Local Approximation of the Holstein Polaron Problem

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1   Introduction

The Holstein model [1] describes non interacting electrons on a lattice cou-
pled to dispersionless phonons. For one electron in the system, the bare
electron is dressed by a cloud of bosonic excitations and is called a polaron.
The properties of this new particle are still puzzling, although this problem
is very old and has been solved numerically for finite or infinite size sys-
tems [2]. Most of these works are devoted to study the Green's function of
the bare electron, $G(\mathbf{k}, \omega)$, which can be measured by photoemission ex-
periments, and not to understand the fundamental nature of the polaron as
a dressed particle [3, 4]. The difficulty arise from the fact that only in the
atomic limit of the problem, a small polaron operator can be mathematically
constructed, and its Green's function $\tilde{G}(\omega)$ defined.

Within the Local Impurity Self-Consistent Approximation [5], which be-
comes exact in the limit of infinite dimensions, the analytical expression of
the local Green's function for the electron [6] has strong simililarities with
its counterpart in the atomic limit, so it is worth to review this local approxi-
mation in the spirit of the small polaron physics, and to learn how to compute
the Green's function $\tilde{G}(\mathbf{k}, z)$ of the small polaron.

For one electron in the system, the Hamiltonian reads

$$H = \varepsilon_0 \sum_j c_j^\dagger c_j - t_0 \sum_{j,\delta} c_{j+\delta}^\dagger c_j + \omega_0 \sum_j b_j^\dagger b_j \qquad (1)$$

$$-g_0 \omega_0 \sum_j c_j^\dagger c_j (b_j^\dagger + b_j),$$

where $c_j^\dagger$ and c_j creates and annihilates an electron at site $\mathbf{R}_j$, $b_j^\dagger$ and b_j
creates and annihilates a bosonic excitation at site $\mathbf{R}_j$. The sum over j runs
over the M sites of the lattice, the sum over δ runs over nearest neighbors,
ω_0 is the optical frequency of the phonons, ε_0 is the atomic energy, t_0 is the
hopping energy, and g_0 is a dimensionless coupling constant. We define the
basis states of the phonons as $|\mathbf{n}\rangle$, with $b_j^\dagger b_j |\mathbf{n}\rangle = n_j |\mathbf{n}\rangle$. For one electron
in the system, the basis states are $c_j^\dagger |\mathbf{n}\rangle$. At zero temperature, the polaron
problem is to compute the Green's function for the electron

$$G_{i,j}^{\mathbf{m},\mathbf{n}}(z) = \langle \mathbf{m}|c_i \frac{1}{z-H} c_j^\dagger |\mathbf{n}\rangle \qquad (2)$$

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This Green's function contains all the physics of the problem. On the ground state of the phonons, that is $G_{i,j}^{\mathbf{0,0}}(z)$, we have just access to the excitations of the bare electron, $G(\mathbf{k}, \omega)$. In this paper, we focus on the Green's function of the small polaron,

$$\tilde{G}_{i,j}^{\mathbf{0,0}}(z) = \langle \mathbf{0}|U_i^\dagger c_i \frac{1}{z - H} c_j^\dagger U_j|\mathbf{0}\rangle \tag{3}$$

where U_j is a local operator defined from the atomic limit of the problem.

2   Basic ideas of DMFT

The Dynamical Mean Field Theory, or DMFT, deals with correlated electrons on a lattice and reduces the problem to a single site embedded self-consistently in an effective medium [5], so the the first idea is to focus on a single site, o,

$$H = H^{(o)} - t_0 \sum_\delta c_{o+\delta}^\dagger c_o + H^{(\odot)} \tag{4}$$

with

$$H^{(o)} = \varepsilon_0 c_o^\dagger c_o + \omega_0 b_o^\dagger b_o - g_0 \omega_0 (b_o^\dagger + b_o) c_o^\dagger c_o \tag{5}$$

and to define an effective Hamiltonian for this single site

$$H_o = H^{(o)} + H_W^{(o)}. \tag{6}$$

The term $H_W^{(o)}$ describes the effective medium.

Consider the one particle Green's function for the electron at this site o on the vacuum of the phonons

$$G_{o,o}(t) = \frac{\theta(t)}{i\hbar} \langle \mathbf{0}|c_o(t)c_o^\dagger|\mathbf{0}\rangle. \tag{7}$$

We obtain the equation of evolution

$$i\hbar\partial_t G_{o,o}(t) = \delta(t) + \varepsilon_0 G_{o,o}(t) - t_0 \sum_\delta G_{o+\delta,o}(t) + F_{o,o}(t) \tag{8}$$

with

$$F_{o,o}(t) = \frac{\theta(t)}{i\hbar} \langle \mathbf{0}|[c_o, H^{(o)} - \varepsilon_0 c_o^\dagger c_o](t)c_o^\dagger|\mathbf{0}\rangle. \tag{9}$$

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Going to complex valued frequencies, we get

$$zG_{o,o}(z) = 1 + \varepsilon_0 G_{o,o}(z) - t_0 \sum_\delta G_{o+\delta,o}(z) + F_{o,o}(z). \qquad (10)$$

We see that we can obtain a closed solution for the local Green's function if we can define a local Weiss's self-energy

$$-t_0 \sum_\delta G_{o+\delta,o}(z) = W_{o,o}(z)G_{o,o}(z) \qquad (11)$$

and a local interaction self-energy

$$F_{o,o}(z) = \Sigma_{o,o}(z)G_{o,o}(z). \qquad (12)$$

Then the solution is

$$G_{o,o}(z) = \frac{1}{z - \varepsilon_0 - W_{o,o}(z) - \Sigma_{o,o}(z)}. \qquad (13)$$

Now, without approximation, for a periodic lattice, we know that the equation of evolution has the form

$$zG(\mathbf{k}, z) = 1 + \varepsilon_0 G(\mathbf{k}, z) + \xi_k G(\mathbf{k}, z) + \Sigma(\mathbf{k}, z)G(\mathbf{k}, z). \qquad (14)$$

We have introduced the Fourier transforms

$$c_j = \frac{1}{\sqrt{M}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_j} c_{\mathbf{k}}, \qquad (15)$$

$$G_{i,j}(z) = \frac{1}{M} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} G(\mathbf{k}, z), \qquad (16)$$

$$-t_0 \sum_\delta G_{i+\delta,i}(z) = \sum_{\mathbf{k}} \xi_{\mathbf{k}} G(\mathbf{k}, z). \qquad (17)$$

If we choose $\Sigma(\mathbf{k}, z) = \Sigma(z)$, we obtain

$$\frac{1}{M} \sum_{\mathbf{k}} \xi_{\mathbf{k}} G(\mathbf{k}, z) = W(z)G(z) \qquad (18)$$

with

$$G(\mathbf{k}, z) = \frac{1}{z - \varepsilon_0 - \xi_{\mathbf{k}} - \Sigma(z)} \qquad (19)$$

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and

$$G(z) = \frac{1}{M} \sum_{\mathbf{k}} G(\mathbf{k}, z) = \frac{1}{z - \varepsilon_0 - W(z) - \Sigma(z)}. \qquad (20)$$

We thus see that we can set up a local approximation for our lattice Hamiltonian if we put by hand that the self-energy is local, and get a Weiss's self-energy that depends only of the lattice and of this local self-energy.

Let us consider a two-site problem. In this case we have $\xi_{\mathbf{k}} = \pm t_0$, so the local Green's function is given by

$$G(z) = \frac{1}{2} \left[\frac{1}{z - \varepsilon_0 - t_0 - \Sigma(z)} + \frac{1}{z - \varepsilon_0 + t_0 - \Sigma(z)} \right], \qquad (21)$$

and we obtain the expression of the Weiss's self-energy

$$W(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma(z)}. \qquad (22)$$

At this stage, we introduce the Renormalized Perturbation Expansion, or RPE [7]. Within the DMFT, the equation of evolution of the Green's function, for a periodic lattice, is

$$z G_{i,j}(z) = \delta_{i,j} + \varepsilon_0 G_{i,j}(z) - t_0 \sum_{\delta} G_{i+\delta,j}(z) + \Sigma(z) G_{i,j}(z). \qquad (23)$$

We can thus define a free propagator

$$G_{i,j}^{(0)}(z) = \frac{\delta_{i,j}}{z - \varepsilon_0 - \Sigma(z)} \qquad (24)$$

and set a Dyson's equation with the hopping term as the non diagonal part of the Hamiltonian. Figure 1(a) corresponds to the contribution

$$G_{i,j} = G_{i,i}^{(0)} \, t_0 G_{n1,n1}^{(0)} \, t_0 G_{j,j}^{(0)} \qquad (25)$$

and Figure 1(b) corresponds to the contribution

$$G_{i,i} = G_{i,i}^{(0)} \, t_0 G_{n1,n1}^{(0)} \, t_0 G_{n2,n2}^{(0)} \, t_0 G_{n3,n3}^{(0)} \, t_0 G_{i,i}^{(0)}. \qquad (26)$$

The RPE states that one uses renormalized Green's functions as we sum over all paths. The above contribution for $G_{i,j}$ becomes

$$G_{i,j} = G_{i,i} \, t_0 G_{n1,n1[i]} \, t_0 G_{j,j,[i,n1]} \qquad (27)$$
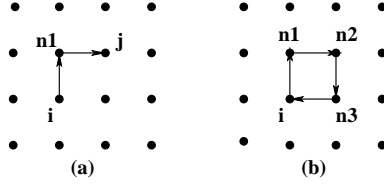
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Figure 1: Path (a) is a contribution to $G_{i,j}$ and path (b) to $G_{i,i}$.

where $G_{n1,n1[i]}$ is the renormalized Green's function for site $n1$ for a lattice where the site i has been removed, and $G_{j,j,[i,n1]}$ is the renormalized Green's function for site j where sites i and $n1$ have been removed from the lattice. The contribution for $G_{i,i}$ becomes

$$G_{i,i} = G_{i,i} \, t_0 G_{n1,n1[i]} \, t_0 G_{n2,n2[i,n1]} \, t_0 G_{n3,n3[i,n1,n2]} \, t_0 G_{i,i}^{(0)}. \qquad (28)$$

The last factor $G_{i,i}^{(0)}$ is the unrenormalized Green's function since the first factor $G_{i,i}$ takes account of the renormalization.

Let us consider a one dimensional infinite lattice. The equation for $G_{i,i}$ is

$$G_{i,i} = G_{i,i}^{(0)} + t_0^2 G_{i,i} G_{i+1,i+1[i]} G_{i,i}^{(0)} + t_0^2 G_{i,i} G_{i-1,i-1[i]} G_{i,i}^{(0)}. \qquad (29)$$

Within the RPE, the path $i \rightarrow i+1 \rightarrow i+2 \rightarrow i+1 \rightarrow i$ is not allowed since the site $i+1$ has been removed of the lattice. Next, we get

$$G_{i+1,i+1[i]} = G_{i+1,i+1}^{(0)} + t_0^2 G_{i+1,i+1[i]} G_{i+2,i+2[i,i+1]} G_{i+1,i+1}^{(0)}. \qquad (30)$$

We notice that $G_{i+2,i+2[i,i+1]} = G_{i+2,i+2[i+1]}$. We thus obtain the solution for the local Green's function as a continued fraction expansion,

$$G_{i,i}(z) = \frac{1}{z - \varepsilon_0 - \Sigma(z) - 2t_0^2 \Phi(z)} \qquad (31)$$

with the self-consistent equation for $\Phi(z)$,

$$\Phi(z) = \frac{1}{z - \varepsilon_0 - \Sigma(z) - t_0^2 \Phi(z)}. \qquad (32)$$

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For the two-site cluster, we obtain the equations

$$G_{1,1} = G_{1,1}^{(0)} + t_0^2 G_{1,1} G_{2,2[1]} G_{1,1}^{(0)} \tag{33}$$

and $G_{2,2[1]} = G_{2,2}^{(0)}$. The local Green's function is thus

$$G_{1,1}(z) = \cfrac{1}{z - \varepsilon_0 - \Sigma(z) - \cfrac{t_0^2}{z - \varepsilon_0 - \Sigma(z)}}. \tag{34}$$

For the Bethe lattice with Z neighbors, we obtain

$$G_{i,i} = G_{i,i}^{(0)} + \sum_{\delta} t_0^2 G_{i,i} G_{i+\delta,i+\delta[i]} G_{i,i}^{(0)} \tag{35}$$

and

$$G_{i+\delta,i+\delta[i]} = G_{i+\delta,i+\delta}^{(0)} \tag{36}$$

$$+ \sum_{\delta'} t_0^2 G_{i+\delta,i+\delta[i]} G_{i+\delta+\delta',i+\delta+\delta'[i,i+\delta]} G_{i+\delta,i+\delta}^{(0)}.$$

For the site i there is Z indentical contributions, while for site $i + \delta$ there is only $Z - 1$ contributions since the path back to i is forbiden. We obtain the solution for the local Green's function

$$G_{i,i}(z) = \frac{1}{z - \varepsilon_0 - \Sigma(z) - Z t_0^2 \Phi(z)} \tag{37}$$

with the recursive expansion

$$\Phi(z) = \frac{1}{z - \varepsilon_0 - \Sigma(z) - (Z-1)t_0^2 \Phi(z)}. \tag{38}$$

Now, if we take the limit $Z \to \infty$ with the scaling $t_0 \to t_0/\sqrt{Z}$, we obtain $W(z) = t_0^2 G(z)$.

Consider now a non periodic lattice. In this case the equations of evolution, within the DMFT, are

$$z G_{i,j}(z) = \delta_{i,j} + \varepsilon_0 G_{i,j}(z) + \Sigma_i(z) G_{i,j}(z) - t_0 \sum_{\delta} G_{i+\delta,j}(z) \tag{39}$$

and we define the free propagators of the RPE as

$$G_{i,i}^{(0)}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_i(z)}. \tag{40}$$

For a three-site problem, with open boundary conditions, we get the equations of evolution

$$\begin{cases} zG_{1,1}(z) = 1 + (\varepsilon_0 + \Sigma_1(z))G_{1,1}(z) - t_0 G_{1,2}(z) \\[2mm] zG_{2,1}(z) = (\varepsilon_0 + \Sigma_2(z))G_{2,1}(z) - t_0 G_{1,1}(z) - t_0 G_{3,1}(z) \\[2mm] zG_{3,1}(z) = (\varepsilon_0 + \Sigma_3(z))G_{3,1}(z) - t_0 G_{2,1}(z) \end{cases} \tag{41}$$

In the language of the RPE, we write

$$\begin{cases} G_{1,1}(z) &= G_{1,1}^{(0)}(z) + t_0^2 G_{1,1}(z)G_{2,2[1]}(z)G_{1,1}^{(0)}(z) \\[2mm] G_{2,2[1]}(z) &= G_{2,2}^{(0)}(z) + t_0^2 G_{2,2[1]}(z)G_{3,3[1,2]}(z)G_{2,2}^{(0)}(z) \\[2mm] G_{3,3[1,2]}(z) &= G_{3,3}^{(0)}(z) \end{cases} \tag{42}$$

and obtain the solution as

$$G_{1,1}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_1(z) - W_1(z)} \tag{43}$$

with

$$W_1(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma_2(z) - \dfrac{t_0^2}{z - \varepsilon_0 - \Sigma_3(z)}}. \tag{44}$$

For $G_{2,2}(z)$, we obtain

$$G_{2,2}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_2(z) - W_2(z)} \tag{45}$$

with

$$W_2(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma_1(z)} + \frac{t_0^2}{z - \varepsilon_0 - \Sigma_3(z)}. \tag{46}$$

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In this case, $\Sigma_1(z) = \Sigma_3(z)$ and $W_1(z) = W_3(z)$. We notice that $G_{1,2}(z) = -t_0 G_{1,1}(z) G_{2,2[1]}(z)$ and $G_{1,3}(z) = t_0^2 G_{1,1}(z) G_{2,2[1]}(z) G_{3,3[1,2]}(z)$, i.e. that all the non-diagonal Green's functions can be expressed in terms of local Green's functions (that may differ by their Weiss's self-energies). We notice, also, that the Weiss's self-energy of a given site involves only the interacting self-energies of the other sites.

3   Atomic Solution

For a single site, the Hamiltonian reads

$$H_{at} = \varepsilon_0 c^\dagger c + \omega_0 b^\dagger b - g_0 \omega_0 c^\dagger c (b^\dagger + b). \tag{47}$$

The basis states of the phonons are $|n\rangle$, with $b^\dagger b |n\rangle = n|n\rangle$. The Hamiltonian commutes with the number of electron $c^\dagger c$, so one can diagonalize it in each subspace. For $c^\dagger c = 0$, one gets an harmonic oscillator with $H_{at}|n\rangle = n\omega_0 |n\rangle$. For $c^\dagger c = 1$, one gets a displaced harmonic oscillator with $H_{at}|n) = (\varepsilon_0 - g_0^2 \omega_0 + n\omega_0)|n)$. The eigenstates are $|n) = U|n\rangle$ where U is the unitary operator

$$U = e^{g_0(b^\dagger - b)} = e^{-\frac{1}{2}g_0^2} e^{g_0 b^\dagger} e^{-g_0 b} \tag{48}$$

with the properties $U^\dagger b U = b + g_0$ and $U^\dagger b^\dagger U = b^\dagger + g_0$ [8]. The Green's function of the electron is given by

$$G_{at}^{m,n}(z) = \langle m | c \frac{1}{z - H_{at}} c^\dagger | n \rangle. \tag{49}$$

Since we compute it for one electron, we get

$$G_{at}^{m,n}(z) = \langle m | \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 (b^\dagger + b)} | n \rangle. \tag{50}$$

Next, we define the atomic polaron, or small polaron, creation operator as $\tilde{c}^\dagger = U c^\dagger$. When acting on the state $|n\rangle$ it creates an electron and a coherent state $|n) = U|n\rangle$. The Green's function of the small polaron is given by

$$\tilde{G}_{at}^{m,n}(z) = \langle m | U^\dagger c \frac{1}{z - H_{at}} c^\dagger U | n \rangle = \frac{\delta_{m,n}}{z - \varepsilon_0 + g_0^2 \omega_0 - m\omega_0}. \tag{51}$$

Instead of writing matrix elements, one can directly write the operator form of these local Green's functions:

$$\mathbf{G}_{at}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 X} \tag{52}$$

and

$$\tilde{\mathbf{G}}_{at}(z) = \frac{1}{z - \tilde{\varepsilon}_0 - \omega_0 b^\dagger b} \tag{53}$$

with $\tilde{\varepsilon}_0 = \varepsilon_0 - g_0^2 \omega_0$ and $X = b^\dagger + b$. We notice the relation $\tilde{\mathbf{G}}_{at}(z) = U^\dagger \mathbf{G}_{at}(z) U$.

Finally, we introduce the unitary transformation that diagonalize H_{at}, such that $e^S = 1$ for $c^\dagger c = 0$ and $e^S = U$ for $c^\dagger c = 1$. This is just $S = g_0 c^\dagger c (b^\dagger - b)$. One obtains the transformed Hamiltonian as

$$\tilde{H}_{at} = e^{-S} H e^S = \tilde{\varepsilon}_0 c^\dagger c + \omega_0 b^\dagger b. \tag{54}$$

It describes a free fermionic small polaron and free bosonic excitations.

4 Standard DMFT solution

In the Local Impurity Self-Consistent Approximation [5], one defines a local Hamiltonian H_{loc} for an given site o, which contains the atomic Hamiltonian H_{at} and a Weiss's Hamiltonian H_W, given by

$$H_W = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k v_k [c_k^\dagger c + c^\dagger c_k]. \tag{55}$$

Here, c_k and $c_k^\dagger$ are auxiliary fermionic annihilation and creation operators. They mimic the contribution of the other sites of the lattice. The parameters ε_k and v_k are chosen to fit the Weiss's self-energy of this given site, $W(z)$. Since there is only one electron in our problem, we have the condition $c^\dagger c + \sum_k c_k^\dagger c_k = 1$. The basis states of the problem are $c^\dagger |n\rangle$ and $c_k^\dagger |n\rangle$, so we can define Green's functions for these auxiliary fermions as

$$G_{k,k}^{m,n}(z) = \langle m | c_k \frac{1}{z - H_{loc}} c_k^\dagger | n \rangle. \tag{56}$$

The problem is to compute the local Green's function for the electron

$$\mathbf{G}_{loc}^{m,n}(z) = \langle m | c \frac{1}{z - H_{loc}} c^\dagger | n \rangle. \tag{57}$$

Let us first compute the local Green's function for $g_0 = 0$. We define diagonal Green's functions for $v_k = 0$ and then use the Dyson's equation. The diagonal Green's functions are

$$G_{o,o}^{(0)}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b} \tag{58}$$

and

$$G_{k,k}^{(0)}(z) = \frac{1}{z - \varepsilon_k - \omega_0 b^\dagger b}. \tag{59}$$

The Dyson's equations are

$$\begin{cases} G_{o,o}(z) = G_{o,o}^{(0)}(z) + \sum_k v_k G_{o,o}^{(0)}(z) G_{k,o}(z) \\ \\ G_{k,o}(z) = v_k G_{k,k}^{(0)}(z) G_{o,o}(z) \end{cases} \tag{60}$$

with the solution

$$\mathbf{G}_{loc}^{(0)}(z) = G_{o,o}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b - W(z - \omega_0 b^\dagger b)} \tag{61}$$

and

$$W(z) = \sum_k \frac{v_k^2}{z - \varepsilon_k}. \tag{62}$$

For $g_0 \neq 0$, we consider the local Hamiltonian for the small polaron $\tilde{H}_{loc} = e^{-S} H_{loc} e^S$. The diagonal part is given by

$$\tilde{H}_{loc}^{(0)} = \tilde{\varepsilon}_0 c^\dagger c + \omega_0 b^\dagger b + \sum_k \varepsilon_k c_k^\dagger c_k \tag{63}$$

so we define the free Green's functions

$$\tilde{G}_{o,o}^{(0)}(z) = \frac{1}{z - \tilde{\varepsilon}_0 - \omega_0 b^\dagger b} \tag{64}$$

and

$$G_{k,k}^{(0)}(z) = \frac{1}{z - \varepsilon_k - \omega_0 b^\dagger b}. \tag{65}$$

The interaction part is given by

$$\tilde{H}_{loc}^{(1)}(z) = \sum_k v_k [U c_k^\dagger c + U^\dagger c^\dagger c_k]. \tag{66}$$

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One obtains the Dyson's equations

$$\begin{cases} \tilde{G}_{o,o}(z) = \tilde{G}^{(0)}_{o,o}(z) + \sum_k v_k \tilde{G}^{(0)}_{o,o}(z) U^\dagger G_{k,o}(z) \\ \\ G_{k,o}(z) = v_k G^{(0)}_{k,k}(z) U \tilde{G}_{o,o}(z) \end{cases} \tag{67}$$

and the solution

$$\tilde{\mathbf{G}}_{loc}(z) = \tilde{G}_{o,o}(z) = \frac{1}{z - \tilde{\varepsilon}_0 - \omega_0 b^\dagger b - \tilde{\mathbf{W}}(z)} \tag{68}$$

with $\tilde{\mathbf{W}}(z) = U^\dagger W(z - \omega_0 b^\dagger b) U$. Finally, we use $\tilde{\mathbf{G}}_{loc}(z) = U^\dagger \mathbf{G}_{loc}(z) U$ and get the solution of the problem

$$\mathbf{G}_{loc}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g\omega_0 X - W(z - \omega_0 b^\dagger b)}. \tag{69}$$

We notice that $\mathbf{G}_{loc}(z) = \mathbf{G}_{at}(z - W(z - \omega_0 b^\dagger b))$. Once again, we use the Dyson's equation to compute $\mathbf{G}^{0,0}_{loc}(z)$ with

$$\mathbf{G}^{(0)}_{loc}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b - W(z - \omega_0 b^\dagger b)} \tag{70}$$

and

$$\mathbf{G}_{loc}(z) = \mathbf{G}^{(0)}_{loc}(z) - g_0 \omega_0 \mathbf{G}^{(0)}_{loc}(z) X \mathbf{G}_{loc}(z). \tag{71}$$

We obtain the solution

$$\mathbf{G}^{0,0}_{loc}(z) = \frac{1}{z - \varepsilon_0 - W(z) - g_0^2 \omega_0^2 \Lambda_1(z; W(z))} \tag{72}$$

with

$$\Lambda_n(z; W(z)) = \tag{73}$$

$$\frac{1}{z - \varepsilon_0 - n\omega_0 - W(z - n\omega_0) - (n+1)g_0^2 \omega_0^2 \Lambda_{n+1}(z; W(z))}.$$

Writing the solution as

$$\mathbf{G}^{0,0}_{loc}(z) = \frac{1}{z - \omega_0 - W(z) - \Sigma(z)} \tag{74}$$

we identify the self-energy.

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We have thus obtained the desired local interaction self-energy $\Sigma_i(z)$ of a given site as a function only of its local Weiss's self-energy, i.e. $\Sigma_i(z) = g_0^2 \omega_0^2 \Lambda_1(z; W_i(z))$. Now, since we can obtain the local Weiss's self-energy as a function of the local interaction self-energies of all the other sites, we have solved the problem.

5   General Framework

Consider the Green's function of the small polaron

$$\tilde{G}_{i,j}^{\mathbf{m},\mathbf{n}}(z) = \langle \mathbf{m}|U_i^\dagger c_i \frac{1}{z-H} c_j^\dagger U_j|\mathbf{n}\rangle \tag{75}$$

with $U_j = e^{g_0(b_j^\dagger - b_j)}$. Writing the Hamiltonian $H = H^{(0)} + V$, where V is the hopping part, one obtains

$$\langle \mathbf{m}|U_i^\dagger c_i \frac{1}{z-H^{(0)}} c_j^\dagger U_j|\mathbf{n}\rangle = \frac{\delta_{i,j}\delta_{\mathbf{m},\mathbf{n}}}{z - \langle \mathbf{m}|U_j^\dagger H^{(0)} U_j|\mathbf{m}\rangle}. \tag{76}$$

We thus define the free local Green's function as

$$\tilde{G}_{i,i}^{(0)}(z) = \frac{1}{z - \tilde{\varepsilon}_0 - \omega_0 \sum_j b_j^\dagger b_j} \tag{77}$$

and get the Dyson's equation

$$\tilde{G}_{i,i}(z) = \tilde{G}_{i,i}^{(0)}(z) - t_0 \sum_\delta \tilde{G}_{i,i}^{(0)}(z) U_i^\dagger U_{i+\delta} \tilde{G}_{i+\delta,i}(z). \tag{78}$$

Now, we use the relation $\tilde{G}_{i,j}(z) = U_i^\dagger G_{i,j}(z) U_j$ to obtain the Dyson's equation for the Green's function of the electron

$$G_{i,i}(z) = G_{i,i}^{(0)}(z) - t_0 \sum_\delta G_{i,i}^{(0)}(z) G_{i+\delta,i}(z) \tag{79}$$

with

$$G_{i,i}^{(0)}(z) = \frac{1}{z - \varepsilon_0 + g_0\omega_0 X_i - \omega_0 \sum_j b_j^\dagger b_j}. \tag{80}$$

This is the Dyson's equation for a free electron on the lattice.

For a two-site problem, the local Green's functions are given by

$$G_{1,1}(z) = \frac{1}{z - \varepsilon_0 - \omega_0(b_1^\dagger b_1 + b_2^\dagger b_2) + g_0\omega_0 X_1 - t_0^2 G_{2,2}^{(0)}(z)} \tag{81}$$

and

$$\tilde{G}_{1,1}(z) = \frac{1}{z - \tilde{\varepsilon}_0 - \omega_0(b_1^\dagger b_1 + b_2^\dagger b_2) - t_0^2 U_1^\dagger G_{2,2}^{(0)}(z) U_1} \tag{82}$$

with

$$G_{2,2}^{(0)}(z) = \frac{1}{z - \varepsilon_0 - \omega_0(b_1^\dagger b_1 + b_2^\dagger b_2) + g_0\omega_0 X_2}. \tag{83}$$

We now consider a finite chain of length M. The interaction part reads

$$V = -t_0 \sum_{j=1}^{M-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j). \tag{84}$$

Consider the problem to compute the Green's function for the first site of the chain, that is $G_{1,1}(z)$, and call it, for a while, the local Green's function of the problem.

In the language of the RPE one gets

$$G_{1,1}(z) = \frac{1}{K_{1,1}^{(0)}(z) - t_0^2 G_{2,2[1]}(z)} \tag{85}$$

with $K_{i,i}^{(0)}(z) = [G_{i,i}^{(0)}(z)]^{-1}$ and $G_{2,2[1]}(z)$ the Green's function with interaction between site 1 and site 2 removed. Next, we obtain

$$G_{2,2[1]}(z) = \frac{1}{K_{2,2}^{(0)}(z) - t_0^2 G_{3,3[1,2]}(z)} \tag{86}$$

and so on, until the end of the chain,

$$G_{M,M[1,\dots,M-1]}(z) = G_{M,M}^{(0)}(z). \tag{87}$$

We notice that $G_{2,2[1]}(z)$ is diagonal in the basis of site 1, that $G_{3,3[1,2]}(z)$ is diagonal in the basis of site 1 and 2, and so on. This means that one can compute $G_{2,2[1]}(z)$ in the basis of all the sites but site 1. If we write $G_{2,2[1]}^{[1]}(z)$

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this Green's function, then one gets $G_{2,2[1]}(z) = G_{2,2[1]}^{[1]}(z - \omega_0 b_1^\dagger b_1)$. The same way, one gets $G_{3,3[1,2]}(z) = G_{3,3[1,2]}^{[1]}(z - \omega_0 b_2^\dagger b_2)$ or $G_{3,3[1,2]}(z) = G_{3,3[1,2]}^{[1,2]}(z - \omega_0 b_1^\dagger b_1 - \omega_0 b_2^\dagger b_2)$. We also notice that $G_{2,2[1]}^{[1]}(z)$ is the local Green's function for the chain with site 1 removed, that $G_{3,3[1,2]}^{[1,2]}(z)$ is the local Green's function with sites 1 and 2 removed, and so on. The Dyson's equations become

$$
\begin{aligned}
G_{1,1}(z) &= G_{1,1}^{(0)}(z) + t_0^2 G_{1,1}(z) G_{2,2[1]}^{[1]}(z - \omega_0 b_1^\dagger b_1) G_{1,1}^{(0)}(z) \\
G_{2,2[1]}^{[1]}(z) &= G_{2,2}^{[1](0)}(z) + t_0^2 G_{2,2[1]}^{[1]}(z) G_{3,3[1,2]}^{[1,2]}(z - \omega_0 b_2^\dagger b_2) G_{2,2}^{[1](0)}(z) \\
\vdots \quad &\quad \vdots \quad \vdots
\end{aligned}
$$

(88)

Finally, we consider a Bethe lattice with coordination number Z. The Dyson's equation for the central site o is

$$
G_{o,o}(z) = G_{o,o}^{(0)}(z) + t_0^2 \sum_\delta G_{o,o}(z) G_{\delta,\delta[o]}(z) G_{o,o}^{(0)}(z).
$$

(89)

The sum δ runs over its Z nearest neighbors. Again, $G_{\delta,\delta[o]}(z)$ is a diagonal operator in the basis of site o and we write $G_{\delta,\delta[o]}(z) = G_{\delta,\delta[o]}^{[o]}(z - \omega_0 b^\dagger b)$. Next, for one of the neighbors, the Dyson's equation reads

$$
G_{\delta,\delta[o]}(z) = G_{\delta,\delta}^{(0)}(z) + t_0^2 \sum_{\delta'} G_{\delta,\delta[o]}(z) G_{\delta+\delta',\delta+\delta'[o,\delta]}(z) G_{\delta,\delta}^{(0)}(z).
$$

(90)

The sum δ' runs overs its $Z - 1$ nearest neigbhors (not the site o). Again $G_{\delta+\delta',\delta+\delta'[o,\delta]}(z)$ is a diagonal operator in the basis of sites o and δ.

Notice that for a Bethe lattice in infinite dimensions, we can use the cavity method [5] and obtain directly the solution of the DMFT for $\mathbf{G}_{loc}(z)$. Consider a central site o, on the lattice, with Z neighbors. Starting from the Dyson's equation (89), we develops in power of t_0^2,

$$
\begin{aligned}
G_{o,o}(z) &= G_{o,o}^{(0)}(z) \\
&+ t_0^2 \sum_\delta G_{o,o}^{(0)}(z) G_{\delta,\delta[o]}(z) G_{o,o}^{(0)}(z) \\
&+ t_0^4 \sum_{\delta,\delta'} G_{o,o}^{(0)}(z) G_{\delta,\delta[o]}(z) G_{o,o}^{(0)}(z) G_{\delta',\delta'[o]}(z) G_{o,o}^{(0)}(z) \\
&+ \dots
\end{aligned}
$$

(91)

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and then take the expectation value on the vacuum of all the sites, but the central site. We introduce the unknown local Green's function $\mathbf{G}_{loc}(z)$, since for $Z \to \infty$, the expectation value of $G_{o,o}(z)$ and $G_{\delta,\delta[o]}(z)$ should correspond to $\mathbf{G}_{loc}^{0,0}(z)$. At order t_0^2 one obtains the contribution to the Weiss's self-energy

$$Z t_0^2 \mathbf{G}_{loc}^{0,0}(z - \omega_0 b^\dagger b). \tag{92}$$

At order t_0^4 one obtains two contributions. The first is just

$$Z(Z-1)[t_0^2 \mathbf{G}_{loc}^{0,0}(z - \omega_0 b^\dagger b)]^2, \tag{93}$$

while the other contribution is

$$Z t_0^4 \sum_q \mathbf{G}_{loc}^{0,q}(z - \omega_0 b^\dagger b) \mathbf{G}_{at}(z - q\omega_0) \mathbf{G}_{loc}^{q,0}(z - \omega_0 b^\dagger b). \tag{94}$$

For $Z \to \infty$ and the rescaling $t_0 \to t_0/\sqrt{Z}$ only a single term survives at each step in the development in power of t_0^2 and we get the Weiss's self energy $t_0^2 \mathbf{G}_{loc}^{0,0}(z - \omega_0 b^\dagger b)$. Since, $G_{o,o}(z)$ should also correspond to $\mathbf{G}_{loc}(z)$, we obtain $\mathbf{G}_{loc}^{-1}(z) = \mathbf{G}_{at}^{-1}(z) - W(z - \omega_0 b^\dagger b)$ and the self-consistent equation $W(z) = t_0^2 \mathbf{G}_{loc}^{0,0}(z)$.

6   Revisited DMFT solution

Consider the two-site problem with the following effective Hamiltonian for site 1

$$H_1 = \varepsilon_0 c_1^\dagger c_1 + \omega_0 b_1^\dagger b_1 - g_0 \omega_0 X_1 c_1^\dagger c_1 + H_W \tag{95}$$

with

$$H_W = \varepsilon_0 c_2^\dagger c_2 - t_0(c_1^\dagger c_2 + hc) + \sum_k a_k \alpha_k^\dagger \alpha_k + \sum_k b_k (c_2^\dagger \alpha_k + hc). \tag{96}$$

The parameters a_k and b_k are choosen such that

$$\Sigma_2(z) = \sum_k \frac{b_k^2}{z - a_k}. \tag{97}$$

We use the equations of evolution to compute $G_{1,1}^{0,0}(z)$. We get

$$i\hbar \partial_t G_{1,1}^{0,0}(t) = \delta(t) + \varepsilon_0 G_{1,1}^{0,0}(t) - t_0 G_{2,1}^{0,0}(t) - g_0 \omega_0 G_{1,1}^{1,0}(t) \tag{98}$$

and

$$i\hbar\partial_t G_{1,1}^{n,0}(t) = (\varepsilon_0 + n\omega_0)G_{1,1}^{n,0}(t) - t_0 G_{2,1}^{n,0}(t) \qquad (99)$$

$$-g_0\omega_0\sqrt{n}G_{1,1}^{n-1,0}(t) - g_0\omega_0\sqrt{n+1}G_{1,1}^{n+1,0}(t).$$

Now, we use the fact that

$$G_{2,1}^{n,0}(z) = \frac{-t_0 G_{1,1}^{n,0}(z)}{z - \varepsilon_0 - n\omega_0 - \Sigma_2(z - n\omega_0)} \qquad (100)$$

so we get the solution

$$zG_{1,1}^{0,0}(z) = 1 + (\varepsilon_0 + \Sigma_1(z))G_{1,1}^{0,0}(z) - t_0 G_{2,1}^{0,0}(z) \qquad (101)$$

or

$$G_{1,1}^{0,0}(z) = \frac{1}{z - \omega_0 - \Sigma_1(z) - W_1(z)} \qquad (102)$$

with $\Sigma_1(z) = g_0^2\omega_0^2\Lambda_1(z; W_1(z))$ and

$$W_1(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma_2(z)}. \qquad (103)$$

If we use the equations of evolution to compute $G_{2,2}^{0,0}(z)$, we obtain

$$G_{2,2}^{0,0}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_2(z) - \dfrac{t_0^2}{z - \varepsilon_0 - \Sigma_1(z)}}. \qquad (104)$$

We thus obtain the desired self-consistent result, given by the standard solution.

For a given site o, the effective Hamiltonian is

$$H_o = \varepsilon_0 c_o^\dagger c_o + \omega_0 b_o^\dagger b_o - g_0\omega_0 X_o c_o^\dagger c_o + H_W \qquad (105)$$

with

$$H_W = \varepsilon_0 \sum_{i\neq o} c_i^\dagger c_i - t_0 \sum_{i,\delta} c_{i+\delta}^\dagger c_i \qquad (106)$$

$$+ \sum_{i\neq o}\sum_k [a_{k,i}\alpha_{k,i}^\dagger\alpha_{k,i} + b_{k,i}(c_i^\dagger\alpha_{k,i} + hc)]$$

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The parameters $a_{k,i}$ and $b_{k,i}$ correspond to

$$\Sigma_i(z) = \sum_k \frac{b_{k,i}^2}{z - a_{k,i}} \tag{107}$$

The Hamiltonian H_W is quadratic, and correspond exactly to the Weiss's Hamiltonian of the standard theory.

Our mean field Hamiltonian H_o emphasises the fact that no excitation of phonon are allowed for the other sites of the lattice, when dealing with the excitations of a given site.

7 Restricted basis

Consider a restricted basis for the phonons, where excited states are allowed only for a single site at a time. For the two-site problem, the basis states are $|n_1, 0\rangle$ and $|0, n_2\rangle$. For a three-site problem, the basis states are $|n_1, 0, 0\rangle$, $|0, n_2, 0\rangle$, and $|0, 0, n_3\rangle$. For a lattice with M sites, the dimension of the phonon basis is $(MP + 1)$, if we allow P excitations for a given site.

If we compute the local Green's fonction for the site i, with the equations of evolution, we obtain the simple result, which corresponds to a local approximation,

$$zG_{i,i}^{\mathbf{0,0}}(z) = 1 + (\varepsilon_0 + \Sigma_i^{(0)}(z))G_{i,i}^{\mathbf{0,0}}(z) - t_0 \sum_\delta G_{i+\delta,i}^{\mathbf{0,0}}(z) \tag{108}$$

or

$$G_{i,i}^{\mathbf{0,0}}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_i^{(0)}(z) - W_i^{(1)}(z)} \tag{109}$$

with

$$\Sigma_i^{(0)}(z) = g_0^2 \omega_0^2 \Lambda_1(z; W_i^{(0)}(z)) \tag{110}$$

and $W_i^{(0)}(z)$ is the free Weiss's self-energy, that is corresponding, in the RPE, to

$$G_{i,i}^{(0)}(z) = \frac{1}{z - \varepsilon_0} \tag{111}$$

while $W_i^{(1)}(z)$ is the Weiss's self-energy corresponding, in the RPE, to

$$G_{i,i}^{(0)}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_i^{(0)}(z)}. \tag{112}$$

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As an example, consider a one dimensional periodic lattice. First, we compute $W^{(0)}(z)$ via

$$\frac{1}{M} \sum_{\mathbf{k}} \frac{1}{z - \varepsilon_0 + 2t_0 \cos(\mathbf{k})} = \frac{1}{z - \varepsilon_0 - W^{(0)}(z)}. \tag{113}$$

Then, we obtain $\Sigma^{(0)}(z) = g_0^2 \omega_0^2 \Lambda_1(z; W^{(0)}(z))$, and then, we get

$$\frac{1}{M} \sum_{\mathbf{k}} \frac{1}{z - \varepsilon_0 + 2t_0 \cos(\mathbf{k}) - \Sigma^{(0)}(z)} = \frac{1}{z - \varepsilon_0 - \Sigma^{(0)}(z) - W^{(1)}(z)}. \tag{114}$$

It is interesting to notice that the expression for this local Green's function, Eq (109), corresponds to some Momentum Average Approximation [9] and to the first iteration of the DMFT solution [10].

The nice thing with this restricted basis, is that we can easily compute numerically exactly all the Green's function $G_{i,j}^{\mathbf{m,n}}(z)$ or $\tilde{G}_{i,j}^{\mathbf{m,n}}(z)$ for small systems. If we perform exact diagonalizations with P excitations, then we can compare with the analytical results by computing $\Sigma_i(z)$ also with P excitations, i.e. by limiting the continued fraction to $\Lambda_P(z; W_i(z))$. Since excitations of phonon are allowed only for a given site at a time, we expect the same structure for these Green's functions and those of the DMFT, so we can check the decoupling scheme of the Green's functions in terms of the local Green's functions.

First we can check that the local Green's functions of the problem

$$G_{i,i}^{m,n}(z) = \langle 0, \dots m, \dots, 0 | c_i \frac{1}{z - H} c_i^\dagger | 0, \dots, n, \dots, 0 \rangle \tag{115}$$

correspond to

$$\mathbf{G}_{i,i}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 X - \mathbf{W}_{i,i}(z)} \tag{116}$$

where $\mathbf{W}_{i,i}(z)$ is the diagonal operator given by

$$\begin{cases} \mathbf{W}_{i,i}^{0,0}(z) = W_i^{(1)}(z) \\ \mathbf{W}_{i,i}^{n,n}(z) = W_i^{(0)}(z - n\omega_0) \ \text{ for } n > 0 \end{cases} \tag{117}$$

We guess the form of $\mathbf{W}_{i,i}(z)$ from the fact that, when computing $\mathbf{G}_{i,i}^{0,0}(z)$, we get $W_i(z) = \mathbf{W}_{i,i}^{0,0}(z)$, while $\Sigma_i(z)$ involves only $\mathbf{W}_{i,i}^{n,n}(z)$ for $n > 0$.

Let us consider the open chain of lenght $M = 3$. For site 1 and 3 we have

$$W_1^{(0)}(z) = \frac{t_0^2}{z - \varepsilon_0 - \dfrac{t_0^2}{z - \varepsilon_0}} \tag{118}$$

and for site 2 we have

$$W_2^{(0)}(z) = \frac{2t_0^2}{z - \varepsilon_0}. \tag{119}$$

From these free Weiss's self-energies, we compute

$$\Sigma_1^{(0)}(z) = g_0^2 \omega_0^2 \Lambda_1(z; W_1^{(0)}(z)) \tag{120}$$

and

$$\Sigma_2^{(0)}(z) = g_0^2 \omega_0^2 \Lambda_1(z; W_2^{(0)}(z)). \tag{121}$$

Then we get

$$W_1^{(1)}(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma_2^{(0)}(z) - \dfrac{t_0^2}{z - \varepsilon_0 - \Sigma_1^{(0)}(z)}} \tag{122}$$

and

$$W_2^{(1)}(z) = \frac{2t_0^2}{z - \varepsilon_0 - \Sigma_1^{(0)}(z)}. \tag{123}$$

Then we compute $G_{1,1}^{0,0}(z)$ and $G_{2,2}^{0,0}(z)$ with our local approximation

$$\mathbf{G}_{1,1}^{0,0}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_1^{(0)}(z) - W_1^{(1)}(z)} \tag{124}$$

and

$$\mathbf{G}_{2,2}^{0,0}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_2^{(0)}(z) - W_2^{(1)}(z)}. \tag{125}$$

We obtain a perfect agreement with the exact result.

Next we compute $G_{1,2}^{0,0}(z)$. We start from the exact expression

$$G_{1,2}(z) = -t_0 G_{1,1}(z) G_{2,2[1]}(z) \tag{126}$$

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and make the decoupling

$$G_{1,2}^{\mathbf{0,0}}(z) = -t_0 \mathbf{G}_{1,1}^{0,0}(z)\mathbf{G}_{2,2[1]}^{0,0}(z). \tag{127}$$

We guess that the local Green's function $\mathbf{G}_{2,2[1]}(z)$ is given by

$$\mathbf{G}_{2,2[1]}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 X - \mathbf{W}_{2,2[1]}(z)} \tag{128}$$

with the diagonal operator

$$\begin{cases} \mathbf{W}_{2,2[1]}^{0,0}(z) = W_{2[1]}^{(1)}(z) \\ \mathbf{W}_{2,2[1]}^{n,n}(z) = W_2^{(0)}(z - n\omega_0) \text{ for } n > 0 \end{cases} \tag{129}$$

and the Weiss's function

$$W_{2[1]}^{(1)}(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma_3^{(0)}(z)}. \tag{130}$$

We thus obtain

$$\mathbf{G}_{2,2[1]}^{0,0}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_2^{(0)}(z) - W_{2[1]}^{(1)}(z)}. \tag{131}$$

We obtain a perfect agreement with the exact result.

Next we compute $G_{1,3}^{\mathbf{0,0}}(z)$. We start from the exact expression

$$G_{1,3}(z) = -t_0 G_{1,2}(z) G_{3,3[1,2]}(z) \tag{132}$$

and make the decoupling

$$G_{1,3}^{\mathbf{0,0}}(z) = +t_0^2 \mathbf{G}_{1,1}^{0,0}(z)\mathbf{G}_{2,2[1]}^{0,0}(z)\mathbf{G}_{3,3[1,2]}^{0,0}(z). \tag{133}$$

We Guess that $\mathbf{G}_{3,3[1,2]}(z)$ is given by

$$\mathbf{G}_{3,3[1,2]}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 X - \mathbf{W}_{3,3[1,2]}(z)} \tag{134}$$

with the diagonal operator

$$\begin{cases} \mathbf{W}_{3,3[1,2]}^{0,0}(z) = 0 \\ \mathbf{W}_{3,3[1,2]}^{n,n}(z) = W_3^{(0)}(z - n\omega_0) \text{ for } n > 0 \end{cases}. \tag{135}$$

We get

$$\mathbf{G}^{0,0}_{33[1,2]}(z) = \frac{1}{z - \varepsilon_0 - \Sigma_3^{(0)}(z)}. \tag{136}$$

We obtain a perfect agreement with the exact result.

For $\tilde{G}^{0,0}_{i,i}(z)$, we compute

$$\tilde{G}^{0,0}_{1,1}(z) = \sum_m \sum_n U^{m,0} \mathbf{G}^{m,n}_{1,1}(z) U^{n,0} \tag{137}$$

and

$$\tilde{G}^{0,0}_{2,2}(z) = \sum_m \sum_n U^{m,0} \mathbf{G}^{m,n}_{2,2}(z) U^{n,0}. \tag{138}$$

We obtain a perfect agreement with the exact results.

For $\tilde{G}^{0,0}_{i,j}(z)$, we compute

$$\tilde{G}^{0,0}_{1,2}(z) = -t_0 \sum_m \sum_n U^{m,0} \mathbf{G}^{m,0}_{1,1}(z) \mathbf{G}^{0,n}_{2,2[1]}(z) U^{n,0} \tag{139}$$

and

$$\tilde{G}^{0,0}_{1,3}(z) = t_0^2 \sum_m \sum_n U^{m,0} \mathbf{G}^{m,0}_{1,1}(z) \mathbf{G}^{0,0}_{2,2[1]}(z) \mathbf{G}^{0,n}_{3,3[1,2]}(z) U^{n,0}. \tag{140}$$

We obtain a perfect agreement with the exact results.

8   Decoupling scheme

We apply the decoupling scheme obtained within the restricted basis to compute $G^{0,0}_{i,j}(z)$ and $\tilde{G}^{0,0}_{i,j}(z)$, within the DMFT, that is, instead to deal with $W_i^{(0)}(z)$ and $W_i^{(1)}(z)$, we use the self-consistent solution $W_i(z)$ given by the DMFT.

Consider a lattice with M sites and solve the DMFT equations to get $\Sigma_i(z)$ and $W_i(z)$. Then construct all the local Green's functions

$$\mathbf{G}^{(0)}_{i,i}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0 \omega_0 X - \mathbf{W}_{i,i}(z)} \tag{141}$$

with the diagonal operator

$$\begin{cases} \mathbf{W}^{0,0}_{i,i}(z) = 0 \\ \mathbf{W}^{n,n}_{i,i}(z) = W_i(z - n\omega_0) \ \text{ for } n > 0 \end{cases} \tag{142}$$

Then use the RPE to express any Green's function in term of these local Green's functions and take the expectation value individually.

For the electron, the RPE is just the equation of free particle on the lattice, so we just need

$$G_{i,i}^{(0)}(z) = [\mathbf{G}_{i,i}^{(0)}(z)]^{0,0} = \frac{1}{z - \varepsilon_0 - \Sigma_i(z)}. \tag{143}$$

For an infinite system, $\Sigma_i(z) = \Sigma(z)$, and for a periodic lattice, we obtain

$$G(\mathbf{k}, z) = \frac{1}{z - \varepsilon_0 - \xi_\mathbf{k} - \Sigma(z)}. \tag{144}$$

For the small polaron, the RPE involve the operators U_i, so we need to compute $[U^\dagger \mathbf{G}_{i,i}^{(0)}(z)]^{0,0} = [\mathbf{G}_{i,i}^{(0)}(z)U]^{0,0}$ or $[U^\dagger \mathbf{G}_{i,i}^{(0)}(z)U]^{0,0}$.

Let us compute $G(\mathbf{k}, z)$ and $\tilde{G}(\mathbf{k}, z)$ for a one-dimensional lattice with M sites. In this case, we have $\Sigma_i(z) = \Sigma(z)$ and $W_i(z) = W(z)$. We start with

$$W_{M[1,...,M-1]}(z) = 0 \tag{145}$$

then compute

$$W_{i[1,...,i-1]}(z) = \frac{t_0^2}{z - \varepsilon_0 - \Sigma(z) - W_{i+1[1,...,i]}(z)} \tag{146}$$

until $W_{2[1]}(z)$, and then

$$W_1(z) = W(z) = \frac{2t_0^2}{z - \varepsilon_0 - \Sigma(z) - W_{2[1]}(z)}. \tag{147}$$

We solve the self-consistent equations for $\Sigma(z) = g_0^2 \omega_0^2 \Lambda_1(z; W(z))$ and $W(z)$. Notice that this way to compute $W(z)$, instead of Eq (114), gives a slightly different result that vanishes for M large enough.

In order to compute $G(\mathbf{k}, z)$, we just have to consider

$$\mathbf{G}_{i,i[1,...,i-1]}^{0,0}(z) = \frac{1}{z - \varepsilon_0 - \Sigma(z) - W_{i[1,...,i-1]}(z)}. \tag{148}$$

We start to compute the local Green's function $G_{1,1}^{0,0}(z)$ that is $\mathbf{G}_{1,1}^{0,0}(z)$, and then compute

$$G_{1,j+1}^{\mathbf{0,0}}(z) = -t_0 G_{1,j}^{\mathbf{0,0}}(z) \mathbf{G}_{j+1,j+1[1,...,j]}^{0,0}(z) \tag{149}$$

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until $G_{1,M}^{0,0}(z)$. Then we use the Fourier transform. From a numerical point of view, it is safer to choose M odd and to compute

$$G(k,z) = G_{o,o}^{0,0}(z) + \sum_{n=1}^{(M+1)/2} 2\cos(2\pi kn/M) \, G_{o,n}^{0,0}(z) \qquad (150)$$

In this case, we can compare the numerical result with the standard result of the DMFT, i.e. Eq (144).

Next, for $\tilde{G}(\mathbf{k}, z)$, we have to compute the full local operators

$$\mathbf{G}_{i,i[1,\ldots,i-1]}(z) = \frac{1}{z - \varepsilon_0 - \omega_0 b^\dagger b + g_0\omega_0 X - \mathbf{W}_{i,i[1,\ldots,i-1]}(z)} \qquad (151)$$

with

$$\begin{cases} \mathbf{W}_{i,i[1,\ldots,i-1]}^{0,0}(z) = W_{i[1,\ldots,i-1]}(z) \\ \\ \mathbf{W}_{i,i[1,\ldots,i-1]}^{n,n}(z) = W(z - n\omega_0) \text{ for } n > 0 \end{cases} \qquad (152)$$

Then we compute

$$\tilde{G}_{1,1}^{0,0}(z) = \sum_{m,n} U^{m,0} U^{n,0} \mathbf{G}_{1,1}^{m,n}(z), \qquad (153)$$

$$\tilde{G}_{1,2}^{0,0}(z) = -t_0 \sum_{m,n} U^{m,0} U^{n,0} \mathbf{G}_{1,1}^{m,0}(z) \mathbf{G}_{2,2[1]}^{0,n}(z), \qquad (154)$$

$$\tilde{G}_{1,3}^{0,0}(z) = t_0^2 \sum_{m,n} U^{m,0} U^{n,0} \mathbf{G}_{1,1}^{m,0}(z) \mathbf{G}_{2,2[1]}^{0,0}(z) \mathbf{G}_{3,3[1,2]}^{0,m}(z), \qquad (155)$$

$$\tilde{G}_{1,4}^{0,0}(z) = -t_0^3 \sum_{m,n} U^{m,0} U^{n,0} \mathbf{G}_{1,1}^{m,0}(z) \mathbf{G}_{2,2[1]}^{0,0}(z) \mathbf{G}_{3,3[1,2]}^{0,0}(z) \mathbf{G}_{4,4[1,2,3]}^{0,m}(z), \qquad (156)$$

and so on, until $\tilde{G}_{1,M}^{0,0}(z)$. Then we get

$$\tilde{G}(k,z) = \tilde{G}_{o,o}^{0,0}(z) + \sum_{n=1}^{(M+1)/2} 2\cos(2\pi kn/M) \, \tilde{G}_{o,n}^{0,0}(z). \qquad (157)$$

In this case, we can check that the sum over $\mathbf{k}$ corresponds to the local Green's function

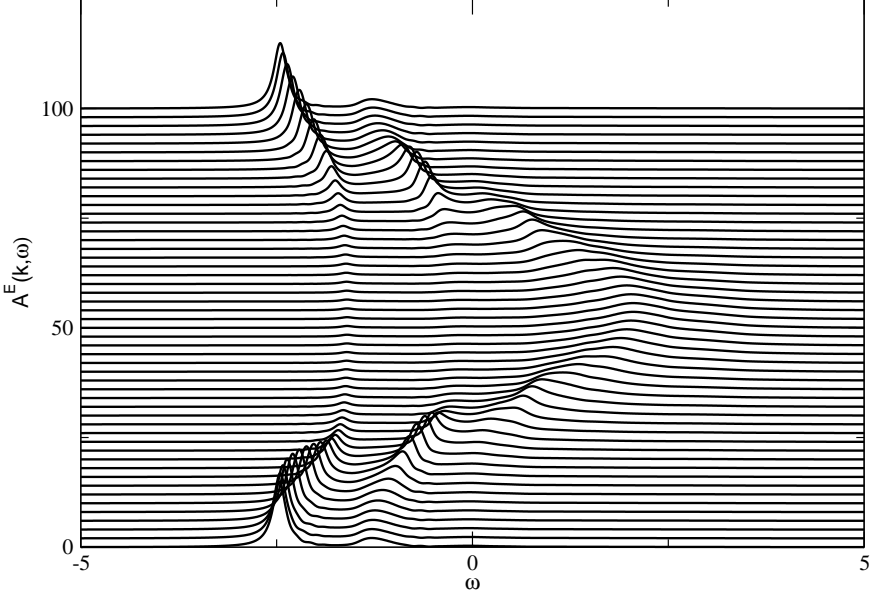$$\tilde{G}_{1,1}^{0,0}(z) = \frac{1}{M} \sum_k \tilde{G}(k,z). \qquad (158)$$

Figure 2: Spectral functions for the electron

In Fig 2 and Fig 3 we show the result for the spectral functions of the electron

$$A(k, \omega) = -2\,\mathcal{I}mG(k, z = \omega + i\eta) \tag{159}$$

and for the spectral functions of the small polaron

$$\tilde{A}(k, \omega) = -2\,\mathcal{I}m\tilde{G}(k, z = \omega + i\eta) \tag{160}$$

The parameters are $t_0 = \omega_0 = g_0 = 1$, $\varepsilon_0 = 0$, $M = 51$, and $\eta = 0.1$.

For these values of the parameters, we obtain that $A(k = 0, \omega)$ and $\tilde{A}(k = 0, \omega)$ have exactly the same main pic, but we obtain a rather different physics for the electron and the small polaron. The small polaron of the atomic limit remains a good quasiparticle.

9   Dressing an electron

We would like to emphasis that they are many ways to define a small polaron operator, i.e. to dress localy an electron with phonons [4].
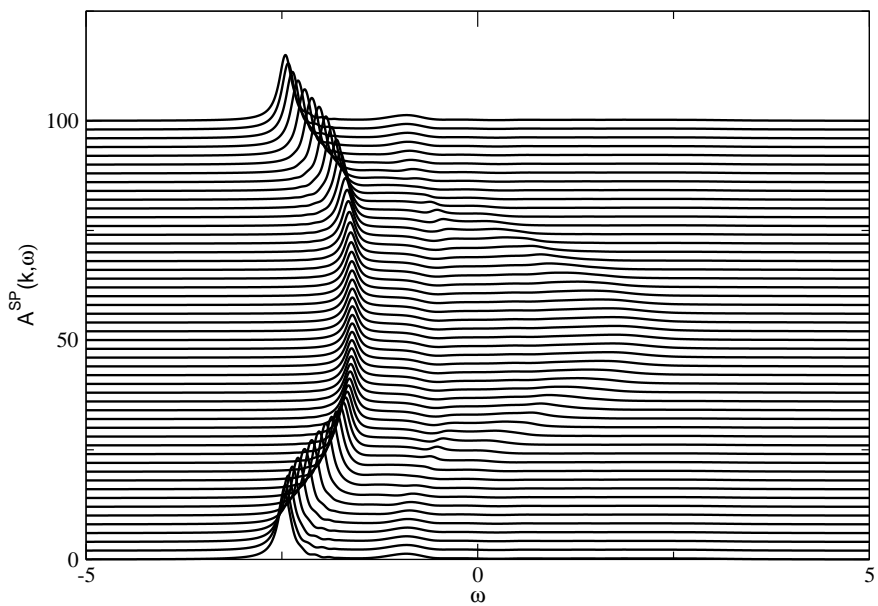
Figure 3: Spectral functions for the small polaron

Consider the two-site problem and compute the Green's functions for the electron

$$G_{1,1}^{m,n}(z) = \langle m, 0 | c_1 \frac{1}{z - H} c_1^\dagger | n, 0 \rangle \tag{161}$$

and

$$G_{1,2}^{m,n}(z) = \langle m, 0 | c_1 \frac{1}{z - H} c_2^\dagger | 0, n \rangle. \tag{162}$$

If we use the operator U to compute the Green's functions for the small polaron $\tilde{G}_{1,1}^{00,00}(z)$ and $\tilde{G}_{1,2}^{00,00}(z)$, with

$$\tilde{G}_{i,j}^{00,00}(z) = \sum_{m,n} U^{m,0} G_{i,j}^{m,n}(z) U^{n,0} \tag{163}$$

we obtain, for the first poles, that correspond to the fundamental energy and the first excited state,

$$\begin{array}{cc} E_p & \mathcal{Z}_p \\ -1.68848 & 0.43015 \\ -1.14106 & \pm 0.37575 \end{array} \tag{164}$$

So $\tilde{G}(k = 0, z)$ has a main pic with $\mathcal{Z} \simeq 0.86$ while $\tilde{G}(k = \pi, z)$ has a main pic with $\mathcal{Z} \simeq 0.75$.

Next, following Ref [4], we can also define a small polaron using the reduced density matrix for a single site. We have, for the eigenstates,

$$|p) = \sum_{j,m_1,m_2} \Psi_{j,m_1,m_2}(p) \, c_j^\dagger | m_1, m_2 \rangle \tag{165}$$

so, targetting only on one of the eigenstates, we obtain the reduced density matrix

$$\rho^{m,n}(p) = \sum_{m_2} \Psi_{1,m,m_2}^*(p) \Psi_{1,n,m_2}(p) \tag{166}$$

Then, we diagonalize $\rho(p)$ and get $U(p)$. The first eigenstate with $E_0 \simeq -1.688$ corresponds to the symmetry $\mathbf{k} = 0$ and the next with $E_1 \simeq -1.141$, corresponds to the symmetry $\mathbf{k} = \pi$. For $U(0)$, we get the result

$$\begin{array}{cc} E_p & \mathcal{Z}_p \\ -1.68848 & 0.46065 \\ -1.14106 & \pm 0.28247 \end{array} \tag{167}$$

So $\tilde{G}(k = 0, z)$ has a main pic with $\mathcal{Z} \simeq 0.92$ while $\tilde{G}(k = \pi, z)$ has a main pic with $\mathcal{Z} \simeq 0.57$. For $U(\pi)$, we get the result

$$
\begin{array}{cc}
E_p & \mathcal{Z}_p \\
-1.68848 & 0.35216 \\
-1.14106 & \pm 0.41841
\end{array}
\tag{168}
$$

So, this time, $\tilde{G}(k = 0, z)$ has a main pic with $\mathcal{Z} \simeq 0.70$ while $\tilde{G}(k = \pi, z)$ has a main pic with $\mathcal{Z} \simeq 0.84$.

The formalism to compute the non local Green's functions of the small polaron within the Dynamical Mean Field Theory, presented in the last section, can be used with any local transformation.

10   Conclusion

In this paper we revisited the Dynamical Mean Field Theory of the Holstein Polaron Problem in order to compute the all dynamical correlation functions for the electron and the small polaron. We introduced a restricted basis for the phonons in order to check numerically the right decoupling scheme of the Green's functions within a local approximation.

References

[1] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959).

[2] H. Fehske and S. A. Trugman, in *Polarons in Advanced Materials*, edited by A. S. Alexandrov, Springer Series in Material Sciences 103 pp. 393-461, Springer Verlag, Dordrecht (2007).

[3] J. M. Robin, Phys. Rev. B **58**, 14335 (1998).

[4] C. Zhang, E. Jeckelmann, and S. R. White, Phys. Rev. B **60**, 14092 (1999).

[5] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13-125 (1996).

[6] S. Ciuchi, F. de Pasquale, S. Fratini, and D. Feinberg, Phys. Rev. B **56**, 4494 (1997).

[7] E. N. Economou, *Green's Function in Quantum Physics*, Springer-Verlage, Berlin.

[8] H. Haken, *Quantum field theory of solids*, North Holland Publishing, Amsterdam, 1976.

[9] M. Berciu, Phys. Rev. Lett. **97**, 036402 (2006).

[10] O. S. Barisic, Phys. Rev. B **76**, 193106 (2007).

Numerical Stuff

Local self-energy

We make the program `berciu.cc` to compute the local self-energy for a system with M sites. First, we compute the free local Green's function

$$G_0(z) = \frac{1}{M} \sum_{k=0}^{M-1} \frac{t_0^2}{z - \varepsilon_0 - \xi_k} \tag{169}$$

with

$$\xi_k = -2t_0 \cos(\frac{2\pi}{M}k) \tag{170}$$

and then extract the free Weiss's function using the formula

$$G_0(z) = \frac{1}{z - \varepsilon_0 - W_0(z)} \tag{171}$$

Then we compute the self-energy

$$\Sigma_0(z) = g_0^2 \omega_0^2 \Lambda_1(z) \tag{172}$$

with

$$\Lambda_n(z) = \frac{1}{z - \varepsilon_0 - n\omega_0 - W_0(z - n\omega_0) - (n+1)g_0^2\omega_0^2\Lambda_{n+1}(z)} \tag{173}$$

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