# Statistical dynamical mean field description of strongly correlated disordered electron-phonon systems


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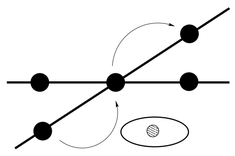
*Abstract:* Combining the self-consistent theory of localization and the dynamical mean-field theory, we present a theoretical approach capable of describing both self-trapping of charge carriers during the process of polaron formation and disorder-induced Anderson localization. By constructing random samples for the local density of states (LDOS) we analyze the distribution function for this quantity and demonstrate that the typical rather than the mean LDOS is a natural measure to distinguish between itinerant and localized states. Significant polaron effects on the mobility edge are found.


## Motivation

The question of how the electron-phonon (EP) interaction influences the localization transition caused by disorder [1], i.e. by strong impurity-induced spatial fluctuations in the potential energy, has been addressed by Anderson about thirty years ago [2]. He called attention to the particular importance of EP coupling effects in the vicinity of the so-called "mobility edge", separating itinerant (extended) and localized states.

Nevertheless, there is as yet not much theoretical work even for the simplest case of a single electron moving in a disordered, deformable medium.



As a first step towards addressing this problem, in Ref. [3] the single-particle Holstein model with site-diagonal, binary-alloy-type disorder was studied within the dynamical mean field approximation (DMFA) [4]. The DMFA, however, cannot (fully) discriminate between itinerant and localized states, mainly because the randomness is treated at the level of the coherent potential approximation.

## Model

In order to remedy this shortcoming, recently the authors [5] adopted the statistical DMFA (statDMFA) [6] to the Anderson-Holstein Hamiltonian,

$$\mathcal{H} = \sum_i \epsilon_i n_i - J\sum_{\langle ij\rangle}(c_i^\dagger c_j + \text{H.c.}) - \sqrt{E_p\Omega}\sum_i (b_i + b_i^\dagger)n_i + \Omega\sum_i b_i^\dagger b_i\,,$$

where $J$ denotes the electron transfer amplitude, $\Omega$ is the frequency of the optical phonon, $E_p$ is the polaron shift, and the on-site energies $\{\epsilon_i\}$ are assumed to be independent random variables with probability density $p(\epsilon_i) = (1/\gamma)\theta(\gamma/2 - |\epsilon_i|)$.

## Localization criterion

As a natural measure of the itinerancy of a polaron state, we consider the tunneling rate from a given site, defined - on a Bethe lattice with connectivity $K$ ($\tilde{J} = J\sqrt{K}$) - as the imaginary part of the hybridization function

$$\Gamma_i(\omega) = (\pi\tilde{J}^2/K)\sum_{l=1}^{K} N_l(\omega), \quad \text{where} \quad N_l(\omega) = -(1/\pi)\text{Im}\mathcal{G}_l(\omega)$$

is the local density of states (LDOS). The LDOS, directly connected to the local amplitude of the electron wave function, undergoes a qualitative change upon localization implying a vanishing tunneling rate $\Gamma_i(\omega)$ for a localized state at energy $\omega$.

## Method

The statDMFA [6] is essentially a probabilistic method (in the sense of the self-consistent theory of localization [7]), based on the construction of random samples for the physical quantities of interest.

The local single-particle Green function and the related hybridization function are given by ($z = \omega + i\eta$)

$$\mathcal{G}_i(z) = \frac{1}{z - \epsilon_i - H_i(z) - \Sigma_i(z)} \quad \text{and}$$

$$H_i = \frac{\tilde{J}^2}{K}\sum_{l=1}^{K+1}\frac{1}{z - \epsilon_l - \bar{H}_l^i - \bar{\Sigma}_l^i},$$

respectively. We now ignore that the functions on the rhs of $H_i$ should be calculated for the Bethe lattice with the site $i$ removed, i.e. we make the replacement $\{\bar{\mathcal{G}}_l^i,\ \bar{H}_l^i,\ \bar{\Sigma}_l^i\} \rightsquigarrow \{\mathcal{G}_l,\ H_l,\ \Sigma_l\}$, and furthermore take $K$ as the typical number of terms even for the central site. Finally, the EP self-energy contribution is determined in the limit $K \to \infty$. The self-energy is then local and, in terms of a continuous fraction expansion, takes the form

$$\Sigma_l(z) = \frac{E_p 1\Omega}{[F_l^{(1)}(z)]^{-1} - \frac{E_p 2\Omega}{[F_l^{(2)}(z)]^{-1} - \ldots}},$$

with $[F_l^{(p)}(z)]^{-1} = z - p\Omega - \epsilon_i - H_l^{(p)}(z)$ and $H_l^{(p)}(z) = H_l(z - p\Omega)$. Here the energy shift keeps track of the number of virtual phonons ($0 < p < M$). Regardless of the local EP self-energy, the statDMFA takes spatial fluctuations of, e.g., the LDOS into account and provides an adequate description of disorder effects. Due to the randomness in the on-site energies, the tunneling rate and the LDOS is a random variables, and the question of whether they vanish or not depends on the probability density exhibiting different features for itinerant and localized states [1, 7]. In particular, the difference between the mean and typical LDOS,

$$N^{\text{mean}}(\omega) = \frac{1}{N}\sum_i^N N_i(\omega) \quad \text{and}$$

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

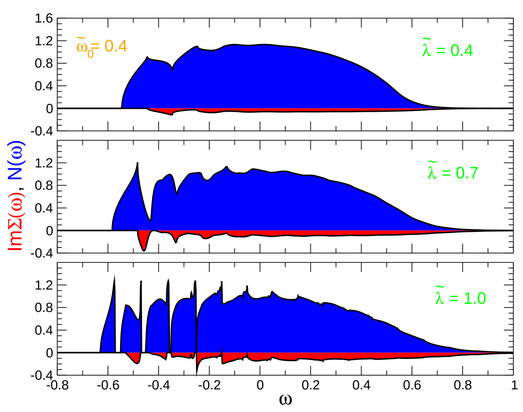
obtained by the arithmetic and geometric mean of the LDOS, respectively, is a useful measure to discriminate between extended and localized states. $N^{\text{mean}}(\omega) > 0$ but $N^{\text{typ}}(\omega) = 0$ indicates a localized state at energy $\omega$.

In the numerical work, we calculated the LDOS by solving a recursion scheme for $H_l^{(p)}$ which depends on $K\varepsilon_j'$s, $KH_j^{(p)}{}'$s, ..., and $KH_j^{(p_{max})}{}'$s. Starting from an initial random configuration for the independent variables $H_l^{(p)}$, which is successively updated with a sampling technique similar to the one described in Ref. [7], we constructed self-consistent random samples for $H_l^{(p)}$, using $K = 2$, $N = 100\,000$, $M = 35$, and $\eta = 10^{-8}$.

## Numerical results and discussion

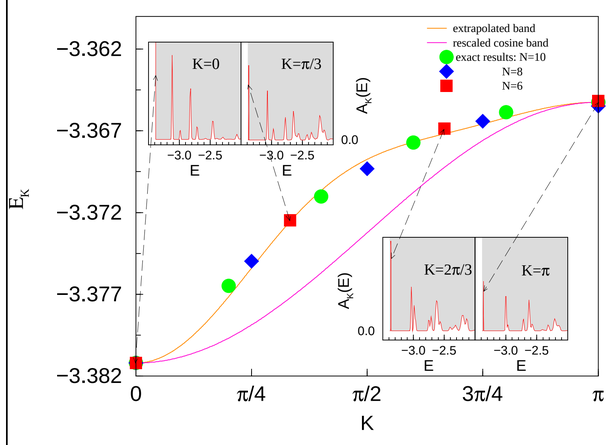
### A. Polaron formation without disorder

The physical properties of the Holstein model are determined by two interaction parameters, $\tilde{\lambda} = E_p/2\tilde{J}$ and $g^2 = E_p/\Omega$, and the adiabaticity ratio $\tilde{\alpha} = \Omega/\tilde{J}$. Polaron formation sets in provided that $\tilde{\lambda} \gtrsim 1/\sqrt{K}$ and $g^2 \gtrsim 1$. Of course, the internal structure of the polaron depends on $\tilde{\alpha}$.




*Evolution of the LDOS $N(\omega)$ (blue) and the imaginary part of the EP self-energy $\text{Im}\Sigma(\omega)$ (red) for the ordered Holstein model ($\gamma = 0$) with increasing EP coupling $\tilde{\lambda} = 0.4, 0.7,$ and $1.0$ (from top to bottom). Results are given for $\tilde{\alpha} = 0.4$ and $\tilde{W}_0 = 1.0$.*

In the crossover regime the typical polaron band dispersion exhibits several striking features: (i) The coherent bandwidth is by about a factor of 10 times larger than predicted by the standard Lang-Firsov formula $\Delta E_{LF} = 4t\exp[-g^2]$. (ii) The effective polaronic band dispersion deviates substantially from a simple rescaled bare band due to further than nearest-neighbour ranged hopping processes induced by the residual polaron-phonon interaction. (iii) The flattening of the band dispersion at large momenta persists to surprisingly large interaction strengths, even if the renormalized band width is by one order of magnitude smaller than the bare phonon frequency.



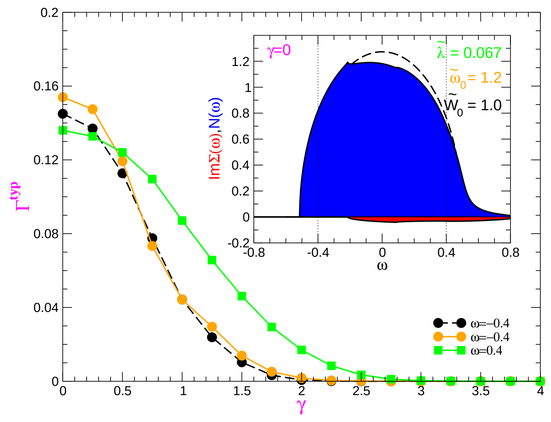

*Band dispersion $E(K)$ of a single electron described by the Holstein model on 1D rings with $N$ sites, where $g = 2.73$ and $\Omega = 0.4$. The insets show the low-energy part of the one-particle spectral function $A_K(E)$ for selected momenta $K$. The magenta line corresponds to the dispersion of a free particle with a renormalized bandwidth. The orange line gives a least-squares fit to an effective band dispersion $\tilde{E}_K = \sum_{l=0}^{3} a_l \cos lK$.*

## B. Interplay of localization & self-trapping phenomena

Without EP coupling, i.e. in the pure Anderson model, the critical disorder strength needed to localize all states is $(\gamma_c/\tilde{W}_0)_{\text{complete}} \approx 2.25$, where $\tilde{W}_0 = 4\tilde{J}$. Disorder affects polaron states quite differently in the adiabatic ($\tilde{\alpha} \ll 1$), non-adiabatic ($\tilde{\alpha} \sim 1$), and antiadiabatic ($\tilde{\alpha} \gg 1$) cases.

*I. Weak EP-coupling case:*

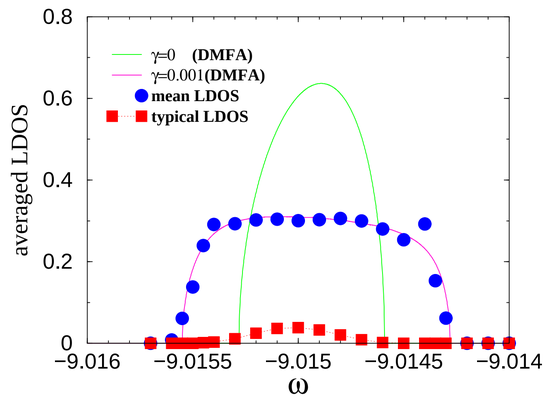
In the weak EP coupling regime, it has been shown that the quantum interference needed for localization is significantly suppressed by inelastic polaron-phonon scattering processes [5]: States above the optical phonon emission threshold are more difficult to localize than the corresponding bare electron states.




*Typical tunneling rates $\Gamma^{\text{typ}}(\omega;\gamma)$ in the (non-to-antiadiabatic) weak EP coupling regime ($\tilde{W}_0 = 1.0$, $\tilde{\alpha} = 1.2$, and $\tilde{\lambda} = 0.067$). Filled circles denote data for $\tilde{\lambda} = 0$. The inset shows the LDOS $N(\omega)$ and the imaginary part of the EP self-energy $\text{Im}\Sigma(\omega)$ for $\gamma = 0$; dashed and (vertical) dotted lines indicate, respectively, the density of states for $\tilde{\lambda} = 0$ and the energies $\omega$ for which $\Gamma^{\text{typ}}(\omega;\gamma)$ is plotted.*

*II. Strong EP-coupling case:*

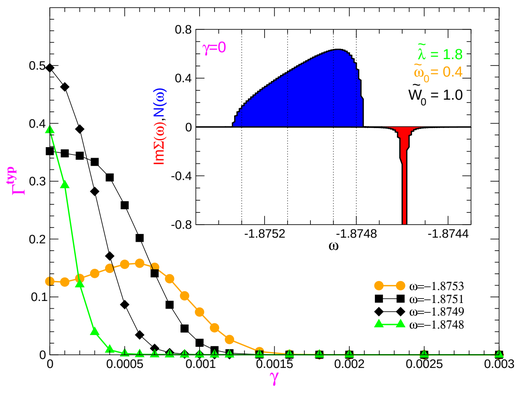
In the very strong EP coupling regime, extremely weak disorder turns itinerant into localized polaron states. Surprisingly, the ratio $(\gamma_c/\tilde{W})_{\text{complete}}$, where $\tilde{W}$ is the band width of the lowest polaron subband, is almost the same as for a bare electron. In fact, in the non-adiabatic strong EP coupling regime, where the band collapse changes only the overall energy scale, disorder affects a polaron in a similar way as a bare electron. For example, the LDOS and mobility edges are symmetric.



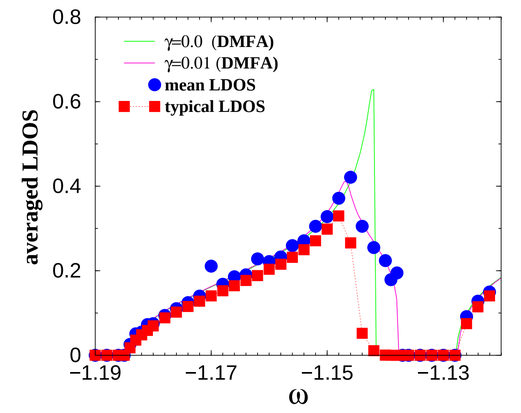

*Mean and typical LDOS for the lowest polaron subband in the non-adiabatic strong EP coupling region ($\tilde{\lambda} = 9.0$, $\tilde{\alpha} = 2.25$, and $J = 0.5$). The pronounced disorder-induced broadening of the LDOS occurs because the variation of the on-site energies $\gamma = 0.001$ is on the order of the strongly renormalized band width $\tilde{W}$.*

*III. Crossover regime:*

In the adiabatic intermediate-to-strong EP coupling regime the physics is much more involved. Here the band dispersion of the lowest subband significantly deviates from a rescaled bare band [8], leading to a strong asymmetric LDOS. Specifically, the states at the bottom of the subband are mostly electronic and rather mobile due to long-range tunneling induced by EP coupling, whereas the states at the top of the subband are rather phononic and immobile [8]. As a direct consequence, the states at the zone boundary are very susceptible to disorder, i.e. the critical disorder strength needed to localize these states is much smaller than for states at the bottom, and, from the results for the typical LDOS, we find asymmetric mobility edges. Moreover, $(\gamma_c/\tilde{W})_{\text{complete}} \approx 2.8$, which is larger than the corresponding ratio for a bare electron. Thus, contrary to naive expectations, at intermediate EP couplings, an adiabatic polaron is even more difficult to localize than a bare electron.

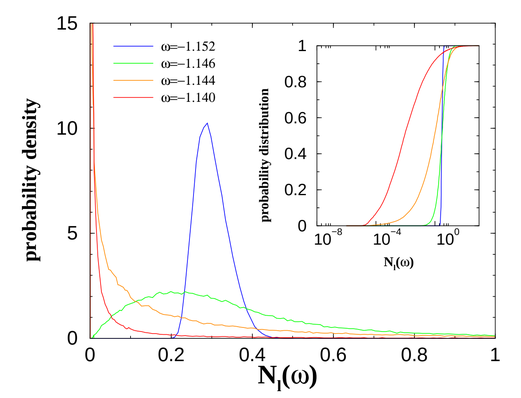



*Typical tunneling rates $\Gamma^{\text{typ}}(\omega;\gamma)$ in the (adiabatic) intermediate EP coupling regime ($\tilde{\alpha} = 0.4$, $\tilde{\lambda} = 1.8$, $\tilde{W}_0 = 2.0$). The inset display the subband LDOS $N(\omega)$ and the imaginary part of the EP self-energy $\text{Im}\Sigma(\omega)$ for $\gamma = 0$ (vertical dotted lines indicate the energies $\omega$ for which $\Gamma^{\text{typ}}(\omega;\gamma)$ is plotted). Note the small spectral weight of the lowest polaron subband.*




*Mean and typical LDOS in the adiabatic intermediate-to-strong EP coupling region ($\tilde{\lambda} = 1.0$, $\tilde{\alpha} = 0.25$, $J = 0.5$). Note that $N^{\text{mean}}(\omega)$ is almost perfectly approximated by the DMFA. At about $\omega = -1.13$ the second polaronic subband starts.*

It is very instructive to discuss the behavior of the probability density of the LDOS and the corresponding probability distribution. Note that both quantities have to be calculated self-consistently within our sampling procedure. The results demonstrate the dramatic change of the probability density of $N_l(\omega)$ when the system undergoes the localization transition by crossing the mobility edge. In the region of localized states, the probability density for the LDOS is broad and very asymmetric and, as a consequence, the mean LDOS is not representative.




*Probability density of the LDOS for four representative energies. The inset shows the probability distribution, i.e., the cumulant of the probability density.*

*Conclusions:* To summarize, in terms of the Anderson Holstein model, we have demonstrated that the statDMFA, which according to the spirit of Anderson's early work [1] focuses on distribution functions and associates typical rather than mean values to physical quantities, yields a proper description of disordered electron-phonon systems.

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