Anderson localization in disordered electron-phonon systems
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Introduction

While the localization of a single non-interacting electron is successfully studied with a variety of methods the question how localization and electron-phonon interaction compete has been addressed considerably less. As a first step towards more realistic systems we studied in the work presented here phonon interaction competition has been addressed concerning local (retarted) Green’s function. While the localization of a single non-interacting Anderson model (green curve) and the lowest polaron subband in the antiadiabatic strong coupling regime.

The Anderson-Holstein model

The Anderson-Holstein model (AAM) consists of tight-binding electrons in a medium with compositional disorder, which are locally coupled to dispersionless Einstein phonons.

The “Holstein” properties of this model are determined by two interaction parameters, \( \lambda = E_2/2J \) and \( g^2 = E_p/\hbar \), and the adiabaticity ratio \( \alpha = \beta \). Polaron formation sets in provided that \( \lambda \ll 1 \) and \( g^2 \ll 1 \). The “Anderson” properties of this model are determined by the distribution of the site energies \( \epsilon_i \) which are assumed to be independent random variables with a box distribution \( \rho(\epsilon_i) = \frac{1}{2}(\epsilon_i^2 - \epsilon_i) \). We will consider a single electron (polaron) at \( \tau = 0 \).

The method

Conceptually the statDMFT is a combination of the selfconsistent theory of localization [1] (AAT) and the DMFT [2]. Its construction proceeds in two steps. One starts by expressing the local Green’s function \( G_{0\omega}(\epsilon_i) \) through Green’s functions \( G_{0\omega}(\epsilon_i) \) which are determined for the lattice with site \( i \) removed. Continuing this expansion yields an infinite hierarchy of equations for general lattices. If one neglects contributions from nontrivial hopping which is equivalent to working on a Bethe lattice – one finds a single equation relating \( G_{0\omega}(\epsilon_i) \) to the local Green’s functions \( G_{0\omega}(\epsilon_i) \) on the \( K \) neighbouring sites \( i \).

\[
G_{\omega}(\epsilon_i) = \frac{1}{\omega - \epsilon_i + \sum_{\epsilon_f} \rho(\epsilon_f) G_{\omega}(\epsilon_f)}
\]

Here the contribution from electron-phonon coupling is included through the electronic phonon selfenergy \( \Sigma_{\omega}(\epsilon_i) \) which is calculated in the limit \( K \to \infty \) (i.e. within DMFT). Note that \( \Sigma_{\omega}(\epsilon_i) \) is a spatially varying quantity. For a single Holstein polaron \( \Sigma_{\omega}(\epsilon_i) \) is given by a continued fraction

\[
\Sigma_{\omega}(\epsilon_i) = \frac{\lambda g^{2}}{\omega - \epsilon_i - \sum_{\epsilon_f} \rho(\epsilon_f) G_{\omega}(\epsilon_f)}
\]

whose \( N \) steps account for the emission and reabsorption of \( N \) at \( T = 0 \) virtual phonons. Here \( F_{\omega}(\epsilon_i) = \rho(\epsilon_i)^{1/2} \sum_{\epsilon_f} \rho(\epsilon_f) G_{\omega}(\epsilon_f) \) denotes the Green’s function without e-ph-interaction at site \( i \). For the second step of the construction one observes that \( G_{\omega}(\epsilon_i) \) is a random variable due to the randomness of the on site potential \( \epsilon_i \). The distribution of

\[
G_{\omega}(\epsilon_i) = \text{independent from the lattice site. Moreover the local Green’s functions on the rhs of the above written equation are independently distributed. Hence this equation can be reinterpreted as a stochastic selfconsistency equation for a random variable \( G_{\omega}(\epsilon_i) \) and the rhs of this selfrepetition and } \mathbf{i} \) denote no longer specific lattice sites but particular realizations of the random variable \( G_{\omega}(\epsilon_i) \). We solve the stochastic selfconsistency equation numerically through a Monte-Carlo procedure (Gibbs sampling) which constructs a selfconsistent random sample for \( G_{\omega}(\epsilon_i) \) from which all relevant distributions can be obtained.

Remark: all results are given for \( K = 2 \). Energies are measured in units of the bare bandwidth \( W = \sqrt{2J} \).

Localization condition

The quality of interest is the probability distribution of the local density of states (LDOS)

\[
N_{\omega}(\epsilon_i) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \text{Im} \ln G_{\omega}(\epsilon + i\epsilon)
\]

This distribution contains all spatial fluctuations and hence the full information about localization. For small disorder the distribution is nearly symmetric and centered at its arithmetic mean value \( N_{\omega}(\epsilon) \). With increasing disorder heavy tails evolve and the distribution becomes strongly asymmetric, the mean value is no longer representative. At the localization transition the distribution becomes even singular. The mean values is however still finite due to the rare events in the tail of the distribution. Therefore the transition from extended to localized states is accompanied by a qualitative change in the distribution that is not detected by the arithmetic mean value.

\[
\text{Typical density of states}
\]

Although the distribution of the LDOS should be understood as the primary object of the theory, it is sometimes more convenient to work with certain averaged quantities. It is however crucial to choose an appropriate average which accounts for the asymmetric form of the distribution in the strongly disordered regime. Defining the typical density of states as

\[
\langle \rho(\epsilon_i) \rangle = \frac{1}{\omega - \epsilon_i + \sum_{\epsilon_f} \rho(\epsilon_f) G_{\omega}(\epsilon_f)}
\]

for \( \omega = 0 \), we can define the localization parameter as

\[
\text{Typical density of states}
\]

For strong coupling and large phonon frequency \( \lambda \ll 0 \), \( \alpha = 2.25 \) the lowest polaron subband is completely coherent \( \rho(\epsilon_f) = 0 \) with a rather symmetric DOS. The localization parameter of the zero polaron subband is expected to be the same as for the pure Anderson model. As a comparison of \( N_{\omega}(\epsilon) \) and the mobility edge trajectories shows this is indeed the case.

Conclusions

We reexamined how the probability distribution of the states at the mobility edge \( \epsilon = \gamma \) reflects the spatial fluctuation analysis of localization. Furthermore we studied the localization of a Holstein polaron by means of the statDMFT in its application to strongly correlated parameter regimes. The important physical lesson is that the localization properties of a Holstein polaron are highly renormalized within a subband without affecting the overall polaronic features of the system.

Adiabatic intermediate coupling

For intermediate coupling and small phonon frequency \( \lambda = 1.0 \), \( \alpha = 0.1 \) the localization properties of the polaron do substantially differ from that of the bare electron. States at bottom of the lowest polaron subband are rather mobile and remain nearly unaffected for small disorder. In contrast states at the top are rather sluggish and very susceptible to disorder. Although the two lowest subbands which correspond to different number of phonons remain separated over a large range of disorder they eventually begin to merge. The relevant energy scale changes before complete localization of the lowest subband can occur.

References