Calculation of Optical Conductivity of Anderson Impurity Model for Various Model Parameters

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Abstract: Materials classified as strongly-correlated systems often exhibit complex and fascinating properties due to interactions among electrons as well as between electrons and other constituents of the material. A common model to describe electronic system with strong on-site Coulomb interaction is Hubbard model. One very powerful approximation method for solving Hubbard model having been widely used over the last few decades is dynamical mean-field theory (DMFT). This method maps the original lattice problem into an impurity problem embedded in a self-consistent bath. Apart from the many variants of implementation of DMFT, it relies on using an impurity solver as part of its algorithm. In this work, rather than solving a Hubbard model, we propose to explore the impurity solver itself for solving a problem of metallic host doped with correlated elements, commonly referred to as Anderson impurity model (AIM). We solve the model using the distributional exact diagonalisation method. Our particular aim is to show how the metal-insulator transition (MIT) occurs in the system and how the phenomenon reflects in its optical conductivity for various model parameters.

Keywords: Strongly-correlated systems, impurity solver, Anderson impurity model, optical conductivity, metal-insulator transition.

1. Introduction

Among various kinds of metal-insulator transition (MIT), the most well known one may be that originating from Coulomb repulsive interactions between two electrons occupying d or f orbital of the same atom. The explanation of this phenomenon was first proposed by Nevill Francis Mott in 1949 [1]. One of the theoretical approximations that explains the phenomenon quite nicely is Hubbard model [2], where each atomic site is assumed to have one correlated orbital, presumably d orbital, electrons can hop between sites, and every two electrons occupying the same site undergo Coulomb repulsion. The MIT phenomenon fit with this model is referred to as Mott-Hubbard transition [3]. Another well known model in correlated systems is Anderson impurity model (AIM) [4], which is usually used to describe a problem of metallic host doped with correlated elements. In AIM each atomic site is assumed to have one uncorrelated orbital, presumably s, p, or d orbital, but there is one atomic site (called the impurity site) that has one uncorrelated and one correlated (presumably f) orbitals. In AIM electrons hop between uncorrelated orbitals of different sites. At the impurity site an electron can hybridise between the two orbitals, but two electrons undergo Coulomb repulsion only if they occupy the correlated orbital.
Despite its simple Hamiltonian, Hubbard model generally cannot be solved exactly except for very few situations, such as Hubbard model applied to a small molecule solved using exact diagonalisation method [5], 1D-Hubbard model solved using Bethe ansatz [6], or infinite-D Hubbard model solved within mean-field theory [7]. For other situations one may solve Hubbard model within some approximation method. Among the popular and reliable method for solving Hubbard model in two or three dimensions is the so-called dynamical mean-field theory (DMFT). It maps the originally interacting lattice problem into an effective impurity problem embedded in a self-consistent host. The resulting mapped problem has the Hamiltonian structure that looks like AIM [4]. The part in the DMFT algorithm to solve this resulting impurity problem is referred to as the impurity solver [8]. It is in this regard that AIM has a close connection with Hubbard model.

A new impurity solver of DMFT for solving Hubbard model that employs distributional exact diagonalisation method was recently proposed by Granath and Strand [9]. Other than to be used as an impurity solver of DMFT for solving Hubbard model, the method can also be used independently to solve AIM [4]. In a previous study [10], we used the distributional exact diagonalisation method to explore AIM for various model parameters. In this study, we calculate the optical conductivity from the results of the self-consistent calculations performed in the previous study. Our particular goal is to explore AIM for various model parameters. In this study, we calculate the optical conductivity spectra, considering various values of model parameters.

2. Model

Taking uncorrelated orbital as the d orbital, while the correlated one to be the f orbital, generically the Hamiltonian for finite-dimensional AIM may be written in second-quantized form as follows

$$H = \sum_{\sigma} \sum_{k}^{N} \epsilon(k) d_{k\sigma}^d d_{k\sigma} + \sum_{\sigma}^{\epsilon_f} f_{\sigma}^d + V \sum_{\sigma} \sum_{k}^{N} (d_{k\sigma}^d f_{\sigma} + f_{\sigma}^d d_{k\sigma}) + U f_{\sigma}^d f_{\sigma}^d f_{\sigma}^d f_{\sigma}.$$  (1)

Here, since each atomic site has d orbital with the same on-site energy, $\epsilon_d$, the translational symmetry possessed by the system in the absence of the impurity site allows one to write the part of Hamiltonian for the d band in k-space, where $N$ is the number of k-points in the Brillouin zone, which is essentially equal to the number of atomic sites. In Eq. (2) operator $d_{k\sigma}^\dagger$ ($d_{k\sigma}$) creates (annihilates) electron with momentum $k$ and spin $\sigma$, where $\epsilon(k)$ is the energy dispersion of the d band, while operator $f_{\sigma}^\dagger$ ($f_{\sigma}$) creates (annihilates) electron at orbital $f$ with spin $\sigma$ in the impurity site. The first term is the kinetic part representing the hopping of electrons among the d orbitals of different sites. The second term represents the energy corresponding to the occupation of f orbital by one electron with spin $\sigma$, with $\epsilon_f$ being the f-orbital on-site energy. The third term represents the hybridisation allowing an electron to move between d and f orbitals in the impurity site, with $V$ being the hybridisation parameter. The last term represents the repulsive interaction when two electrons of opposite spins occupy the f orbital at the impurity site, with $U$ being the Coulomb repulsion parameter.

3. Methods

As mentioned earlier, we shall solve the AIM using distributional exact diagonalisation method proposed by Granath and Strand [9]. The idea is that we sample at random only a small number, $N_d$, of k-points among k-points in the Brillouin zone for the d states, along with one f state. Equivalently, rather than selecting k-points, one may select the corresponding energy $\epsilon$ among the $\epsilon(k)$ values. Thus, for one particular sampling, let say the $\nu$-th sampling, we have the Hamiltonian looking like

$$H_\nu = \sum_{\alpha=1}^{N_d} \sum_{\sigma}^{\epsilon_{d\alpha}^\nu} d_{d\sigma}^\dagger d_{d\sigma} + \sum_{\sigma}^{\epsilon_f} f_{\sigma}^\dagger f_{\sigma} + V \sum_{\sigma} \sum_{\alpha=1}^{N_d} (d_{d\sigma}^\dagger f_{\sigma} + f_{\sigma}^\dagger d_{d\sigma}) + U f_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma}.$$  (2)

Here, we are interested in the half-filled system with a particle-hole symmetry, for which we set $\epsilon_f = -U/2$, while the $N_d$ values of $\epsilon_{d\alpha}^\nu$ are to be chosen randomly.
In order to solve this Hamiltonian using exact diagonalisation method we first have to define a set of basis states $|\phi_k\rangle$ which depends on the number of single-particle states and the number of electrons involved. For instance, we take $N_d = 4$, then there are $2(4 + 1) = 10$ available single particle states. Since our system is half-filled we have $\frac{10}{2} = 5$ electrons. With this, our basis set consists of $\frac{10!}{5!(10-5)!} = 252$ configurations, and hence we can form a $252 \times 252$ Hamiltonian matrix whose elements are $\langle \phi_k | H | \phi_l \rangle$. The Hamiltonian matrix can then be exactly diagonalised to give us a set of energy eigenvalues and eigenstates. These energy eigenvalues and eigenstates are to be used to obtain the retarded Green function through Lehmann representation. But in order to do so, we need to diagonalise two other Hamiltonian matrices corresponding to $5 - 1 = 4$ and $5 + 1 = 6$ electrons. From the resulting retarded Green function for the corresponding sampling we can then extract the corresponding retarded self-energy matrix. We need to repeat this procedure with as many samplings as possible, let say upto 10000 samplings. The “true” self-energy matrix is to be obtained by averaging all the sampling results. With this “true” self-energy matrix we can then construct all the corresponding “true” retarded Green functions for the $d$ and $f$ orbitals. All this process has been described in our previous paper [10], so we shall not repeat it in this paper.

Finally, having the $d$ retarded Green function in hand we compute the optical conductivity through Kubo formula which in our case reads as

$$
\sigma(\omega) = \frac{\pi e^2}{\hbar a} \int dv \sum_\lambda v^2 \ A_{d\lambda}(v) A_{d\lambda}(v + \omega) \ \frac{f(v, T, \mu) - f(v + \omega, T, \mu)}{\omega},
$$

where $v \equiv ta/\hbar$ is the velocity parameter with $a$ being the lattice constant of the material, $A_{d\lambda}(v) = -\frac{1}{\pi} \text{Im} \ G_{d\lambda}(v)$ is the spectral function of the $d$ electron at single-particle state $\lambda$, with $G_{d\lambda}(v)$ being the corresponding retarded Green function of the $d$ electron, $f(v, T, \mu)$ is the Fermi distribution function at energy $v$, temperature $T$, and chemical potential $\mu$.

4. Results and Discussion

Throughout our calculations we vary the energy variable $\varepsilon$ of the $d$ band dispersion following Bethe lattice such that $-t < \varepsilon < t$, with $t$ taken to be 1 eV, while $\varepsilon_f$ is set following the $U$ value, $\varepsilon_f = -U/2$. We take the number of samplings $N_{\text{sampling}} = 10000$. We vary the parameters $U, V, T, \text{and } x$. Here, $x$ is the impurity concentration which we define as $x = \frac{1}{N_d}$, such that we can vary $x$ through $N_d$. In addition, we use the following numerical parameters: $N_\varepsilon = 3001$ (number of $\varepsilon$-points), $\eta = 0.03$ eV (artificial broadening parameter).

4.1. Variation of $x$

First, we set our system at the ground state, i.e. $T = 0$. We choose $U = 4$ eV and $V = 1.8$ eV just so the density of states (DOS($\omega$) = $-\frac{1}{\pi} \text{Im} \ \Sigma_d G_{d\lambda}(\omega)$) has a noticeable pseudogap. We perform the calculations for $x = 1/2$, $x = 1/4$, and $x = 1/5$. Figure 1(a) shows the DOS of the system for various $x$ values at fixed $U, V, \text{and } T$. It is seen that once the pseudogap has been formed, by increasing $x$ the pseudogap tends to become a full gap. Meanwhile, the optical gap also tends to increase with increasing $x$, making the system be more and more insulating.
4.2. Variation of $V$

Next, we analyse the effect of hybridisation parameter, $V$. This parameter measures how strong the tendency for an electron previously occupying the $d$ orbital to move to the $f$ orbital, or vice versa, at the impurity site. In Figure 2(a) we show how the DOS at fixed $x = \frac{1}{5}$, $U = 6.5$ eV, and $T = 0$ K, evolves as $V$ is introduced and increased. As we see from the figure, the presence of $V$ causes some states around the chemical potential ($\omega = \mu = 0$) to get repelled towards the left and the right of the centre of the DOS symmetrically, leading to the formation of pseudogap, hence the system starts to transform from metallic to insulating-like. As $V$ increases, the pseudogap deepens and eventually forms a full gap at large $V$. Figure 2(b) displays how the corresponding optical conductivity evolves with variation of $V$ accordingly. It is clearly seen that, when $V = 0$, the optical conductivity has a Drude peak, signifying a good metallic character. Upon introducing and increasing $V$, the Drude peak vanishes, while an optical gap forms and becomes larger and larger, indicating that the system becomes more and more insulating.

Figure 2. (a) Density of states (DOS) and (b) optical conductivity of the system with variation of hybridisation parameter $V$, for $x = 1/5, U = 6.5$ eV, $T = 0$ K.

4.3. Variation of $U$

Further, we analyse the effect of variation of the on-site Coulomb repulsion parameter $U$. Here we set the other parameters fixed at $x = 1/4$, $V = 2.1$ eV, $T = 0$ K. From we can observe in Figure 3(a), once a hybridisation pseudogap has been well established, increasing the $U$ value from 3 to 6 eV does not change the profile of DOS that much. However, if we look more closely at the pseudogap region (see the inset of Figure 3(a)) there is a tendency that pseudogap becomes narrower, indicating that the system
becomes less insulating. Accordingly, in Figure 3(b) we can see the evolution of the optical conductivity with the variation of $U$, where the optical gap tends to decrease with increasing $U$.

![Figure 3](image)

**Figure 3.** (a) Density of states (DOS) and (b) optical conductivity of the system with variation of on-site Coulomb repulsion parameter $U$, for $x = 1/4$, $V = 2.1$ eV, $T = 0$ K.

### 4.4. Variation of $T$

Lastly, we analyse the effect of variation of temperature, $T$. Here we take the other parameters fixed at $x = 1/4$, $V = 3$ eV, $U = 6$ eV. At those fixed parameters values, the ground state of the system ($T = 0$ K) is insulating indicated by the full gap in the DOS (see Figure 4(a)). As the system starts to be thermally excited ($T > 0$ K), new quasi-particle states form in the gap region, weakening the presence of the gap itself. As temperature becomes very large, the gap becomes much narrowed, and in addition, a sharp quasi-particle peak emerges. Figure 4(b) shows how the evolution of the DOS with increasing $T$ manifests in the evolution of the optical conductivity. In particular, in the low photon energy region ($\omega < 0.2$ eV) we can clearly see the emergence of the Drude peak as $T$ increases, indicating transformation from insulating to metallic. Meanwhile, we also observe that the uprise position, i.e. the photon energy value at which the optical conductivity value suddenly increases from almost zero, gets blue-shifted, which may correspond to the increase of the separation between the two symmetry peaks of the DOS. We interpret these as a compensation of the emergence of the new states on the gap region.

![Figure 4](image)

**Figure 4.** (a) Density of states (DOS) and (b) optical conductivity of the system with variation of temperature $T$, for $x = 1/4$, $V = 3$ eV, $U = 6$ eV.
5. Conclusion
We have performed calculations of optical conductivity of Anderson impurity model from the self-consistent Green function obtained through distributional exact diagonalisation followed by implementation of Lehman representation. We focus our attention to the metal-insulator transition occurring in the system and how the phenomenon may be influenced by the change of various parameters \((x, V, U, T)\) of the model. We investigate these effects by observing the evolution of the density of states and optical conductivity. Our results confirm that the peak metal with some impurity can eventually transform the system into an insulator at sufficient amount of doping concentration \((x)\). The increase of hybridisation parameter \(V\) tends to make the system become more insulating, while increasing \(U\) tends to narrow the insulating gap. Once the system has an insulating gap in the ground state, thermal excitation tends to destroy the gap, hence transforming into a metal at sufficiently high temperature. Overall our study has confirmed that the distributional exact diagonalisation method is reliable to solve the Anderson impurity model.

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