Anderson localization in disordered electron-phonon systems

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In order to study the competition between Anderson localization and polaron formation we adopt the statistical dynamic mean field theory to a generic model for a strongly coupled electron-phonon system. The localization properties of a single polaron are discussed in detail.

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 adressed considerably less. As a first step towards more realistic systems we studied in the work presented here the localization properties of a single Holstein polaron within a microscopic approach, the *statistical dynamic mean-field theory* (statDMFT) which has been previously applied to the disordered Hubbard model [2]. The statDMFT is an extension of the DMFT to include spatial fluctuations on a finite dimensional lattice. In the spirit of Anderson's first work on localization it adresses the question of localization through distributions of local quantities. Its basic idea is to set up a Monte-Carlo scheme for the local (retarted) Green's function $G_{ii}(\omega)$ whose distribution (but not average) is critical at the localization transition.

Anderson-Holstein model

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

$$H = \sum_i \epsilon_i c_i^\dagger c_i + J \sum_{\langle ij \rangle} c_i^\dagger c_j + c_j^\dagger c_i + \Omega \sum_i b_i^\dagger b_i - \sqrt{E_P \Omega} \sum_i c_i^\dagger c_i (b_i^\dagger + b_i)$$

The "Holstein" properties of this model are determined by two interaction parameters, $\lambda = E_p/2J$ and $g^2 = E_p/\Omega$, and the adiabaticity ratio $\alpha = \Omega/J$. Polaron formation sets in provided that $\lambda \gtrsim 1$ and $g^2 \gtrsim 1$. The "Anderson" properties of this model are determined by the distribution of the on site energies ϵ_i which are assumed to be independent random variables with a box distribution $p(\epsilon_i) = \frac{1}{\gamma}\,\theta\left(\frac{\gamma}{2} - |\epsilon_i|\right)$.

We will consider a single electron (polaron) at $T = 0$.

The method

Conceptionally the statDMFT is a combination of the selfconsistent theory of localization [4] (AAT) and the DMFT [5]. Its construction proceeds in two steps. One starts by expressing the local Green's function $G_{ii}(\omega)$ through Green's functions $G^{(i)}_{jk}(\omega)$ which are obtained 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 loops – which is equivalent to working on a Bethe lattice – one finds a single equation relating $G_{ii}(\omega)$ to the local Green's functions $G_{jj}(\omega)$ on the K neighbouring sites to i.

$$G_{ii}(\omega) = \frac{1}{\omega - \epsilon_i - J^2 \sum_{j=1}^{K} G_{jj}(\omega) - \Sigma_{ii}(\omega)}$$

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

$$\Sigma_{ii}(\omega) = \cfrac{E_p\Omega}{F_{ii}^{-1}(\omega-\Omega) - \cfrac{2E_p\Omega}{F_{ii}^{-1}(\omega-2\Omega) - \cdots}}$$

whose N-th level accounts for the emission and reabsorption of N (at $T = 0$ virtual) phonons. Here $F_{ii}(\omega) = (\omega - \epsilon_i - J^2 \sum_{j=1}^{K} G_{jj}(\omega))^{-1}$ denotes the Green's function without e-ph-interaction at site i.

For the second step of the construction one observes that $G_{ii}(\omega)$ is a random variable due to the randomness of the on site potential ϵ_i. The distribution of $G_{ii}(\omega)$ is independent from the lattice site. Moreover the K 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 $G_{ii}(\omega)$ (in turn of this reinterpretation i and j denote no longer specific lattice sites but particular realizations of the random variable $G_{ii}(\omega)$). We solve the stochastic selfconsistency equation numerically through a Monte-Carlo procedure (Gibbs sampling) which constructs a selfconsistent random sample for $G_{ii}(\omega)$ from which all relevant distributions can be obtained.

Remark: all result are given for $K = 2$. Energies are measured in units of the bare bandwidth $W_0 = 4J\sqrt{K} = 1$. Due to the scaling of the hopping matrix element J as $J = \tilde{J}/\sqrt{K}$ in the $K\to\infty$-limit we work with rescaled interaction parameters $\tilde{\lambda} = E_p/2\tilde{J} = \lambda/\sqrt{K}$ and $\tilde{\alpha} = \Omega/\tilde{J} = \alpha/\sqrt{K}$.

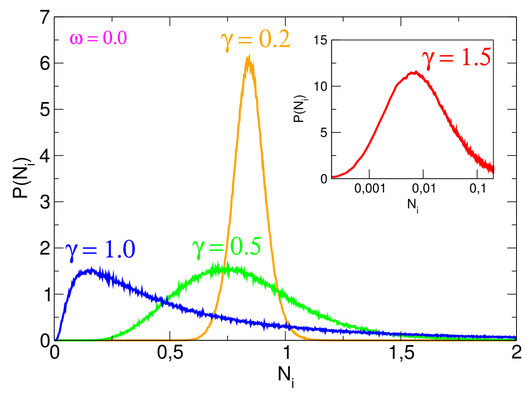
Localization criterion

Distributions

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

$$N_i(\omega) = -\frac{1}{\pi} \lim_{\eta\to 0+} \operatorname{Im} G_{ii}(\omega + \mathrm{i}\eta)$$

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 $N^{\mathrm{ave}}(\omega)$. 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.



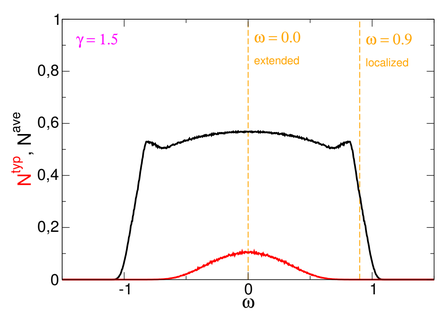
Probability distribution of the LDOS for the pure Anderson model (no e-ph-interaction) in the band center $\omega = 0$, for four values of disorder γ. Note the logarithmic scale in the inset.

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 appropiate average which accounts for the asymmetric form of the distribution in the strongly disordered regime. Defining the typical density of states as

$$N^{\mathrm{typ}}(\omega) = \exp\left(\frac{1}{N}\sum_i \log N_i(\omega)\right)$$

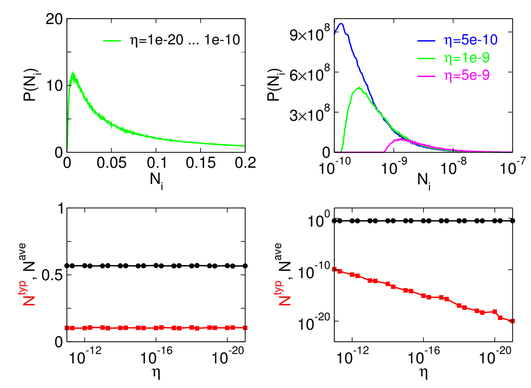
states at energy ω are classified as extended if $N^{\mathrm{typ}}(\omega) > 0$, and localized if $N^{\mathrm{typ}}(\omega) = 0$. In *both* cases $N^{\mathrm{ave}}(\omega) > 0$ (otherwise one had no states at ω). So the typical (but not the averaged) density of states plays the role of an "order parameter" for localization.



Anderson-Model, average and typical density of states for $\gamma = 1.5$.

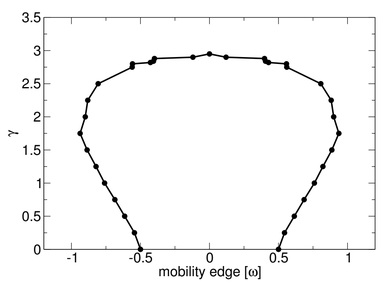
$\eta \to 0$ -limit

The LDOS $N_i = -\frac{1}{\pi}\operatorname{Im} G_{ii}(\omega + \mathrm{i}\eta)$, hence its distribution, is defined in the limit $\eta \to 0$. While no strict distinction between extended and localized states can be made for finite η the limiting distribution for $\eta \to 0$ exhibits clearly different features in the two regimes.



Probability distribution of the LDOS, N^{ave} and N^{typ} with respect to η for extended ($\omega = 0.0$, left column) and localized ($\omega = 0.9$, right column) states, with $\gamma = 1.5$.

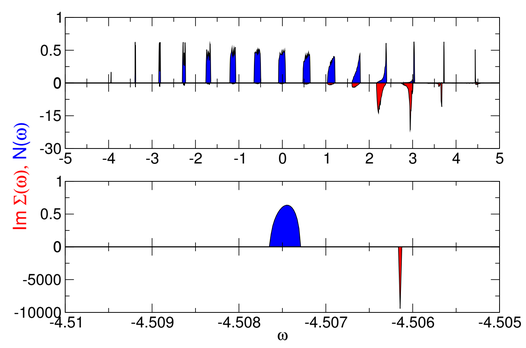
This is the key observation: localization manifests in the distribution of the LDOS for $\eta \to 0$. Exploiting the limit $\eta \to 0$ numerically allows for a clear distinction of localized versus extended states.



Mobility edges for the Anderson model on a Bethe lattice with $K = 2$. The critical disorder for complete localization is $\gamma_c(\omega = 0) \approx 2.9$.

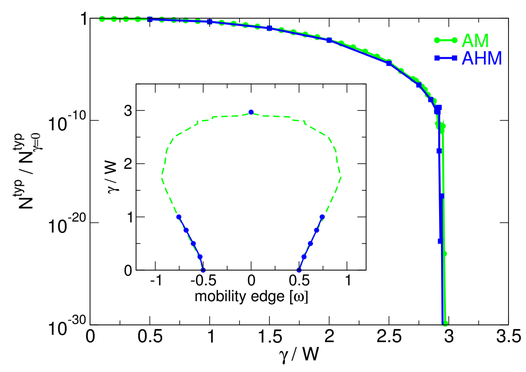
Localization of a polaron

Antiadiabatic strong coupling



Antiadiabatic strong coupling $\tilde{\alpha} = 2.25$, $\tilde{\lambda} = 9.0$ (DMFT result). The lowest polaron subband has a renormalized bandwidth $W = 3.45 \times 10^{-4}$ and is fully coherent.

For strong coupling and large phonon frequency ($\tilde{\lambda} = 9.0$, $\tilde{\alpha} = 2.25$) the lowest polaron subband is completely coherent ($\operatorname{Im}\Sigma(\omega) = 0$) with a rather symmetric DOS. The localization properties of this band are expected to be same as for the pure Anderson model. As a comparison of N^{typ} and the mobility edge trajectories shows this is indeed the case.

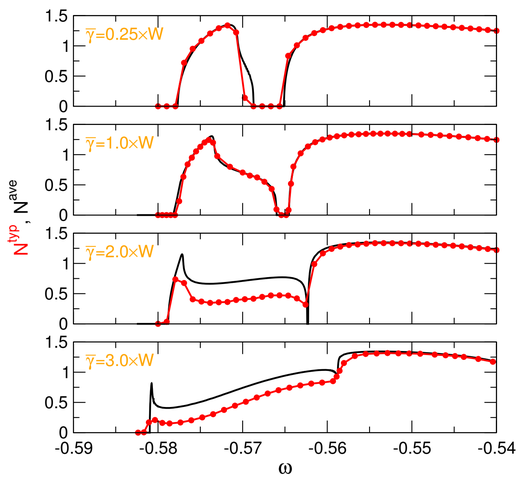


Comparison of N^{typ} in the bandcenter of the pure Anderson model (green curve) and the lowest polaron subband in the antiadiabatic strong coupling regime $\tilde{\lambda} = 9.0$, $\tilde{\alpha} = 2.25$ (blue curve). The respective bandwidth is denoted by W. The inset displays part of the corresponding mobility edge trajectories. The energy ω is scaled to the respective bandwidth and -center.

The two mobility edge trajectories do match even for very strong disorder when all states in the polaron subband become localized. However the critical disorder is orders of magnitude smaller than the separation of the subbands because of the strong renormalization of the bandwidth. So disorder can localize all states within a single subband without affecting the overall polaronic features of the system.

Adiabatic intermediate coupling

For intermediate coupling and small phonon frequency ($\tilde{\lambda} = 1.0$, $\tilde{\alpha} = 0.2$) 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 a 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.

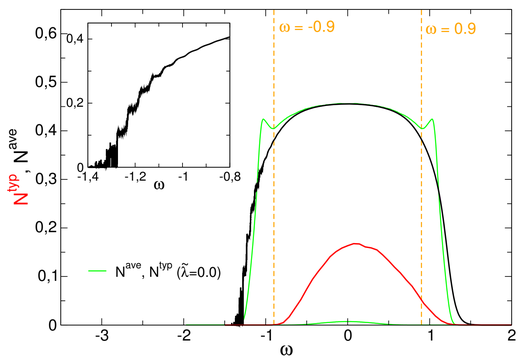


N^{ave} and N^{typ} for $\tilde{\lambda} = 1.0$, $\tilde{\alpha} = 0.2$ and four values of γ. $W \approx 8.123 \times 10^{-3}$ is the width of the lowest polaron subband of the pure Holstein model ($\gamma = 0$).

Anderson regime

Up to now we discussed the "Holstein regime" regime when disorder is comparable to the width of the lowest polaron subband. We can as well consider the "Anderson regime" when disorder is large on the energy scale set by e-ph interaction.

For $\gamma = 2$ in the pure Anderson model localized and extended states are separated by mobility edges at $\omega \approx \pm 0.9$. If electron-phonon interaction is switched on (here with $\tilde{\alpha} = 0.2$, $\tilde{\lambda} = 0.75$) states at energy ω begin to couple to states at energies less than ω (recall that $T = 0$). States at the lower mobility edge can only couple to states which are already localized. Hence disorder and e-ph-interaction work in the same direction. As a consequence polaron like defect states do form as is indicated by the step-like structure of the average DOS (this can be readily understood in terms of the independent boson model). At the upper mobility edge formerly localized states delocalize due to the coupling to extended states towards the band center. Here e-ph-interaction weakens the tendency towards localization. As a consequence the upper mobility edge is shifted to higher energies.



N^{ave} (DMFT) and N^{typ} for $\tilde{\alpha} = 0.2$, $\tilde{\lambda} = 0.75$, $\gamma = 2.0$. The green curves show N^{ave} and N^{typ} for $\tilde{\lambda} = 0$. The vertical slashed lines indicate the mobility edges for $\tilde{\lambda} = 0$.

Conclusions

We reexamined how the probability distribution of the local density of states can be used for an analysis of localization. Furthermore we studied the localization of a Holstein polaron by means of the statDMFT and demonstrated its applicability in various parameter regimes. The important physical lesson is that the localization properties of a Holstein polaron are highly non universal.

References

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