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Theoretical study of the dependence of single impurity Anderson model on various parameters within distributional exact diagonalization method

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Abstract. Single impurity Anderson model describes a system consisting of non-interacting conduction electrons coupled with a localized orbital having strongly interacting electrons at a particular site. This model has been proven successful to explain the phenomenon of metalinsulator transition through Anderson localization. Despite the well-understood behaviors of the model, little has been explored theoretically on how the model properties gradually evolve as functions of hybridization parameter, interaction energy, impurity concentration, and temperature. Here, we propose to do a theoretical study on those aspects of a single impurity Anderson model using the distributional exact diagonalization method. We solve the model Hamiltonian by randomly generating sampling distribution of some conducting electron energy levels with various number of occupying electrons. The resulting eigenvalues and eigenstates are then used to define the local single-particle Green function for each sampled electron energy distribution using Lehmann representation. Later, we extract the corresponding self-energy of each distribution, then average over all the distributions and construct the local Green function of the system to calculate the density of states. We repeat this procedure for various values of those controllable parameters, and discuss our results in connection with the criteria of the occurrence of metal-insulator transition in this system.

1. Introduction

Systems of non-interacting electrons have been pretty well understood in how the electronic, magnetic, and optical properties arise. Further, systems with weak electron-electron interactions are usually still understandable as they may still behave qualitatively similar to the noninteracting ones. However, the theories established for non- or weakly-interacting electrons fail to describe the properties of the electron systems in which the strength of the electron-electron interactions is comparable to or larger than the kinetic energy. These systems are now referred to as strongly-correlated electron systems. Discoveries on these systems include, for instance, heavy-fermion compounds[1], superconductors[2], and Mott-Hubbard metal-insulator transition (MIT)[3]. Nowadays many new concepts have been constructed to explain these phenomena, but the understanding of these systems are not complete until now. A Mott insulator, as an example, can undergo phase change from metal to insulator and vice versa at certain condition. Its physical properties change dramatically with variation of control parameters such as carrier concentration, temperature, the interaction energy, or external magnetic field[4].

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One of basic models that can theoretically describe strongly correlated electron systems is Anderson impurity model, or more specifically, the single impurity Anderson model (SIAM). This model describes the influence of the presence of transition element impurity in non-interacting host metal. Rigorous theoretical solutions (both analytic and numeric) for such an impurity problem are still quite complicated or demanding high computational cost. Hence, alternative methods which are simple, effective, and computationally inexpensive are still needed to be developed. Despite the existance of many impurity-problem solvers that have been tested, the distributional exact diagonalization (DED) method proposed by Granath *et al* [5] seems promising for the possibility of its application in small computer cluster. In this research, we develop computational algorithm of the DED method for solving our SIAM problem with various values of impurity concentration. The behavior of each impurity system is observed by varying temperature, interaction energy and hybridization parameters.

2. Model

SIAM which is proposed by P. W. Anderson[6] is a simple model to describe the interplay of charge and spin fluctuations of a localized interacting impurity in a metallic host environment. This magnetic impurity could be for example the d- or f-level of a transition metal atom or rare-earth atom embedded in a non-magnetic metal. In such systems one observes an anomalous minimum in the electrical resistivity at very low temperatures, which is caused by the interaction of the conduction bath electrons with the electron of impurities.

The Hamiltonian of the SIAM consists of three parts

$$\hat{H}_{SIAM} = \hat{H}_{bath} + \hat{H}_{hyb} + H_{imp}.$$
(1)

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 \hat{H}_{bath} serves as the unperturbed Hamiltonian term describing the non-interacting conduction electrons. It is given by $\hat{H}_{bath} = \sum_{\mathbf{k},\sigma} \epsilon_{d\mathbf{k}} \hat{d}^{\dagger}_{\mathbf{k}\sigma} \hat{d}_{\mathbf{k}\sigma}$; where $\epsilon_{d\mathbf{k}}$ is the kinetic energy of the bath state d with momentum \mathbf{k} . The expression $\hat{d}^{\dagger}_{\mathbf{k}\sigma} \hat{d}_{\mathbf{k}\sigma}$ acts as the number operator describing the occupation number of electrons with spin σ in the band state with wave vector \mathbf{k} .

The coupling of the impurity site and the bath levels due to hybridization is described by the Hamiltonian term $\hat{H}_{hyb} = \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} \left(\hat{f}_{\sigma}^{\dagger} \hat{d}_{\mathbf{k}\sigma} + \hat{d}_{\mathbf{k}\sigma}^{\dagger} \hat{f}_{\sigma} \right)$. This type of *d*-*f* coupling is characterized by the hybridization parameter $V_{\mathbf{k}}$. The bath electron with with momentum \mathbf{k} and spin σ is annihilated by operator $\hat{d}_{\mathbf{k}\sigma}$ and then created in the impurity site with spin σ by operator $\hat{f}_{\sigma}^{\dagger}$. Meanwhile, electron which formerly occupies the impurity site is annihilated by operator \hat{f}_{σ} and then created in the bath with momentum \mathbf{k} by operator $\hat{d}_{\mathbf{k}\sigma}^{\dagger}$. In this model, for simplicity, we assume that the hybridization strength is constant in momentum space, giving us $V_{\mathbf{k}} = V = const$. Hence, the hybridization Hamiltonian term can be simplified to be $\hat{H}_{hyb} = V \sum_{\mathbf{k},\sigma} \left(\hat{f}_{\sigma}^{\dagger} \hat{d}_{\mathbf{k}\sigma} + \hat{d}_{\mathbf{k}\sigma}^{\dagger} \hat{f}_{\sigma} \right)$.

The last term of SIAM Hamiltonian, \hat{H}_{imp} , describes the impurity site that is defined as $\hat{H}_{imp} = \sum_{\sigma} \epsilon_f \hat{f}_{\sigma}^{\dagger} \hat{f}_{\sigma} + U \hat{f}_{\uparrow}^{\dagger} \hat{f}_{\uparrow} \hat{f}_{\downarrow}^{\dagger} \hat{f}_{\downarrow}$. It consists of two parts: the first part describes the on-site energy of the localized f-state on the impurity atom, while the second term describes the local electron-electron Coulomb interaction for two electrons occupying the impurity state.

3. Computational method

We aim to address problem of impurity systems with various impurity concentrations. For this, we choose to use the symmetric SIAM and solve it using a stochastic ED method on several small systems containing one f-state and N_d d-states, where N_d is to be varied. To mimic different impurity concentrations, we define the impurity concentration x, such that $x = 1/N_d$ is the ratio of the number of impurity sites to the total number of sites in the entire crystal sample. For

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every system with a fixed x or N_d , the energies of d-states (ϵ_d) are generated randomly with a constraint that they are distributed symmetrically with respect to zero, while the f-on-site energy (ϵ_f) is set fixed at $\epsilon_f = -U/2$. The symmetry of our model implies that the chemical potential (μ) is 0 for all temperatures. Accordingly, we sample the corresponding representative **k** points of ϵ_{d_k} with only N_d base states denoted by an index α running from 1 to N_d . Thus, the simplified model Hamiltonian for each v^{th} - sampling reads as

$$\mathcal{H} = \sum_{\sigma} \sum_{\alpha=1}^{N_d} \epsilon_{d_\alpha} \hat{d}^{\dagger}_{\alpha\sigma} \hat{d}_{\alpha\sigma} + \sum_{\sigma} \epsilon_f \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} + V \sum_{\sigma} \sum_{\alpha=1}^{N_d} \left(\hat{d}^{\dagger}_{\alpha\sigma} \hat{f}_{\sigma} + \hat{f}^{\dagger}_{\sigma} \hat{d}_{\alpha\sigma} \right) + U \hat{f}^{\dagger}_{\uparrow} \hat{f}_{\uparrow} \hat{f}^{\dagger}_{\downarrow} \hat{f}_{\downarrow}.$$
(2)

Our particular goal is to compute the retarded Green's function (GF) of SIAM from ED results for zero and finite temperatures. For this purpose, we need to obtain the eigenstates of \mathcal{H} for N, N + 1, and N - 1 particle systems, respectively. Here, for the symmetric SIAM, N is always set to be half of the total number of orbitals considered in the system, i.e. $N = N_d + 1$. The calculated eigenvalues and eigenstates are then used to compute the retarded GF, G_{ff} , for the f-state, through Lehmann representation [7]. The need for obtaining $G_{\rm ff}$ is particularly for the purpose of extracting the self-energy of system[8]. In Lehmann representation, the corresponding retarded GF for the f electrons can be defined as:

For zero temperature (T = 0)

$$G_{ff_{\sigma v}}^{R}(\omega + i0^{+}) = \frac{1}{Z} \sum_{N=1}^{N_{max}} \left\{ \sum_{l=1}^{\#N+1} \frac{|\langle l|\hat{f}_{\sigma}^{\dagger}|GS^{(N)}\rangle|^{2}}{\omega + i0^{+} - (E_{l}^{(N+1)} - E_{GS}^{(N)} - \mu)} + \sum_{n=1}^{\#N-1} \frac{|\langle n|\hat{f}_{\sigma}|GS^{(N)}\rangle|^{2}}{\omega + i0^{+} + (E_{n}^{(N-1)} - E_{GS}^{(N)} + \mu)} \right\}.$$
(3)

For finite temperature (T > 0)

DOS as follows

$$G_{ff\sigma\upsilon}^{R}(\omega+i0^{+}) = \frac{1}{Z} \sum_{N=1}^{N_{max}} \left\{ \sum_{l=1}^{\#N+1} \sum_{m=1}^{\#N} \frac{\left(e^{-\beta(E_{l}^{(N+1)}-\mu_{(N+1)})} + e^{-\beta(E_{m}^{(N)}-\mu_{(N)})}\right) |\langle l|\hat{f}_{\sigma}^{\dagger}|m\rangle|^{2}}{\omega+i0^{+} - (E_{l}^{(N+1)}-E_{m}^{(N)}-\mu)} + \sum_{n=1}^{\#N-1} \sum_{m=1}^{\#N} \frac{\left(e^{-\beta(E_{n}^{(N-1)}-\mu_{(N-1)})} + e^{-\beta(E_{m}^{(N)}-\mu_{(N)})}\right) |\langle n|\hat{f}_{\sigma}|m\rangle|^{2}}{\omega+i0^{+} + (E_{n}^{(N-1)}-E_{m}^{(N)}+\mu)} \right\}$$
(4)

In SIAM, we believe that under no external magnetic field spontaneous magnetization would not occur. Hence, we would always have $G_{\uparrow} = G_{\downarrow}$. Thus, after obtaining GF of the system at both zero and finite temperature from Eq. (3) and (4), we can then drop the spin index using either $\sigma = \uparrow$ or $\sigma = \downarrow$. The self-energy of the SIAM problem for every v^{th} sampling can be extracted through $\Sigma_v(\omega) = \left(G_{ff_v}^0(\omega + i0^+)\right)^{-1} - \left(G_{ff_v}(\omega + i0^+)\right)^{-1}$; where $G_{vff}^0(\omega + i0^+)$ is bare GF for the *f*-state which is defined as $G_{ff_v}^0(\omega + i0^+) = \frac{1}{\omega + i0^+ - \epsilon_f - \frac{1}{x}\sum_{\alpha} \rho(\epsilon_{d_{\alpha}}) \frac{V^2}{\omega + i0^+ - \epsilon_{d_{\alpha}}}}$. not occur. Hence, we would always have $G_{\uparrow} = G_{\downarrow}$. Thus, after obtaining GF of the system Here, as mentioned before, $x = 1/N_d$ is the concentration of impurity in the system. Finally, after a sufficient number of samplings $(N_{sampling})$, the complete self-energy is the average over all self-energy samples, that is $\Sigma(\omega) = \frac{1}{N_{sampling}} \sum_{v=1}^{N_{sampling}} \Sigma_v(\omega)$. After obtaining the averaged self-energy, we can construct the full CD of the full CD of the self-energy. self-energy, we can construct the full GF of d- electrons $(G_{dd}(\omega + i0^+))$ and the corresponding

$$G_{dd}(\omega + i0^{+}) = \int d\varepsilon \frac{\rho(\varepsilon)}{\omega + i0^{+} - \varepsilon - \frac{V^{2}}{\omega + i0^{+} - \epsilon_{f} - \Sigma(\omega)}} \text{ and } DOS_{d}(\omega) = -\frac{1}{\pi} \text{Im}G_{dd}(\omega + i0^{+}).$$
(5)

In this calculation, we simplify the bare density of states of the metallic host (i.e. the d electron density of states) to be semicircular, that is $\rho(\varepsilon) = \frac{2}{\pi} \sqrt{(1-\varepsilon^2)}$.

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4. Results and discussion

As our specific research goal is to understand the influence of the parameter values in the SIAM problem, we vary temperature (T), hybridization parameter (V), interaction energy (U), and impurity concentration (x). We start with the most concentrated impurity system by taking $x = \frac{1}{2}$. For this x value, we search for the right combination of critical U and V values that lead to metal-insulator phase transition. Then, subsequently we do the same for more dilute systems with $x = \frac{1}{3}, \frac{1}{4}$ and $\frac{1}{5}$. However, for brevity, we only show the results of variation of U, V, and T for the most concentrated system $(x = \frac{1}{2})$ and the most dilute system $(x = \frac{1}{5})$ that we have modeled.

When the d - f hybridization parameter is set to 0 (V = 0, the electrons in d-orbitals do not feel any effect of the presence of impurity. Therefore, the d-orbital band shows bare density of states that represents half-filled metallic band with Fermi energy lying at the middle of the band. If we turn on the hybridization parameter (V > 0), the existence of impurity will influence the movement of the bath electrons. As we increase the hybridization parameter, the charge fluctuations become larger, electrons can hop from bath to the impurity sites. This causes the dband to redistribute into wider range of energy. Instead of gathering around the Fermi level, the electrons spread out and occupy the lower energy states. At some critical values of hybridization parameter V_c and interaction strength U_c , the coupling between d and f orbitals becomes large enough to allow the electrons to more easily go back and forth from d to f states, however the strong interaction at the f site tends to prevent the electrons to do. As a result, this situation leads the d band to split into two parts separated by an energy gap, while the Fermi energy falls inside the energy gap. Hence the metallic band undergoes a transition to become insulating band. Note that the formation of energy gap depends on all the parameters x, V, U, and T. The smaller x, the larger V and U, and the lower T we need, in order for the gap to form. The transitions of the d electron density of states from having no gap until the gap forms upon variation of the parameters x, V, U, and T are illustrated in Figures 1, 2, 3.

To vary the impurity concentration, we change the number of bath (d) states while keeping one impurity (f) state for every system. Therefore, the effect of impurity scattering will be different although we do not change the number of impurity state for our models. As we keep our systems to be always at half filling, the larger number of bath states implies the larger number of non-interacting electrons. It means that the possibility of impurity to scatter the conduction electron becomes more diminished since the entire electrons experience less disorder potential. From Figure 4, we can see that at those specific values of U and V, the MIT occurs for system $x = \frac{1}{2}$.



Figure 1: *d*-band DOS with various V values for system with $x = \frac{1}{2}$ at T = 0 K and with $x = \frac{1}{2}$ at T = 0 K $U_c =$ U = 4 eV



Figure 2: *d*-band DOS with various U values for system 4 eV, $V_c = 1.8$ eV, $E_g = 0.32$ eV)



Figure 3: *d*-band DOS with various U values for system with $x = \frac{1}{5}$ at T = 0 K ($U_c =$ $6.5 \text{ eV}, V_c = 3.6 \text{ eV}, E_g = 0.28$ eV)

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Figure 4: *d*-band DOS for various impurity concentration at T = 0 K ($U_c = 4$ eV, $V_c = 1.8$ eV, $E_q = 0.32$ eV)

Figure 5: *d*-band DOS at some temperatures for system with $x = \frac{1}{2}$ having $T_c = 1600$ K



Figure 6: *d*-band DOS at some temperatures for system with $x = \frac{1}{5}$ having $T_c = 250$ K

When we apply those values of U and V to more dilute systems $(x = \frac{1}{3} \text{ and } \frac{1}{4})$, the gap starts to dissapear and insulating-like band will become 'bad' metallic band that has poor conducting ability. Then, for the last system, $(x = \frac{1}{5})$, the metallic properties get more obvious since the dip of band around Fermi energy become shallow. Thus, the higher impurity concentration, the more probable MIT to occur. In real materials pure Anderson transition often appeas to be temperature-independent. That is because such disorder-induced insulating phase usually has robust gap that remains existing up overy high temperatures[9]. In our model, however, we also vary the interaction energy, so that our systems can undergo Mott-Anderson transition which is temperature-dependent. This hypothesis is verified by our model and calculation, which is shown in the Figure 5 and 6 respectively for system with $x = \frac{1}{2}$ and $x = \frac{1}{5}$.

5. Conclusions

We have developed detailed computational algorithm to implement the DED method on SIAM for various parameter values. Our calculation has proven that DED is a reliable method to solve SIAM problem. From the results, our modeled systems capture the occurrence of Mott-Anderson metal to insulator transition (MIT) at some critical values of impurity concentration (x), temperature (T), interaction energy (U), and hybridization parameter (V). Overall, our study has demonstrated that doping a metallic system with a strongly-correlated element can transform the system into an insulator, depending on the values of controllable parameters, which is consistent with the picture of Anderson localization.

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