowers the RKKY-type \cite{27, 28} physics, which makes the hybridization mean-field treatment of the DKLM in this letter reasonable.

The quantum phases of heavy fermions in a DW potential are characterized by the density $n_g$ and density fluctuation $\Delta n_g$ \cite{28}. The nontrivial density fluctuation is consistent with the transport of $g$ atoms between the subwells in the fractional density conducting phases, while the integral density and zero density fluctuation indicates the insulating phases, where the half-filling Kondo insulator is protected by the hybridization gap, and the unity-filling insulator with the vanished hybridization is actually a band insulator of noninteracting $g$ atoms.

By varying the strength of the disorder, the QPTs of heavy fermions in a disordered DW potential can be accessed. In the metallic phase (Fig. 1a), disorder suppresses the density fluctuation and at strong disorder a poorly conducting phase is reached. In the DW picture, it is obvious that in the metallic phase the tilting tends to freeze the $g$ atoms in the potential valley as the transport is suppressed by the barrier $\Delta$, then in the disorder landscape the $g$ atoms are isolated in the randomly distributed

![Fig. 1: (Color online) In the metallic phases at low and high density ($a$) and the insulating phases near the phase boundary ($e-d$), the quantum phase transitions are accessed by varying the strength of disorder $\Delta$, which are described by the density $n_g$ (blue dotted) and density fluctuation $\Delta n_g$ (red and green dotted, magnified 20 and 5 times respectively).](image)
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deep potential valleys, which explains the poor conductivity at strong disorder and the compressibility anomaly at low density [30]. In the insulating phases near the phase boundary, though the states are robust at the weak disorder, the sufficiently strong disorder creates the nontrivial density fluctuation and the fractional density conducting phases (Fig. 1a-d). The band insulator is doped by holons which activates the hybridization and conductivity, while the hybridization of the Kondo insulator is suppressed by the disorder-doped doublons (holons) at positive (negative) chemical potential and the state evolves into the high (low) density conducting phase. The most striking and undemonstrated feature of the QPTs in the insulating phases near the phase boundary is the reversion of the effect of disorder on the density fluctuation from enhancement to suppression, which creates the poorly conducting phase at strong disorder. For example, in the Kondo insulator phase (Fig. 1a-d), the reversion has been identified at $\Delta / J_K \approx 0.5 - 1.5$, which suggests a possible connection between the reversion and the DW hybridization gap $\Delta_D$. Thus, to reveal the underlying physics behind the reversion of the effect of disorder transparently, we study the corresponding hybridization gap structure.

**Gap structure of the disordered heavy-fermion lattice gas.** The disordered heavy-fermion lattice gas is described by the single-band DKLM Hamiltonian

$$H_{DKLM} = -t_g \sum_{\langle i,j \rangle, \sigma} c_{ig\sigma}^\dagger c_{jg\sigma} + J_K \sum_i \vec{S}_{ig} \cdot \vec{S}_{ic} + \sum_i (\Omega_i^2 + \epsilon_i) n_{ig},$$

where site $i \in [-L, L]$ and $\Omega_i^2$ denotes the harmonic confining potential. The one-dimensional laser speckle is described by the Gaussian correlated random potential $\epsilon_i$

$$\epsilon_i = \frac{1}{\sqrt{2\pi\xi}} \sum_{j=-L}^{L} \exp \left[ -\frac{(i-j)^2}{2\xi} \right] W_j,$$

where $P(W_j) = 1/(2\Delta)$ and $W_j \in [-\Delta, \Delta]$ [31]. In this letter, we choose the correlation length $\xi = 1/2$ to affect the many-body heavy-fermion system microscopically [32].

The hybridization mean-field picture, having been verified in the heavy-fermion materials such as YbFe$_2$Sb$_{12}$ and CeRu$_2$Sb$_{12}$ [33], is introduced by the order parameter

$$\chi_i = \frac{1}{2} \sum_{\sigma} \langle c_{ig\sigma}^\dagger c_{ic\sigma} + c_{ic\sigma}^\dagger c_{ig\sigma} \rangle,$$

and the inhomogeneity of the harmonic confining potential and laser speckle is treated by the local density approximation with the local chemical potential $\mu_{ij} = \mu_j - \Omega_j^2 - \epsilon_j$. At a specified realization of disorder $\epsilon_i$, the ground state of the DKLM can be obtained by the variational procedure following Refs. [23][24], where we predict the clean hybridization gap $\Delta H \sim 3/4J_K$ (Fig. 2 blue). And the ground state observation of an arbitrary operator $O$ in the laser speckle is derived by the statistical averaging over a ensemble of a finite number of disorder realizations $\langle O \rangle_{\text{dis}} = \sum_{\epsilon_i} P(\epsilon_i) \langle O \rangle_{\epsilon_i}$.

Now we continue the discussion of the QPTs in the insulating phases near the phase boundary at $\Omega = 0$. At $\Delta = \Delta_H/10$, though the weak disorder smooths the singularity of the gap, the Kondo insulator phase locating in the gap manifests nontrivial robustness (Fig. 2 red dashed). While with the increasing disorder, the Kondo insulator phase reaches the shrunk gap edge and evolves into the compressible conducting phase, which is consistent with the enhancement of the density fluctuation. Dramatically, we find that the gapped heavy-fermion system turns gapless at $\Delta = \Delta_H/2$ where the reversion in the DW model happens (Fig. 2 green). And with the larger $\partial \mu_{g}/\partial \sigma$ at $\Delta > \Delta_H/2$, it is obvious that disorder reduces the compressibility of the gapless heavy-fermion system, which is consistent with the reversion of the effect of disorder to the suppression of the density fluctuation in the Kondo insulator phase near the phase boundary (Fig. 2 purple). Note that for the Kondo insulator phases not near the phase boundary, the reversion of the effect of disorder is messed up by the metal-insulator transition, which is a too complicated situation to be included in the range of this letter. And straightforwardly, the gap structure in the band insulator phase near the phase boundary shall play a similar role. Thus, the underlying physics behind the reversion of the effect of disorder is actually the crucial role of the gap structure in determining the effect of disorder on the heavy-fermion system, in other words, the vanishing of the gap structure reverses the effect of dis-
order on density fluctuation in the insulating phases near the phase boundary from enhancement to suppression.

**Observation of the role of gap structure in the disordered Kondo wedding cake.** – From the experimental side, the strongly correlated lattice gases are usually trapped in the harmonic confinement and manifest the wedding cake structure, the quantum phase transitions of which are probed with density profile and compressibility \[1, 34\]. Subsequently, for heavy fermions, the disordered Kondo wedding cake in the harmonic confining potential \((\Omega \sim \frac{2}{\hbar c} t_g)\) can be probed in the same way.

The disorder-induced melting of the Kondo wedding cake can be explained by the doping picture introduced in the DW model, whose effect on interband hybridization is verified in Fig. 3b. For the density profile, at weak disorder, the robustness of the Kondo wedding cake is obvious, though the slight melting at the edge of the insulating plateau indicates the smoothing of the singularity of the gap structure (Fig. 3a blue and red dashed); while at strong disorder, the Kondo wedding cake has melted completely and manifested the bell-shape density profile consistent with the gapless system, the leakage though the edge of the harmonic confinement has also been observed (Fig. 3a purple). However, the most important result of observing the density profile is we have identified that the Kondo insulator plateau vanishes with the gap structure at \(\Delta = \Delta_H/2\) (Fig. 3a green), around which the compressibility can be probed to verify the reversion of the effect of disorder.

We observe both global and local compressibility of the disordered Kondo wedding cake. The global compressibility is described by the stiffness \(S = \frac{\partial^2}{\partial N_g^2}\), where \(N_g\) is the total number of the \(g\) atoms \[18\]. The singularities on the global compressibility indicate the quantum phase transitions between metallic and insulating phases accessed by varying \(N_g\) (Fig. 4a blue dotted). As the gap structure shrinks, the increasing disorder smooths the singularities out (Fig. 4a red dotted, green dotted and purple dotted). And the anomaly explained in the DW model is very obvious at the low density. The local compressibility is defined as \(\kappa = \frac{\partial n_g(r)}{\partial \Omega_r^2}\). To access the Kondo insulator phase near the phase boundary, we observe the local compressibility near the edge of the Kondo plateau. And we find that the disordered-induced enhancement of the local compressibility turns suppression at \(\Delta = \Delta_H/2\) (Fig. 4b), which verifies that the vanishing of the gap structure reverses the effect of disorder on density fluctuation in the insulating phases near the phase boundary from enhancement to suppression.

**Conclusion.** – To summarize, in this letter, we demonstrate that the gap structure plays a crucial role in determining the effect of disorder on the density fluctuation in the insulating phases near the phase boundary, and we prove that our demonstration can be verified in the harmonic confining potential by the experimentally accessible density profile and compressibility.

We hope this work can serve as a reasonable guide for the underlying physics of the DKLM and contribute to the experimental investigation of the DKLM with ultracold AEMAs in the future.

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Fig. 4: (Color online) (a) The global compressibility of the heavy fermions in the harmonic confinement with the increasing total $g$ atom number at the disorder strength $\Delta = 0$ (blue dotted), $\Delta H/10$ (red dotted), $\Delta H/2$ (green dotted) and $\Delta H$ (purple dotted). (b) The significant reversion of the effect of disorder on the local compressibility at the location near the edge of the Kondo plateau.

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