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EFFECTIVE HAMILTONIANS FOR PHONON AND SPIN POLARONS*

M. Acquarone

C.N.R.–G.N.S.M., I.N.F.M., Dipartimento di Fisica, Universita' di Parma
Parco Area delle Scienze 7A, 43100 Parma, Italy

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Effective Hamiltonians for phonon and spin polarons are obtainedby applying a sequence of displacement and squeezing transformations to electron–phonon, or electron–magnon, interacting Hamiltonians. The basic techniques of calculation are shown in details, with explicit applications to the case of two- and four-sites systems.

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1. Introduction

An interacting fermion–boson Hamiltonian is generally composed of purely fermionic and bosonic parts, plus a term expressing the interaction between the two types of particles. It is often convenient to try to transform the interacting Hamiltonian into another one, from which the interaction term has been eliminated or expressed in a physically more significant way. In some cases, it is possible to obtain an equivalent Hailtonian from which one type of particle is completely absent. These lecture notes will show how, in the case of electrons interacting with phonons or with spin waves, one can build *effective* Hamiltonians, where the Bose operators do not appear, and the fermions interact through renormalized interactions, whose values depend of the phononic properties of the system. Such fermions, *dressed* by bosons, are called *polarons*. The general technique to eliminate bosonic operators consists in applying to the interacting Hamiltonian a sequence of unitary transformations determined by the fermion- boson interaction term, usually called *displacement* transformations. They will be followed by the evaluation of the *displaced* Hamiltonian over a so-called *squeezed* bosonic

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wavefunction, which is a generalization of the harmonic oscillator wavefunction. We shall consider two types of bosons: the phonons and the antiferromagnetic spin waves (or magnons). Their physical effects are quite different, but the formalism is the same in both cases. Therefore we shall first treat in some details the phonon polarons, to establish the procedure. When dealing with the spin waves case, we shall take advantage of many results obtained for the phonon case. As these notes are intended for didactical purposes, we shall not deal with the phenomenology of polarons in real materials.

2. The electron–phonon Hamiltonian

Our starting point will be the so called Hubbard–Holstein Hamiltonian:

$$H = H_{\rm el} + H_{\rm ph} + H_{\rm el-ph}\,, \tag{1}$$

where, in standard notation, the electronic term in the lattice site representation reads:

$$H_{\rm el} = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_{i\langle j\rangle\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\langle j\rangle} V_{ij} n_i n_j\,, \tag{2}$$

ε_i is the atomic on-site energy; U is the Hubbard on-site repulsion energy acting between two particles with opposite spins occupying the same lattice site i, while V_{ij} is the inter-site charge interaction, and $n_i = \sum_\sigma n_{i\sigma}$. We shall use, according to conveniency, both the sum over sites $\sum_{i\langle j\rangle}$, meaning summing over the z nearest neighbours $\langle j\rangle$ of each site $i\,(i = 1...N)$, and the sum over $\langle i,j\rangle$ bonds $\sum_{\langle ij\rangle}$.

The free phonon term is a harmonic oscillator for the deformations u_i of the sites. In terms of the eigenmodes $u_q = 1/\sqrt{N}\sum_j u_j \exp(iqR_j)$ and the associated momenta P_q of the vibrating mass M at frequency Ω_q it reads

$$H_{\rm ph} = \sum_q \frac{P_q P_{-q}}{2M} + \frac{M}{2}\sum_q \Omega_q^2 u_q u_{-q}\,. \tag{3}$$

We shall quantize the deformations and momenta introducing Bose operators $b_q, b_q^{\dagger}$according to the standard rules, yielding:

$$u_q = \sqrt{\frac{\hbar}{2M\Omega_q}}\left(b^{\dagger}_{-q} + b_q\right)\,, \qquad P_q = i\sqrt{\frac{\hbar\Omega_q}{2M}}\left(b^{\dagger}_{-q} - b_q\right)\,. \tag{4}$$

Notice the characteristic length $L_q = \sqrt{\hbar/2M\Omega_q}$. The local phonon operators $b_j^{\dagger}, b_j$ are derived from $b_q, b_q^{\dagger}$ by Fourier transform:

$$b_j^{\dagger} = 1/\sqrt{N}\sum_q b_q^{\dagger}\exp\left(-iqR_j\right).$$

The phonon Hamiltonian is then diagonalized as:

$$H_{\rm ph} = \sum_q \hbar\Omega_q \left(b_q^\dagger b_q + \tfrac{1}{2} \right) . \tag{5}$$

In the following we shall also consider the case of dispersionless phonons, which model the optical phonons, implying $\Omega_q \to \Omega$, $L_q \to L$.

The interacting Hamiltonian will be assumed of the Holstein type [1], *i.e.* a local interaction of strength G betwen the site charge density n_j and its deformation u_j:

$$H_{\rm el-ph} = G \sum_j u_j n_j = g \sum_j \left(b_j^\dagger + b_j \right) n_j = \hbar\Omega\gamma \sum_j \left(b_j^\dagger + b_j \right) n_j \,, \tag{6}$$

where $g = GL$ and $\gamma = g/\hbar\Omega$. The mixed form, where only the Bose operators are Fourier transformed, will also be used, yielding:

$$H_{\rm el-ph} = \hbar\Omega\gamma \sum_q \left(b_{-q}^\dagger + b_q \right) \left[\frac{1}{\sqrt{N}} \sum_j n_j {\rm e}^{iqR_j} \right] = \hbar\Omega\gamma \sum_q \left(b_{-q}^\dagger + b_q \right) n_q \,. \tag{7}$$

Let us remark that n_q introduced above equals $\sqrt{N}$ times the true Fourier tranform of n_j. To have a physical understanding of the formalism, let us consider simple cases: the dimer [2], consisting of two ions at the sites R_j ($j = 1, 2$) spaced by a. Its Brillouin zone consists of two points: $q = 0,\ \pi/a$. Then $b_0 = (b_1 + b_2)/\sqrt{2}$ and $b_{\pi/a} = (b_1 - b_2)/\sqrt{2}$ while the interaction term becomes:

$$H_{\rm el-ph} = \frac{\hbar\Omega\gamma}{\sqrt{2}} \left[(n_1 + n_2) \left(b_0^\dagger + b_0 \right) + (n_1 - n_2) \left(b_{\pi/a}^\dagger + b_{\pi/a} \right) \right] . \tag{8}$$

We see that the zone center mode ($q = 0$) couples to the total charge, while the zone boundary one ($q = \pi/a$) couples to the charge transfer between the sites. The reader might work out the corresponding expressions for the four-site closed chain.

Our goal is to tranform H into a physically equivalent effective Hamiltonian H^* whose operatorial part is expected to have the same shape as $H_{\rm el}$ but with renormalized interaction parameters, and possibly the addition of fermionic interaction terms $H_{\rm new}$ which were not present in $H_{\rm el}$:

$$H^* = H_{\rm el} \left(\varepsilon_i^*, t_{ij}^*, U^*, V_{ij}^* \right) + H_{\rm new} + c - {\rm number} \,. \tag{9}$$

The renormalized interactions will contain the effect of the coupling with the phonons:

$$\varepsilon_i^* = \varepsilon_i^* \left(\varepsilon_i, \Omega, g \right) , \quad t_{ij}^* = t_{ij}^* \left(t_{ij}, \Omega, g \right) , \quad U^* = U^* \left(U, \Omega, g \right) , \quad V_{ij}^* = V_{ij}^* \left(V_{ij}, \Omega, g \right) . \tag{10}$$

Thus the final *polaronic* Hamiltonian will describe fermions "dressed" by bosons, and therefore interacting between themselves with different strengths than in the absence of bosons.

3. The displacement transformation

The first reasonable step in our program might seem to be the diagonalization of H, by eliminating $H_{\mathrm{el-ph}}$. Actually, we shall see that this procedure has serious physical drawbacks. However, let's follow it for the moment. The materials where polarons are supposed to exist, like high temperature superconductors [4] (HTS) or colossal magnetoresistance compounds [5] (CMR) have strong electron–phonon interactions. Therefore $H_{\mathrm{el-ph}}$ can not be dealt with perturbatively. One can instead try to get rid of it by applying to H a unitary transformation e^{R} such that $\mathrm{e}^{R^\dagger}\mathrm{e}^{R} = 1$ (implying that the *generator* R is anti-Hermitian: $R^\dagger = -R$). We hope that a proper choice of R will produce a transformed $H^T = \mathrm{e}^{R} H \mathrm{e}^{-R}$ from where $H_{\mathrm{el-ph}}$ has been removed. A comprehensive treatment of unitary transformations can be found in Ref. [3].

To devise the form of R we learn from the perturbative limit. Suppose we want to diagonalize the general Hamiltonian $H = H_0 + xH_1$ where $x \ll 1$. We guess $R = x\mathcal{R}$ and we develop $\mathrm{e}^{x\mathcal{R}\cdot}$ in series of commutators:

$$H^T = \mathrm{e}^{R} H \mathrm{e}^{-R} = H + [x\mathcal{R}, H] + \frac{1}{2}\left[x\mathcal{R}, [x\mathcal{R}, H]\right] + \mathcal{O}\left(x^3\right) . \tag{11}$$

In the perturbative limit, we neglect $\mathcal{O}\left(x^3\right)$ and we eliminate the terms in H^T linear in x by imposing $H_1 + [\mathcal{R}, H_0] = 0$. Then $H^T = H_0 - \left(x^2/2\right)[\mathcal{R}, [\mathcal{R}, H_0]]$. If $\{|p\rangle\}$ and $\{|n\rangle\}$ are complete sets of eigenstates of H_0 with eigenvalues E_p, E_n, then from:

$$\sum_{p,n} |p\rangle\langle p|\{H_1 + [\mathcal{R}, H_0]\}|n\rangle\langle n| = 0 \tag{12}$$

it follows

$$\sum_{p,n} |p\rangle \left[\langle p|H_1|n\rangle - (E_p - E_n)\langle p|\mathcal{R}|n\rangle\right]\langle n| = 0 \tag{13}$$

yielding the condition:

$$\langle p|\mathcal{R}|n\rangle = \frac{\langle p|H_1|n\rangle}{(E_p - E_n)} \tag{14}$$

which tells us that R has the same operatorial form as the perturbative term H_1, only with different coefficients, because R has to obey the anti-Hermiticity condition.

In order to get rid of the Holstein term, then, let us apply to the Hamiltonian the unitary transformation generated by:

$$R = \sum_q R_q = \gamma \sum_{q\sigma} \delta_q \left(b^\dagger_{-q} - b_q \right) n_q \,, \tag{15}$$

where the wavevector-dependent parameters $\{\delta_q\}$ are, for the moment, undetermined. We have therefore as many generators as there are sites in the Bravais lattice, or as many points in the Brillouin zone. All generators commute among themselves. In the case of the dimer we have:

$$R_0 = \delta_0 \frac{\gamma}{\sqrt{2}} \left(n_1 + n_2\right) \left(b^\dagger_0 - b_0 \right) \,, \qquad R_{\pi/a} = \delta_{\pi/a} \frac{\gamma}{\sqrt{2}} \left(n_1 - n_2\right) \left(b^\dagger_{\pi/a} - b_{\pi/a} \right) . \tag{16}$$

We shall try to perform the transformation rigorously, *i.e.* without any truncation in the development of e^R.

To transform each term of the Hamiltonian, we have to know how the individual Bose and Fermi operators are transformed. Let us consider $B_p^{(\dagger)} = \mathrm{e}^R b_p^{(\dagger)} \mathrm{e}^{-R}$, or

$$B_p^{(\dagger)} = \{\exp[\sum_{jq\sigma} \gamma_q \delta_q \left(b^\dagger_{-q} - b_q \right) n_q]\} b_p^{(\dagger)} \{\exp[\sum_{jq\sigma} \gamma_q \delta_q \left(b_q - b^\dagger_{-q} \right) n_q]\} \,. \tag{17}$$

By using the relation $\exp(X+Y) = \exp(X)\, \exp(Y) \exp(-\frac{1}{2}[X,Y])$, valid if $[X,Y] = c-$number, we can reduce Eq. (17) for, say, B_p to:

$$B_p = [\exp(\gamma_p \delta_p b^\dagger_p n_{-p})] b_p [\exp(-\gamma_p \delta_p b^\dagger_p n_{-p})] \,. \tag{18}$$

If we develop the exponentials in series, Eq. (18) becomes a series of commutators $B_p = b_p + [r, b_p] + \frac{1}{2}[r,[r,b_p]] + \frac{1}{3!}[r,[r,[r,b_p]]] + ...$ with $r = \gamma \delta_p b^\dagger_p n_{-p}$.

Now, $[r, b_p] = \gamma_p \delta_p n_{-p}$ *i.e.* a boson-independent term, so that all higher order commutators vanish, and we obtain (with a similar procedure for $B^\dagger_p$):

$$B_p = b_p - \gamma_p \delta_p n_{-p} \,, \qquad B^\dagger_p = b^\dagger_p - \gamma_p \delta_p n_p \,. \tag{19}$$

The $B_p^{(\dagger)}$'s are *displaced Bose operators:* they describe an oscillator whose equilibrium position has been displaced under the action of an external force. Here the force is due the coupling with the electronic charge. A textbook example is a harmonically oscillating charge acted upon by the electric field, while here the force is due to the coupling with the electronic charge. In the case of the dimer with dispersionless phonons we would obtain:

$$\begin{aligned} (B_0, B^\dagger_0) &= (b^\dagger_0, b_0) - \frac{\gamma}{\sqrt{2}} \delta_0 (n_1 + n_2), \\ (B_{\pi/a}, B^\dagger_{\pi/a}) &= (b^\dagger_{\pi/a}, b_{\pi/a}) - \frac{\gamma}{\sqrt{2}} \delta_{\pi/a} (n_1 - n_2) \,. \end{aligned} \tag{20}$$

When transforming the Fermi operators it is more convenient to use the real space representation for n_q yielding

$$R = N^{-1/2} \sum_{jq\sigma} \gamma_q \delta_q \left(b^\dagger_{-q} - b_q \right) n_{j\sigma} \exp\left(iqR_j\right).$$

The *displaced Fermi operators* $C^{(\dagger)}_{j\sigma} = \mathrm{e}^R c^{(\dagger)}_{j\sigma} \mathrm{e}^{-R}$ are easily obtained by noting that the n-th order commutator in the development of $C_{j\sigma}$ yields $[(-1)N^{-1/2}\sum_q \delta_q\gamma_q \left(b^\dagger_{-q} - b_q\right)\exp\left(iqR_j\right)]^n c_{j\sigma}$ *i.e.* the n-th power of a bosonic operator $[...]^n$ times the same Fermi operator $c_{j\sigma}$ to be transformed. The case for the creation operator $C^\dagger_{j\sigma}$ is similar, but for lacking the factor (-1) inside $[...]^n$ and having $c^\dagger_{j\sigma}$ in place of $c_{j\sigma}$. Therefore the series of commutators can be summed to an exponential of the bosonic operator, yielding

$$C^\dagger_{j\sigma} = c^\dagger_{j\sigma} \exp[\frac{1}{\sqrt{N}} \sum_q \delta_q\gamma_q \left(b^\dagger_{-q} - b_q \right) \mathrm{e}^{iqR_j}]$$

$$C_{j\sigma} = c_{j\sigma} \exp[-\frac{1}{\sqrt{N}} \sum_q \delta_q\gamma_q \left(b^\dagger_{-q} - b_q \right) \mathrm{e}^{iqR_j}]\,. \tag{21}$$

We can now use the above results to transform the whole electron–phonon Hamiltonian.

4. The "displaced" Hamiltonian

Equation (21) implies that the number operators $n_{j\sigma}$ are unaffected by the displacement transformation. The only term in H_{el} affected by the transformation is therefore the hopping term, yielding:

$$\mathrm{e}^R \sum_{l\langle j\rangle\sigma} t_{lj} c^\dagger_{l\sigma} c_{j\sigma} \mathrm{e}^{-R} = \sum_{l\langle j\rangle\sigma} t_{lj} (\mathrm{e}^R c^\dagger_{l\sigma} \mathrm{e}^{-R})(\mathrm{e}^R c_{j\sigma} \mathrm{e}^{-R})$$

$$= \sum_{l\langle j\rangle\sigma} c^\dagger_{l\sigma} c_{j\sigma} t_{lj} \exp\left[\frac{1}{\sqrt{N}} \sum_q \delta_q\gamma_q \left(b^\dagger_{-q} - b_q \right) \left(\mathrm{e}^{iqR_l} - \mathrm{e}^{iqR_j} \right] \right. . \tag{22}$$

A strong non-linear interaction with the phonons, which affects the hopping of the electrons, has been introduced by the transformation.

To see how the terms containing phononic operators are transformed, let us start from the free oscillator term:

$$\mathrm{e}^R \left[\sum_q \hbar\Omega_q \left(b^\dagger_q b_q + \frac{1}{2} \right) \right] \mathrm{e}^{-R} = \sum_q \hbar\Omega_q \left[(b^\dagger_q - \gamma_q\delta_q n_q)(b_q - \gamma_q\delta_q n_{-q}) + \frac{1}{2} \right]$$

$$= \sum_q \hbar\Omega_q \left[b^\dagger_q b_q + \frac{1}{2} - \gamma_q\delta_q n_q \left(b^\dagger_{-q} + b_q \right) + \gamma^2_q \delta^2_q n_q n_{-q} \right]. \tag{23}$$

The Holstein term yields:

$$\mathrm{e}^{R}\left[\sum_{q}\hbar\Omega_{q}\gamma_{q}\left(b_{-q}^{\dagger}+b_{q}\right)n_{q}\right]\mathrm{e}^{-R}=\sum_{q}\hbar\Omega_{q}\left[\gamma_{q}\left(b_{-q}^{\dagger}+b_{q}\right)n_{q}-2\gamma_{q}^{2}\delta_{q}n_{q}n_{-q}\right]. \tag{24}$$

By reordering the terms in Eqs. (23) and (24) we can write the total transformed phononic Hamiltonian $H_{\mathrm{ph}}^{T}=\mathrm{e}^{R}\left[H_{\mathrm{ph}}+H_{\mathrm{el-ph}}\right]\mathrm{e}^{-R}$ as:

$$\begin{aligned}H_{\mathrm{ph}}^{T}=\sum_{q}\hbar\Omega_{q}\left(b_{q}^{\dagger}b_{q}+\frac{1}{2}\right) &+\sum_{q}\hbar\Omega_{q}\gamma_{q}\left(b_{-q}^{\dagger}+b_{q}\right)n_{q}\left(1-\delta_{q}\right)\\ &-\sum_{q}\hbar\Omega_{q}\gamma_{q}^{2}\delta_{q}\left(2-\delta_{q}\right)n_{q}n_{-q}\,.\end{aligned} \tag{25}$$

We see that H_{ph}^{T} has a pure fermionic term in addition to the free oscillator and Holstein terms. The Holstein term might be cancelled if we chose $\delta_{q}=1$ for any q. This was indeed the historic reason for which Lang and Firsov, who first introduced [6] the displacement transformation, made that choice for δ_{q}, realising the *complete displacement transformation* (CDT). We shall follow a different approach, by letting, for the moment, δ_{q} undetermined. The most interesting term in H_{ph}^{T} is the last one, which, going back to the real space representation, reads:

$$\begin{aligned}&\sum_{q}\hbar\Omega_{q}\gamma_{q}^{2}\delta_{q}\left(2-\delta_{q}\right)n_{q}n_{-q}=\sum_{j}\left(n_{j}+2n_{j\uparrow}n_{j\downarrow}\right)\left[\frac{1}{N}\sum_{q}\hbar\Omega_{q}\gamma_{q}^{2}\delta_{q}\left(2-\delta_{q}\right)\right]\\ &+\sum_{j}\sum_{l\neq j}n_{j}n_{l}\left[\frac{1}{N}\sum_{q}\hbar\Omega_{q}\gamma_{q}^{2}\delta_{q}\left(2-\delta_{q}\right)\mathrm{e}^{iq(R_{j}-R_{l})}\right].\end{aligned} \tag{26}$$

We find phonon-induced contributions to the on- site atomic energy ($\approx n_{j}$), to the on-site Hubbard interaction ($\approx n_{j\uparrow}n_{j\downarrow}$), and to the intersite Coulomb interaction ($\approx n_{j}n_{l}$) . Collecting all contributions, we write the *displaced* Hamiltonian $H^{T}\equiv e^{R}\left(H_{\mathrm{el}}+H_{\mathrm{ph}}+H_{\mathrm{el-ph}}\right)\mathrm{e}^{-R}$ as:

$$\begin{aligned}H^{T} \;=\; &\sum_{j\sigma}\varepsilon_{j}^{*}n_{j\sigma}+\sum_{i<j>\sigma}t_{ij}^{*}c_{i\sigma}^{\dagger}c_{j\sigma}+U^{*}\sum_{j}n_{j\uparrow}n_{j\downarrow}+\sum_{i<j>}V_{ij}^{*}n_{i}n_{j}\\ &+\sum_{q}\hbar\Omega_{q}\left(b_{q}^{\dagger}b_{q}+\frac{1}{2}\right)+\sum_{q}\hbar\Omega_{q}\gamma_{q}\left(b_{-q}^{\dagger}+b_{q}\right)n_{q}\left(1-\delta_{q}\right)\end{aligned} \tag{27}$$

where the phonon-renormalized interactions read:

$$\varepsilon_{j}^{*} \;=\; \varepsilon_{j}-\frac{1}{N}\sum_{q}\hbar\Omega_{q}\gamma_{q}^{2}\delta_{q}\left(2-\delta_{q}\right), \tag{28}$$

$$U_j^* \;=\; U_j - 2\left(\frac{1}{N}\right)\sum_q \hbar\Omega_q\gamma_q^2\delta_q\,(2-\delta_q)\;, \tag{29}$$

$$V_{jl}^* \;=\; V_{jl} - \frac{1}{N}\sum_q \hbar\Omega_q\gamma_q^2\delta_q\,(2-\delta_q)\,\mathrm{e}^{iq(R_j-R_l)}\,. \tag{30}$$

As the physical values of δ_q are between 0 and 1, the additional terms decrease the values of the bare interactions. The effect might be so large as to change the sign of U and V_{jl} from positive to negative, with drastic effects on the physics. Moreover, while the bare V_{jl} vanishes if j and l are not first neighbours, in the additional contribution there is no constraint on j and l : the phonons produce an undamped long range oscillating interaction between the charges on the various sites. Here one can appreciate the importance of not adopting the Lang–Firsov choice $\delta_q \to 1$ for any q. Indeed, in that case one would have (recalling $\gamma_q = g/\hbar\Omega_q$ and defining Δ_{jl} =0 if $j \neq l$):

$$V_{jl}^* \Longrightarrow V_{jl} - \frac{1}{N}\sum_q \hbar\Omega_q\gamma_q^2\mathrm{e}^{iq(R_j-R_l)} = V_{jl} - g^2\Delta_{jl} = V_{jl}\,. \tag{31}$$

Namely, the long range interaction disappears in the CDT case. For hystorical reasons, a number of characteristic quantities in the polaron literature has been introduced just for CDT where:

$$\varepsilon_j^* \Longrightarrow \varepsilon_j - \hbar\Omega\gamma^2 = \varepsilon_j - \frac{g^2}{\hbar\Omega}\,, \qquad U_j^* \Longrightarrow U_j - 2\frac{g^2}{\hbar\Omega}\,. \tag{32}$$

The quantity $g^2/\hbar\Omega$ is called *polaronic shift* or *polaron binding energy*, being the phonon-induced shift of the atomic energy, *i.e.* the additional attractive energy which each site acquires due to the phonons. Given this interpretation of $g^2/\hbar\Omega$ one can ask how many phonons dress a polaron. An intuitive answer is provided by dividing the polaron binding energy by the energy $\hbar\Omega$ of each phonon. The result $(g/\hbar\Omega)^2$ is called the *Huang–Rhys factor.* Its evaluation for arbitrary δ_q will be given later on (see Eq. (57)).

4.1. Applications to two- and four-site systems

Let us see now how this general formalism reads when applied to the dimer case [2] with $\Omega_q \to \Omega\,(\gamma_q \to \gamma)$. The transformed Bose operators are now:

$$B_0^{(\dagger)} = b_0^{(\dagger)} - \frac{\delta_0\gamma_0}{\sqrt{2}}\,(n_1+n_2)\;, \qquad B_{\pi/a}^{(\dagger)} = b_{\pi/a}^{(\dagger)} - \frac{\delta_{\pi/a}\gamma_{\pi/a}}{\sqrt{2}}\,(n_1-n_2) \tag{33}$$

so that the phonon-depending part of the transformed Hamiltonian, $H_{\rm ph}^T$, is:

$$H_{\rm ph}^T = {\rm e}^{\left(R_0+R_{\pi/a}\right)}\left(H_{\rm ph}+H_{\rm el-ph}\right){\rm e}^{-\left(R_0+R_{\pi/a}\right)} = \hbar\Omega\left(B_0^\dagger B_0+B_{\pi/a}^\dagger B_{\pi/a}+1\right)$$
$$+\frac{\hbar\Omega\gamma}{\sqrt{2}}\left[\left(1-\delta_0\right)\left(B_0^\dagger+B_0\right)\left(n_1+n_2\right)+\left(1-\delta_{\pi/a}\right)\left(B_{\pi/a}^\dagger-B_{\pi/a}\right)\left(n_1-n_2\right)\right]$$
$$-\frac{\hbar\Omega\gamma^2}{2}\left[\delta_0\left(2-\delta_0\right)\left(n_1+n_2\right)^2+\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\left(n_1-n_2\right)^2\right]. \qquad (34)$$

As $[H_{\rm el},(n_1+n_2)]=0$, then ${\rm e}^{R_0}H_{\rm el}{\rm e}^{-R_0}=H_{\rm el}$, and we can choose $\delta_0=1$ which minimizes the $q=0$ contribution to $H_{\rm ph}^T$. This can not be done for $\delta_{\pi/a}$ because the Fermi operators are transformed into

$$C_{1\sigma}^\dagger = c_{1\sigma}^\dagger{\rm e}^{\delta_{\pi/a}\gamma\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)/\sqrt{2}}, \qquad C_{1\sigma}=c_{1\sigma}{\rm e}^{-\delta_{\pi/a}\gamma\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)/\sqrt{2}},$$
$$C_{2\sigma}^\dagger = c_{2\sigma}^\dagger{\rm e}^{\delta_{\pi/a}\gamma\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)/\sqrt{2}}, \qquad C_{2\sigma}=c_{2\sigma}{\rm e}^{\delta_{\pi/a}\gamma\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)/\sqrt{2}}. \qquad (35)$$

After these transformations, the hopping term reads:

$$t\sum_\sigma\left(C_{1\sigma}^\dagger C_{2\sigma}+C_{2\sigma}^\dagger C_{1\sigma}\right)=t\cosh\left[\sqrt{2}\gamma\delta_{\pi/a}\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)\right]\sum_\sigma\left(c_{1\sigma}^\dagger c_{2\sigma}+c_{2\sigma}^\dagger c_{1\sigma}\right)$$
$$+t\sinh\left[\sqrt{2}\gamma\delta_{\pi/a}\left(b_{\pi/a}^\dagger-b_{\pi/a}\right)\right]\sum_\sigma\left(c_{1\sigma}^\dagger c_{2\sigma}-c_{2\sigma}^\dagger c_{1\sigma}\right) \qquad (36)$$

while the renormalized Coulomb interactions are:

$$\varepsilon_j^* = \varepsilon_j-\frac{\hbar\Omega\gamma^2}{2}\left[1+\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\right],$$
$$U_j^* = U_j-\hbar\Omega\gamma^2\left[1+\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\right],$$
$$V_{ij}^* = V_{ij}-\frac{\hbar\Omega\gamma^2}{2}\left[1-\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\right]. \qquad (37)$$

Notice that, consistently with Eq. (2) one has to write the total inter-site Coulomb term for the dimer as $\sum_{j\langle l\rangle}V_{jl}n_jn_l=V_{12}n_1n_2+V_{21}n_2n_1=2V_{12}n_1n_2$.

To see in a concrete example the long range nature of V_{ij}^* let us consider the four-site chain with $\Omega_q\to\Omega$. There are two orders of neighbours: for nearest neighbours $|R_j-R_l|=a$ and:

$$V_{i,i+1}^*=V_{i,i+1}-\frac{\hbar\Omega\gamma^2}{4}\left[\delta_0\left(2-\delta_0\right)-\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\right]. \qquad (38)$$

For second neighbours $|R_j-R_l|=2a$ and V_{ij}^* has only the long range part, reading:

$$V_{i,i+2}^*=-\frac{\hbar\Omega\gamma^2}{4}\left[\delta_0\left(2-\delta_0\right)-2\delta_{\pi/2a}\left(2-\delta_{\pi/2a}\right)+\delta_{\pi/a}\left(2-\delta_{\pi/a}\right)\right]. \qquad (39)$$

Due to the periodic boundary conditions imposed on the chain, the third neighbours coincide with the first ones.

4.2. The phonon subsystem

Before continuing to study how the electrons are influenced by the phonons, it is interesting to consider briefly the inverse problem, *i.e.* how the phonons respond to the electrons [7]. Let us select from Eq. (27) the phonon-depending terms:

$$\begin{aligned} H_{\rm ph}^T \;=\; & \sum_q \hbar\Omega_q \left(b_q^\dagger b_q + \frac{1}{2} \right) + \frac{1}{\sqrt{N}} \sum_{jq\sigma} \hbar\Omega_q \gamma_q \left(1-\delta_q\right) \left(b_{-q}^\dagger - b_q \right) n_{j\sigma} \mathrm{e}^{iqR_j} \\ & + \sum_{\langle jl\rangle\sigma} t_{jl} \cosh \left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q \right) \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right] \left(c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma} \right) \right. \\ & + \sum_{\langle jl\rangle\sigma} t_{jl} \sinh \left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q \right) \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right] \left(c_{j\sigma}^\dagger c_{l\sigma} - c_{l\sigma}^\dagger c_{j\sigma} \right) . \end{aligned} \tag{40}$$

In the hopping term we have switched from site to bond sum. We shall develop $H_{\rm ph}^T$ in mean field approximation (MFA:$AB \approx A\langle B\rangle + B\langle A\rangle - \langle A\rangle\langle B\rangle$), under the assumption that there are no spontaneous currents ($\langle c_{j\sigma}^\dagger c_{l\sigma} - c_{l\sigma}^\dagger c_{j\sigma}\rangle = 0$) and that translational invariance holds ($\langle c_{j\sigma}^\dagger c_{l\sigma}\rangle = \langle c_{l\sigma}^\dagger c_{j\sigma}\rangle$). Let us define

$$\tau_{jl}\left(\{\delta_q\}\right) \equiv \left\langle \cosh \left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q \right) \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right] \right\rangle , \tag{41}$$

where the expectation value is to be taken over an appropriate phonon state. If we take the phonon vacuum, as shown in the equation (82) later on, $\tau \equiv \exp\left\{ -N^{-1} \sum_q \gamma_q^2 \delta_q^2 \left[1 - \cos\left(qa\right) \right] \right\}$ independently of j, l. The MFA form of the displaced hopping term $H_{\rm hop}^T$ reads:

$$\begin{aligned} H_{\rm hop}^T = & - \sum_{j\langle l\rangle\sigma} t_{jl} \tau_{jl} \langle c_{j\sigma}^\dagger c_{l\sigma}\rangle + \sum_{j\langle l\rangle\sigma} t_{jl} \tau_{jl} c_{j\sigma}^\dagger c_{l\sigma} \\ & + 2 \sum_{j\langle l\rangle\sigma} t_{jl} \langle c_{j\sigma}^\dagger c_{l\sigma}\rangle \cosh \left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q \right) \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right] . \end{aligned} \tag{42}$$

The first line of Eq. (42) contributes to the effective electronic Hamiltonian, while the second one to its phononic counterpart. Indeed, the purely

phononic MFA Hamiltonian now reads:

$$H_{\rm ph}^T = \sum_q \hbar\Omega_q \left(b_q^\dagger b_q + \frac{1}{2} \right) + \sum_{jq\sigma} \hbar\Omega_q \gamma_q \left(1-\delta_q\right) \left(b_{-q}^\dagger - b_q \right) \langle n_q \rangle$$

$$+2 \sum_{j\langle l\rangle\sigma} t_{jl} \langle c_{j\sigma}^\dagger c_{l\sigma} \rangle \cosh \left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q \right) \left({\rm e}^{iqR_j} - {\rm e}^{iqR_l} \right) \right] . \quad (43)$$

We see that the phonon subsystem is apparently influenced by both the density ($\langle n_q \rangle$) and the hopping ($t_{jl}\langle c_{j\sigma}^\dagger c_{l\sigma}\rangle$) of the electrons. To better understand what happens, let us evaluate the phonon Green's Function (GF) $\langle\langle b_q \, ; b_q^\dagger \rangle\rangle$ which obeys the equation of motion (EOM):

$$\hbar\omega_q \langle\langle b_q ; b_q^\dagger \rangle\rangle = \frac{1}{2\pi} \left\langle \left[b_q, b_q^\dagger \right] \right\rangle + \left\langle \left\langle \left[b_q, H_{\rm ph}^T \right] ; b_q^\dagger \right\rangle \right\rangle , \quad (44)$$

where ω_q is the renormalized frequency, in principle different from the bare one Ω_q. Defining for short $T_{jl\sigma} = t_{jl}\langle c_{j\sigma}^\dagger c_{l\sigma}\rangle$ and $X_{qlj} = \left(1/\sqrt{N}\right) \delta_q \gamma_q ({\rm e}^{iqR_j} - {\rm e}^{iqR_l})$ we obtain the first order EOM in the form:

$$(\hbar\omega_p - \hbar\Omega_p) \langle\langle b_p ; b_p^\dagger \rangle\rangle = \frac{1}{2\pi} + \sum_{j\langle l\rangle\sigma} T_{jl\sigma} X_{-plj} \quad (45)$$

$$\times \left\{ \left\langle \left\langle \exp\Big[\sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \Big] ; b_p^\dagger \right\rangle \right\rangle - \left\langle \left\langle \exp\Big[-\sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \Big] ; b_p^\dagger \right\rangle \right\rangle \right\} .$$

Notice that no contribution to the EOM comes from the Holstein term $\approx \langle n_q \rangle$. Its role is to put into contact the electron and phonon subsystems, but only the hopping of the electrons influences quantitatively the phonons. The new GF's obey the second order EOM:

$$\hbar\omega_p \left\langle \left\langle \exp \Big[\pm \sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \Big] ; b_p^\dagger \right\rangle \right\rangle$$

$$= \frac{1}{2\pi} \left\langle \Big[\exp \Big[\pm \sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \Big] ; b_p^\dagger \Big] \right\rangle$$

$$+ \left\langle \left\langle \Big[\exp \Big[\pm \sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \Big] ; H_{\rm ph}^T \Big] ; b_p^\dagger \right\rangle \right\rangle . \quad (46)$$

To break the chain of EOM's we shall assume that the GF's of phonons of different modes $\langle\langle b_q ; b_p^\dagger \rangle\rangle$ vanish (harmonic approximation), and develop in MFA terms like $b_p^\dagger \exp\left[\pm \sum_q X_{qlj} \left(b_{-q}^\dagger - b_q \right) \right]$. The expectation values

will be taken over the *undisplaced* phonon states, so that $\left\langle b_p^\dagger \right\rangle = 0$ and $\left\langle \exp\left[\pm\sum_q X_{qlj}\left(b_{-q}^\dagger - b_q\right)\right]\right\rangle = \tau_{lj}$. The Eq. (46) then reduces to:

$$\left[\hbar\omega_p + \sum_q \hbar\Omega_q X_{qlj} X_{-qlj}\right]\left\langle\left\langle \exp\left[\pm\sum_q X_{qlj}\left(b_{-q}^\dagger - b_q\right)\right]; b_p^\dagger\right\rangle\right\rangle$$
$$= \mp\left[\frac{X_{plj}}{2\pi} + \hbar\Omega_p X_{plj}\langle\langle b_p; b_p^\dagger\rangle\rangle\right]\exp\left[-\frac{1}{2}\sum_q X_{qlj}X_{-qlj}\right]. \tag{47}$$

Finally, by evaluating X_{qlj} for $|R_j - R_l| = a$, we obtain that the phonon GF obeys:

$$\langle\langle b_p; b_p^\dagger\rangle\rangle\left\{\hbar\omega_p - \hbar\Omega_p\left[1 - \frac{4\delta_p^2\gamma_p^2\left[1-\cos(pa)\right](1/N)\sum_{\langle lj\rangle\sigma} T_{lj\sigma}\tau_{lj}}{\hbar\omega_p - (2/N)\sum_q \hbar\Omega_q\delta_q^2\gamma_q^2\left[1-\cos(qa)\right]}\right]\right\}$$
$$= \left(\frac{1}{2\pi}\right)\left\{1 - \left[\frac{1}{N}\sum_{\langle lj\rangle\sigma} T_{lj\sigma}\tau_{lj}\right]\frac{4\delta_p^2\gamma_p^2\left[1-\cos(pa)\right]}{\hbar\omega_p - (2/N)\sum_q \hbar\Omega_q\delta_q^2\gamma_q^2\left[1-\cos(qa)\right]}\right\}. \tag{48}$$

The above results show that the electron hopping modifies both the phonon frequency and the spectral weight. The renormalized frequency follows from the poles of the GF. By defining for short $\Delta_q = \delta_q^2\gamma_q^2\left[1-\cos(qa)\right]$ and $T = (1/N)\sum_{\langle lj\rangle\sigma} T_{lj\sigma}\tau_{lj}$, we obtain:

$$\hbar\omega_p = \frac{1}{2}\left[\hbar\Omega_p + \frac{2}{N}\sum_q \hbar\Omega_q\Delta_q \pm \sqrt{\left(\hbar\Omega_p - \frac{2}{N}\sum_q \hbar\Omega_q\Delta_q\right)^2 - 16\hbar\Omega_p\Delta_p T}\right]. \tag{49}$$

The correct choice of the sign follows from imposing $\lim_{T\to 0}\omega_p = \Omega_p$. The softening or hardening of the phonons then depends on the sign in front of the square root, in turn determined by the ratio $\hbar\Omega_p \,/\left(\frac{2}{N}\right)\sum_q \hbar\Omega_q\Delta_q$. Notice that, even if the bare phonons were dispersionless ($\Omega_p \to \Omega$), the dressed phonons acquire dispersion, due to the itineracy of the electrons, through the T- depending term under the square root. In the case of the dimer, $\Delta_{\pi/a} = 2\gamma^2\delta_{\pi/a}^2$ and the renormalized frequency is:

$$\omega_{\pi/a} = \frac{\Omega}{2}\left[1 + 2\gamma^2\delta_{\pi/a}^2 \pm \sqrt{\left(1 - 2\gamma^2\delta_{\pi/a}^2\right)^2 - 32\gamma^2\delta_{\pi/a}^2\frac{T}{\hbar\Omega}}\right]. \tag{50}$$

The phonon gets softened if $\gamma^2\delta_{\pi/a}^2 \geq 1/2$, a condition easily met when the displacement $\delta_{\pi/a}$is not negligible and the Huang–Rhys factor $(g/\hbar\Omega)^2$

is appreciable. The possibility that the phonon gets hardened might be an artifact of our approximations. A more rigorous treatment [7] yields a softening in all cases.

5. Displaced phonon states

To recall where we are before proceeding, let us write down the total *displaced* Hamiltonian H^T in the general case of dispersive bare phonons:

$$\begin{aligned} H^T \;=\; & \mathrm{e}^{R}\,(H_{\mathrm{el}} + H_{\mathrm{ph}} + H_{\mathrm{el=ph}})\,\mathrm{e}^{-R} = \sum_{j\sigma} \varepsilon_j^* n_{j\sigma} \\ & + \sum_{j<l>\sigma} t_{jl} \exp\left[\frac{1}{\sqrt{N}} \sum_q \delta_q \gamma_q \left(b_{-q}^\dagger - b_q\right) \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l}\right]\right. c_{j\sigma}^\dagger c_{l\sigma} \\ & + U^* \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{j<l>} V_{jl}^* n_j n_l + \sum_q \hbar\Omega_q \left(b_q^\dagger b_q + \frac{1}{2}\right) \\ & + \frac{1}{\sqrt{N}} \sum_{jq\sigma} \hbar\Omega_q \gamma_q \,(1-\delta_q) \left(b_{-q}^\dagger - b_q\right) n_{j\sigma} \mathrm{e}^{iqR_j} \,. \end{aligned} \tag{51}$$

Phonon operators are still present in H^T. To obtain the purely electronic effective Hamiltonian we shall evaluate the expectation value of H^T over some appropriate phonon wavefunction. This will substitute the terms containing phonon operators with $c-$numbers, leaving the Fermi operators unaffected. We shall proceed in two ways, one more traditional, one more modern.

To start with the traditional treatment, let us consider two sites in our lattice: on one, labeled l, there is no charge to interact with its deformation u_l, described by local phonon operators $b_j^\dagger, b_j$. The other one, j, has a local charge ρ_l and a charge-induced deformation $\mathrm{e}^R u_j \mathrm{e}^{-R} = \mathcal{U}_j = u_j - Q_j$, where $Q_j = 2\gamma\delta\rho_l L$. On site j the phonons are displaced and described by $B_j^{(\dagger)} = b_j^{(\dagger)} - Q_j/2L$. Undisplaced $n-$phonon states on l will be indicated as $|n_l\rangle$, while displaced ones on j by $|n_j)$. The vacuum wave function $|0_l\rangle = (M\omega/\pi\hbar)^{1/4} \exp\left[-\,(M\omega/2\hbar)\,u_l^2\right]$ is the one for the harmonic oscillator. For the *displaced vacuum* $|0_j)$ we have instead:

$$\begin{aligned} |0_j) \;&=\; \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\left(\frac{M\omega}{2\hbar}\right)\mathcal{U}_j^2} = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\left(\frac{M\omega}{2\hbar}\right)(u_j - Q_j)^2} \\ &=\; \mathrm{e}^{-\left(\frac{M\omega}{2\hbar}\right)Q_l^2} \mathrm{e}^{\left(\frac{M\omega}{\hbar}\right)Q_l u_j} |0_j\rangle \,. \end{aligned} \tag{52}$$

To rewrite $|0_j)$ in terms of undisplaced phonon operators, we exploit the definition of Q_j and the quantization of u_j, yielding $\left(\frac{M\omega}{2\hbar}\right) Q_j^2 = (\gamma\delta\rho_j)^2$ and

$\left(\frac{M\omega}{\hbar}\right) Q_j u_j = \left(b_j^\dagger + b_j\right) \gamma\delta\rho_j$. Then, by disentangling e^{X+Y}:

$$\begin{aligned} |0_j) &= \mathrm{e}^{-(\gamma\delta\rho_j)^2} \mathrm{e}^{\gamma\delta\rho_j \left(b_j^\dagger + b_j\right)} |0_j\rangle = \mathrm{e}^{-\frac{1}{2}(\gamma\delta\rho_j)^2} \mathrm{e}^{\gamma\delta\rho_j b^{\dagger}{}_j} \mathrm{e}^{\gamma\delta\rho_j b_j} |0_j\rangle \\ &= \mathrm{e}^{-\frac{1}{2}(\gamma\delta\rho_j)^2} \mathrm{e}^{\gamma\delta\rho_j b_j^\dagger} |0_j\rangle \,, \end{aligned} \tag{53}$$

where we have used $\exp\left(\gamma\delta\rho_j b_j\right)|0_j\rangle = \sum_m \frac{(\gamma\delta\rho_j b_j)^m}{m!}|0_j\rangle = |0_j\rangle$ because only the $m = 0$ term gives a non-vanishing contribution. In a similar way one can build the other excited displaced states, yielding:

$$|n) = \frac{1}{\sqrt{N!}} \left[b_j^\dagger - \gamma\delta\rho_j\right]^n |0) = \frac{1}{\sqrt{N!}} \sum_k^{0\ldots n} \binom{n}{k} (-\gamma\delta\rho_j)^k \left(b_j^\dagger\right)^{n-k} |0) \,. \tag{54}$$

One has to be careful in interpreting the notational relation between bare and displaced states: for instance, the displaced vacuum state $|0_j)$ is far from being empty of phonons. Indeed, let us evaluate the number of undisplaced phonons in $|0_j)$:

$$\begin{aligned} \frac{(0_j|b_j^\dagger b_j|0_j)}{\mathrm{e}^{-(\gamma\delta\rho_j)^2}} &= \langle 0_j|\mathrm{e}^{\gamma\delta\rho_j b_j} b_j^\dagger b_j \mathrm{e}^{\gamma\delta\rho_j b_j^\dagger}|0_j\rangle \\ &= \langle 0_j| \sum_{k,p} \frac{(\gamma\delta\rho_j)^{k+p}}{k!p!} b_j^k \left(b_j^\dagger b_j\right) \left(b_j^\dagger\right)^k |0_j\rangle \\ &= \sum_k \frac{(\gamma\delta\rho_j)^{2k}}{(k!)^2} \langle 0_j| b_j^k \left(b_j b_j^\dagger - 1\right) \left(b_j^\dagger\right)^k |0_j\rangle \\ &= \sum_k \frac{(\gamma\delta\rho_j)^{2k}}{(k!)^2} \left[\langle 0_j| b_j^{k+1} \left(b_j^\dagger\right)^{k+1} - b_j^k \left(b_j^\dagger\right)^k |0_j\rangle\right] . \end{aligned} \tag{55}$$

By recalling that normalized phonon states ($\langle k|k\rangle = 1$) obey $\left(b_j^\dagger\right)^k |0_j\rangle = \sqrt{k!}|k_j\rangle$ and $b_j^k|k_j\rangle = \sqrt{k!}|0_j\rangle$ we can write

$$\begin{aligned} (0_j|b_j^\dagger b_j|0_j) &= \mathrm{e}^{-(\gamma\delta\rho_j)^2} \left\{\sum_{k=0}^\infty \frac{(\gamma\delta\rho_j)^{2k}}{k!}(k+1) - \sum_{k=0}^\infty \frac{(\gamma\delta\rho_j)^{2k}}{k!}\right\} \\ &= \mathrm{e}^{-(\gamma\delta\rho_j)^2} \left\{\sum_{k=1}^\infty \frac{(\gamma\delta\rho_j)^{2k}}{(k-1)!} + \sum_{k=0}^\infty \frac{(\gamma\delta\rho_j)^{2k}}{k!} - \mathrm{e}^{(\gamma\delta\rho_j)^2}\right\} \\ &= \mathrm{e}^{-(\gamma\delta\rho_j)^2} \sum_{k=1}^\infty \frac{(\gamma\delta\rho_j)^{2k}}{(k-1)!} \,. \end{aligned} \tag{56}$$

Now, by changing from k to $p = k - 1$ in the series, we have:

$$\begin{aligned}(0_j|b_j^\dagger b_j|0_j) &= \mathrm{e}^{-(\gamma\delta\rho_j)^2}\sum_{p=0}^{\infty}\frac{(\gamma\delta\rho_j)^{2p+2}}{p!} \\ &= \mathrm{e}^{-(\gamma\delta\rho_j)^2}\left[(\gamma\delta\rho_j)^2\,\mathrm{e}^{(\gamma\delta\rho_j)^2}\right] = (\gamma\delta\rho_j)^2\ . \end{aligned} \tag{57}$$

$(0_j|b_j^\dagger b_j|0_j)$ is nothing else that the Huang–Rhys factor in the general case of arbitrary δ value and electron density ρ_j, which measures rigorously the non-vanishing number of bare phonons in the state obtained by displacing their vacuum.

We can go further, showing that, while $\langle 0_j|b_j|0_j\rangle = 0$ (which is the definition of the vacuum state $|0_j\rangle$ of the bare phonons) on the contrary $(0_j|b_j|0_j) = \gamma\delta\rho_j$, so that $|0)$ is an eigenstate of the bare destruction operator b_j. States satisfying $b|0) \neq 0$ are called *coherent states* in the literature. By using Eq. (53),defining for short $x = \gamma\delta\rho_j$ with the site index understood, we have:

$$(0|b|0) = \mathrm{e}^{-x^2}\langle 0|\mathrm{e}^{xb}b\mathrm{e}^{xb^\dagger}|0\rangle\,. \tag{58}$$

Developing the exponentials yields:

$$(0|b|0) = \mathrm{e}^{-x^2}\langle 0|\sum_{p,q}\frac{x^p x^q}{p!q!}b^{p+1}\left(b^\dagger\right)^q|0\rangle\,. \tag{59}$$

Using the properies of the normalized phonon states yields:

$$\langle 0|b^{p+1}\left(b^\dagger\right)^q|0\rangle = \langle 0|\sqrt{q!}\,b^{p+1}|q\rangle = q!\Delta_{p+1,q}\,. \tag{60}$$

Then, after changing the sum index to $n = q - 1$, Eq. (59) yields:

$$(0|b|0) = \mathrm{e}^{-x^2}\sum_n\frac{x^{2n+1}}{n!} = \mathrm{e}^{-x^2}\left(x\mathrm{e}^{x^2}\right) = x\,. \tag{61}$$

Therefore in the displaced (or coherent) state even a single phonon operator has a non-vanishing expectation value.

We saw that only the hopping term was modified in the displacement transformation. Now we can evaluate its value over the displaced phonon states. Let us suppose that initially we have one $\sigma-$electron on site j and none on site l: the electronic state can be described by $|0_l; 1_{j\sigma}\}$. Correspondingly, the phonon vacuum states will be $|0_l\rangle$ and $|0_j)$. The hopping term $t_{jl}c_{l\sigma}^\dagger c_{j\sigma}$ transfers the electron, causing the system to pass from an

initial state $|I\rangle = |0_l; 1_{j\sigma}\}|0_l\rangle|0_j)$ to a final one $|F\rangle = |1_{l\sigma}; 0_j\}|0_l)|0_j\rangle$. We want to evaluate the matrix element $\langle F|t_{jl}c^\dagger_{l\sigma}c_{j\sigma}\ |I\rangle$, that is:

$$\langle F|t_{jl}c^\dagger_{l\sigma}c_{j\sigma}|I\rangle = \{1_{l\sigma}; 0_j|t_{jl}c^\dagger_{l\sigma}c_{j\sigma}|0_l; 1_{j\sigma}\}(0_l|\langle 0_j|0_l\rangle|0_j) = t_{jl}(0_l|0_l\rangle\langle 0_j|0_j)\,. \tag{62}$$

The kinetic energy depends on the degree of overlap between the undisplaced, and the displaced, phonon wavefunctions on each site. By using Eq. (53) we evaluate the *Franck–Condon integrals* $\langle 0_j|0_j)$ as:

$$\langle 0_j|0_j) = \langle 0_j|\mathrm{e}^{-(\gamma\delta\rho_j)^2/2}\mathrm{e}^{\gamma\delta\rho_j b^\dagger_j}|0_j\rangle = \mathrm{e}^{-(\gamma\delta\rho_j)^2/2}\,. \tag{63}$$

It is easy to show that $\langle 0_j|n_j) = \left[(\gamma\delta\rho_j)^n/\sqrt{n!}\right]\langle 0_j|0_j)$. Therefore

$$\langle F|t_{jl}c^\dagger_{l\sigma}c_{j\sigma}|I\rangle = t_{jl}\mathrm{e}^{-(\gamma\delta\rho_j)^2}\,. \tag{64}$$

This result tells us that the phonons are expected to reduce strongly the hopping amplitude due to the reduced overlap between $|n\rangle$ and $|n)$ on each site. We shall comment on the physical implications of this effect later on.

6. The squeezed state

The discussion given above follows a traditional line of argument. More recently, a new approach has been applied [8], based on the concept of *Squeezing transformation* and of *Squeezed wavefunction*. We shall devote some space to describe squeezing in general, as applied to condensed matter: the lectures by Prof. Bialinicky–Birula also deal with squeezing, but mainly in electromagnetism. Further literature is listed under Ref. [9]. Squeezing can also apply to fermions, but we shall limit ourselves to squeezing of bosons.

Given Bose operators $\left\{b^\dagger_p, b_p\right\}$, one can define different squeezing transformations according to conveniency. If the Hamiltonian couples different modes (*e.g.* q and $-q$ in the Holstein case), then the squeezing operator is generally written as:

$$\mathrm{e}^S = \exp\left[-\sum_p \alpha_p\left(b^\dagger_p b^\dagger_{-p} - b_p b_{-p}\right)\right]\,, \qquad \left(\mathrm{e}^S\mathrm{e}^{S^\dagger} = 1\right)\,, \tag{65}$$

where $\alpha_p \geq 0$ is a real number, to be determined according to conveniency. When discussing the spin polarons we shall meet a situation where a different sign for the exponent has to be adopted. Given the phonon vacuum $|0\rangle$ (such that $b_p|0\rangle = 0$) we shall define the squeezed wavefunction $|\Psi_{SQ}\rangle$ as:

$$|\Psi_{SQ}\rangle = \mathrm{e}^{-S}\ |0\rangle = \mathrm{e}^{\sum_p \alpha_p\left(b^\dagger_p b^\dagger_{-p} - b_p b_{-p}\right)}\ |0\rangle\,. \tag{66}$$

If only a single mode q is of interest (*e.g.* in the dimer case, where only $q = \pi/a$ influences the electron hopping) then $S = -\alpha_p \left(b_q^\dagger b_q^\dagger - b_q b_q \right)$. One can use the squeezing also in the real space representation, where p will be a site label. By definition, if $\alpha_p \to 0$ the SQ states go over continuously to the usual harmonic oscillator state, so that they can be considered as extensions of the standard bosonic states.

Let us work out the squeezed form of $b_p^\dagger, b_p$ defined as $\mathcal{B}_p^{(\dagger)} = \mathrm{e}^S b_p^{(\dagger)} \mathrm{e}^{-S}$, by using the equation of motion technique, *i.e.* by considering $\mathcal{B}_p^{(\dagger)}$ a function of α_p and trying to set up a differential equation for $\mathcal{B}_p^{(\dagger)}(\alpha_p)$. The first derivative yields:

$$\frac{d\mathcal{B}_p^\dagger}{d\alpha_p} = \mathrm{e}^S \left[-(b_p^\dagger b_{-p}^\dagger - b_p b_{-p}), b_p^\dagger \right] \mathrm{e}^{-S} = \mathcal{B}_{-p}\,, \qquad \frac{d\mathcal{B}_p}{d\alpha_p} = \mathcal{B}_{-p}^\dagger\,. \tag{67}$$

The two equations are coupled, so we go to the second derivatives, yielding decoupled relations:

$$\frac{d^2\mathcal{B}_p^\dagger}{d\alpha_p^2} = \mathcal{B}_p^\dagger\,, \qquad \frac{d^2\mathcal{B}_p}{d\alpha_p^2} = \mathcal{B}_p \tag{68}$$

whose solution, taking into account the initial conditions $\mathcal{B}_p^{(\dagger)}(\alpha_p = 0) = b_p^{(\dagger)}$ together with $d\mathcal{B}_p^\dagger/d\alpha_p|_0 = b_{-p}$ and $d\mathcal{B}_p/d\alpha_p|_0 = b_{-p}^\dagger$, are:

$$\mathcal{B}_p^\dagger = b_p^\dagger \cosh(\alpha_p) + b_{-p} \sinh(\alpha_p)\,, \qquad \mathcal{B}_p = b_{-p}^\dagger \sinh(\alpha_p) + b_p \cosh(\alpha_p)\,. \tag{69}$$

In the case of a single mode, q say, the result has $2\alpha_q$ in place of α_p. The deformation and momentum operators then transform as:

$$\mathrm{e}^S (b_{-p}^\dagger + b_p) e^{-S} = \mathrm{e}^{\alpha_p} (b_{-p}^\dagger + b_p) \qquad \mathrm{e}^S (b_{-p}^\dagger - b_p) \mathrm{e}^{-S} = \mathrm{e}^{-\alpha_p} (b_{-p}^\dagger - b_p)\,. \tag{70}$$

To understand the reason why such states are called *squeezed (SQ)*, let us evaluate the Heisenberg uncertainty relation

$$\langle \Psi_{SQ} | \sqrt{u_p u_{-p}} | \Psi_{SQ} \rangle \langle \Psi_{SQ} | \sqrt{P_p P_{-p}} | \Psi_{SQ} \rangle \geq \hbar/2$$

by using Eq. (70). By definition:

$$\begin{aligned} u_p u_{-p} &= \left(\frac{\hbar}{2M\Omega_p} \right) (b_{-p}^\dagger + b_p)(b_p^\dagger + b_{-p})\,, \\ P_p P_{-p} &= -\left(\frac{\hbar \Omega_p M}{2} \right) (b_{-p}^\dagger - b_p)(b_p^\dagger - b_{-p})\,. \end{aligned} \tag{71}$$

In the SQ state, by using Eq. (70):

$$\begin{aligned}\langle\Psi_{SQ}|(b^\dagger_{-p}-b_p)(b^\dagger_p-b_{-p})|\Psi_{SQ}\rangle &= \mathrm{e}^{-2\alpha_p}\langle 0|(b^\dagger_{-p}-b_p)(b^\dagger_p-b_{-p})|0\rangle = -\mathrm{e}^{-2\alpha_p},\\ \langle\Psi_{SQ}|(b^\dagger_{-p}+b_p)(b^\dagger_p+b_{-p})|\Psi_{SQ}\rangle &= \mathrm{e}^{2\alpha_p}\langle 0|(b^\dagger_{-p}+b_p)(b^\dagger_p+b_{-p})|0\rangle = \mathrm{e}^{2\alpha_p}, \quad (72)\end{aligned}$$

so that:

$$\langle\Psi_{SQ}|\sqrt{u_p u_{-p}}|\Psi_{SQ}\rangle\langle\Psi_{SQ}|\sqrt{P_p P_{-p}}|\Psi_{SQ}\rangle = \sqrt{-\left(\frac{\hbar^2}{4}\right)\left(\mathrm{e}^{2\alpha_p}\right)\left(-\mathrm{e}^{-2\alpha_p}\right)} = \frac{\hbar}{2}\,. \quad (73)$$

The SQ states are minimal uncertainty states, just like the usual harmonic oscillator states, as they verify the Heisenberg relation with the equality sign. However, the indeterminacy on either the deformation, or the momentum, is reduced (*squeezed*) in amplitude, or correspondingly enhanced (*anti-squeezed)*, according to the sign in front of α_p in Eq. (65).

To better understand the physical meaning of the SQ states, let us consider the inverse problem [7]: given a Hamiltonian for SQ states which has a diagonal form *i.e.* $H_{SQ} = \sum_q \hbar\Omega_q \left(\mathcal{B}^\dagger_p\mathcal{B}_p + 1/2\right)$, we want to determine which is the non-diagonal phonon Hamiltonian $H_{\mathrm{nd}} \equiv \mathrm{e}^{-S}H_{SQ}\mathrm{e}^{S}$ which is diagonalized by the squeezing transformation. By substituting Eq. (69) in H_{SQ} we easily find:

$$\begin{aligned}H_{\mathrm{nd}} &= \sum_q \hbar\Omega_q \sinh^2(\alpha) + \sum_q \hbar\Omega_q \cosh(2\alpha_q)\left[b^\dagger_q b_q + \frac{1}{2}\right]\\ &+ \sum_q \hbar\Omega_q \left[\frac{\sinh(2\alpha_q)}{2}\right]\left(b^\dagger_q b^\dagger_{-q} + b_q b_{-q}\right). \quad (74)\end{aligned}$$

The original Hamiltonian has a harmonic part, with an enhanced frequency $\omega_q = \Omega_q \cosh(2\alpha_q)$ with respect to H_{SQ} and also has an anharmonic term. We can say that the squeezing is a way to treat the simplest (quadratic) anharmonicity, which produces a softening of the phonon frequencies. We shall deal with Eq. (74) again when discussing the spin polarons.

It is also interesting to study how the shape of the SQ wavefunction differs from the unsqueezed one. Let us consider a single q mode squeezing, and write its generator as:

$$\begin{aligned}S &= \alpha_q\left[b_q^2 - \left(b_q^\dagger\right)^2\right] = \alpha_q\left[1 + (b_q^\dagger + b_q)(b_q^\dagger - b_q)\right]\\ &= \alpha_q\left[1 + \left(\sqrt{\frac{2M\Omega}{\hbar}}u_q\right)\left(-\sqrt{\frac{2}{\hbar M\Omega}}\frac{d}{du_q}\right)\right],\\ S &= \alpha_q\left(1 + 2u_q\frac{d}{du_q}\right). \quad (75)\end{aligned}$$

This form of S allows to prove that the squeezing transformation acts on functions of u_q as a scaling transformation *i.e.* that:

$$\mathrm{e}^{-S} F\left(u_q\right) = \mathrm{e}^{-\alpha_q\left(1+2u_q\frac{d}{du_q}\right)} F\left(u_q\right) = \mathrm{e}^{-\alpha_q} F\left(\mathrm{e}^{-2\alpha_q} u_q\right) . \tag{76}$$

The proof is in the Appendix. The consequences of Eq. (76), *e.g.* in the case $F\left(u_q\right)$ is the Gaussian harmonic oscillator wavefunction, are that the SQ function at $u_q = 0$ is smaller (for $\alpha_q > 0$) by a factor $\mathrm{e}^{-\alpha_q}$ than the unsqueezed function, but, for increasing $|u_q|$, it decreases much less quickly than the latter.

Let us now continue our study of SQ operators by considering the boson number operator:

$$\langle \Psi_{SQ} | b_p^\dagger b_p | \Psi_{SQ} \rangle = \langle 0 | \left(\mathrm{e}^S b_p^\dagger \mathrm{e}^{-S}\right)\left(\mathrm{e}^S b_p \mathrm{e}^{-S}\right) | 0 \rangle = \sinh^2\left(\alpha_p\right) . \tag{77}$$

Any appreciable squeezing ($\alpha_p \neq 0$) creates an exponentially large number of phonons.

The hopping term in the displaced Hamiltonian contains an exponential function of Bose operators, whose squeezed form we shall now obtain. Consider the general exponential operator $Y = \exp\left[\sum_q A_q\left(b_{-q}^\dagger - b_q\right)\right]$ where $A_q = A_{-q}^*$ are c-numbers. By using standard tricks [10] for exponential operators, one has:

$$\begin{aligned} \langle \Psi_{SQ} | Y | \Psi_{SQ} \rangle &= \left\langle 0 \middle| \exp\left[\mathrm{e}^S \sum_q A_q\left(b_{-q}^\dagger - b_q\right)\mathrm{e}^{-S}\right] \middle| 0 \right\rangle \\ &= \left\langle 0 \middle| \exp\left[\sum_q A_q \mathrm{e}^{-\alpha_q}\left(b_{-q}^\dagger - b_q\right)\right] \middle| 0 \right\rangle . \end{aligned} \tag{78}$$

By rearranging $\sum_q A_q \mathrm{e}^{-\alpha_q}\left(b_{-q}^\dagger - b_q\right) = \sum_q \mathrm{e}^{-\alpha_q}\left(A_q^* b_q^\dagger - A_q b_q\right)$ we can write:

$$\left\langle 0 \middle| \exp\left[\sum_q \mathrm{e}^{-\alpha_q}\left(A_q^* b_q^\dagger - A_q b_q\right)\right] \middle| 0 \right\rangle = \prod_q \left\langle 0 \middle| \exp\left[\mathrm{e}^{-\alpha_q}\left(A_q^* b_q^\dagger - A_q b_q\right)\right] \middle| 0 \right\rangle . \tag{79}$$

Let us consider each q mode separately. Disentangling the exponential yields:

$$\begin{aligned} &\left\langle 0 \middle| \exp\left[\mathrm{e}^{-\alpha_q}\left(A_q^* b_q^\dagger - A_q b_q\right)\right] \middle| 0 \right\rangle = \left\langle 0 \middle| \exp\left[\mathrm{e}^{-\alpha_q} A_q^* b_q^\dagger\right] \exp\left[-\mathrm{e}^{-\alpha_q} A_q b_q\right] \right. \\ &\left. \times \exp\left[-\mathrm{e}^{-2\alpha_q} |A_q|^2 / 2\right] \middle| 0 \right\rangle . \end{aligned} \tag{80}$$

The only non-vanishing contributions from the series expansions of the exponentials of $b_q^\dagger, b_q$ acting on $|0\rangle$ comes from the zeroth-order term, and equals 1.

Therefore, $\left\langle 0 \left| \exp\left[\mathrm{e}^{-\alpha_q} \left(A_q^* b_q^\dagger - A_q b_q \right) \right] \right| 0 \right\rangle = \exp\left[-\mathrm{e}^{-2\alpha_q} \left| A_q \right|^2 / 2 \right]$ and:

$$\begin{aligned} \langle \Psi_{SQ} | \sum_q A_q \left(b_{-q}^\dagger - b_q \right) | \Psi_{SQ} \rangle &= \prod_q \exp\left[-\mathrm{e}^{-2\alpha_q} \left| A_q \right|^2 / 2 \right] \\ &= \exp\left[-\sum_q \mathrm{e}^{-2\alpha_q} \left| A_q \right|^2 / 2 \right] . \end{aligned} \quad (81)$$

One important feature of this result is that the argument of the exponential carries a minus sign, irrespective of the sign of A_q.

Now we can write down the expectation value of the displaced Hamiltonian, Eq. (51), taken over the SQ wavefunction. The Holstein term yields a vanishing contribution ($\approx \left\langle 0 \left| b_{-q}^\dagger + b_q \right| 0 \right\rangle$), whatever the value of δ_q. The free oscillator term is given by Eq. (77). The bosonic function in the hopping term, by using Eq. (81), yields:

$$\begin{aligned} &\langle \Psi_{SQ} | \exp\left[\frac{1}{\sqrt{N}} \sum_q \gamma_q \delta_q \left(\mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right) \left(b_{-q}^\dagger - b_q \right) \right] | \Psi_{SQ} \rangle \equiv \tau\left(\{\delta_q\} \{\alpha_q\} \right) \\ &= \exp\left[-\frac{1}{2N} \sum_q \gamma_q^2 \delta_q^2 \left| \mathrm{e}^{iqR_j} - \mathrm{e}^{iqR_l} \right|^2 \mathrm{e}^{-2\alpha_q} \right] \\ &= \exp\left\{ -\frac{1}{N} \sum_q \gamma_q^2 \delta_q^2 \left[1 - \cos\left(qa \right) \right] \mathrm{e}^{-2\alpha_q} \right\} , \end{aligned} \quad (82)$$

where we defined $a = |R_j - R_l|$. For a single-mode case, one would obtain $\exp\left(-4\alpha\right)$ in the exponent. In the limit of no squeezing ($\alpha_q \to 0$), this $\tau\left(\{\delta_q\} \{\alpha_q\} \right)$ coincides with the quantity τ introduced in Eq. (41). One sees that the effect of the squeezing is to introduce a factor $\mathrm{e}^{-2\alpha_q}$ into the exponent. This reduces its absolute value, so that, for given coupling γ_q and displacement δ_q, $\tau\left(\{\alpha_q\} \right)$ is larger the stronger is the squeezing.

Now we can write down the effective Hamiltonian for phonon polarons H^*:

$$\begin{aligned} H^* &= \sum_{j\sigma} \varepsilon_j^* n_{j\sigma} + \sum_{j\langle l \rangle \sigma} t_{jl}^* c_{j\sigma}^\dagger c_{l\sigma} + U^* \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{j\langle l \rangle} V_{jl}^* n_j n_l \\ &+ \sum_q \hbar \Omega_q \left[\sinh^2\left(\alpha_p \right) + \frac{1}{2} \right] , \end{aligned} \quad (83)$$

where we defined $t_{jl}^* = \tau\left(\{\alpha_q\} \right) t_{ij}$ as the effective hopping, and now in the V_{jl}^* term the sum over the l sites is not restricted to the nearest neighbours of site j. While ε_j^*, $U^*$and V_{jl}^* are renormalized only by the displacement,

in the case of t^*_{ij} both displacement and squeezing have an effect , but in opposite direction. Displacement, tending to reduce t^*_{ij}, is counteracted by squeezing. The two effects manifest themselves separately in other physical observables. To have a clear example, let us consider in details the case of the dimer, where the calculations can be made in explicit form.

7. Correlation functions in the dimer case

The dimer sites are labeled $i, j = 1, 2$, and, for a non-degenerate orbital, the filling is limited to $N = 1, 2$ due to electron–hole symmetry.

The effective Hamiltonian, which contains only fermionic terms, is analogous to Eq. (2). It can be exactly diagonalized, yielding the eigenvalues and eigenvectors listed in Table I.

TABLE I

Eigenvalues and eigenvectors of the Hamiltonian of Eq. (2) for $N = 1, 2$. D is the degeneracy of the state. The labels a, b indicate *bonding* and *antibonding* character. For $N = 2$ we have defined $E_U = 2\varepsilon + U$, $E_V = 2\varepsilon + V$, $r = \sqrt{(E_U - E_V)^2 + 16t^2}$, $\tan\theta = -4t/(E_U - E_V + r)$.

Filling and energy	D	S, S^z	Eigenvectors
$N=1\ E_1 = \varepsilon - t$	2	$\frac{1}{2}, \frac{1}{2}$	$\|1b,\uparrow\rangle = \frac{1}{\sqrt{2}}[c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}]\|0\rangle$
		$\frac{1}{2}, -\frac{1}{2}$	$\|1b,\downarrow\rangle = \frac{1}{\sqrt{2}}[c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}]\|0\rangle$
$N=1\ E_2 = \varepsilon + t$	2	$\frac{1}{2}, \frac{1}{2}$	$\|1a,\uparrow\rangle = \frac{1}{\sqrt{2}}[c^\dagger_{1\uparrow} - c^\dagger_{2\uparrow}]\|0\rangle$
		$\frac{1}{2}, -\frac{1}{2}$	$\|1a,\downarrow\rangle = \frac{1}{\sqrt{2}}[c^\dagger_{1\downarrow} - c^\dagger_{2\downarrow}]\|0\rangle$
$N=2\ E_3 = \frac{1}{2}(E_U+E_V-r)$	1	0, 0	$\|3\rangle = \frac{1}{\sqrt{2}}[\sin\theta\left(c^\dagger_{1\downarrow}c^\dagger_{1\uparrow} + c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}\right)$ -$\cos\theta\left(c^\dagger_{1\downarrow}c^\dagger_{2\uparrow} + c^\dagger_{2\downarrow}c^\dagger_{1\uparrow}\right)]\|0\rangle$
$N=2\ E_{4,\pm1} = 2\varepsilon + V$	2	$1, 1\,(-1)$	$\|4,\pm1\rangle = c^\dagger_{1\uparrow(\downarrow)}c^\dagger_{2\uparrow(\downarrow)}\|0\rangle$
$N=2\ E_{4,0} = 2\varepsilon + V$	1	1, 0	$\|4,0\rangle = \frac{1}{\sqrt{2}}\left[c^\dagger_{2\downarrow}c^\dagger_{1\uparrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right]\|0\rangle$
$N=2\ E_5 = 2\varepsilon + U$	1	0, 0	$\|5,0\rangle = \frac{1}{\sqrt{2}}\left[c^\dagger_{1\downarrow}c^\dagger_{1\uparrow} - c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}\right]\|0\rangle$
$N=2\ E_6 = \frac{1}{2}(E_U+E_V+r)$	1	0, 0	$\|6\rangle = \frac{1}{\sqrt{2}}[\cos\theta\left(c^\dagger_{1\downarrow}c^\dagger_{1\uparrow} + c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}\right)$ $+\sin\theta\left(c^\dagger_{1\downarrow}c^\dagger_{2\uparrow} + c^\dagger_{2\downarrow}c^\dagger_{1\uparrow}\right)]\|0\rangle$

The value $\langle\langle X\rangle\rangle_{|k\rangle}$ of the correlation function (CF) related to a operator X in one of the eigenstates $|k\rangle$ of the effective Hamiltonian has to be defined as follows:

$$\langle\langle X\rangle\rangle_{|k\rangle} \equiv \langle k|\langle\Psi_{SQ}|\mathrm{e}^R X \mathrm{e}^{-R}|\Psi_{SQ}\rangle|k\rangle\,, \quad |\Psi_{SQ}\rangle = \exp[-\alpha(b^\dagger b^\dagger - bb)]|0\rangle_{\mathrm{ph}}\,, \tag{84}$$

where $|0\rangle_{\rm ph}$ is the phonon vacuum, and $|\Psi_{SQ}\rangle$ is the squeezed state, where $\alpha \equiv \alpha_{\pi/a}$ is the only non-vanishing α_q. The notation $\langle\langle X\rangle\rangle$ here indicates a sequence of two transformations performed on X, and should not be confused with the Green's function notation. If X is a product of operators, then one isolates each operator by inserting $1 = \sum |k\rangle\langle k|$. We need the matrix elements of $n_{i\sigma}, n_i, n_i^2$ and $n_1^2 - n_2^2$ over the electronic eigenstates, which are listed below.

$\underline{N = 1 \text{ (quarter filled orbital)}}$.

The states are the bonding and antibonding combinations labelled $|1b\sigma\rangle, |1a\sigma\rangle$ in the Table. The spin- resolved matrix elements are:

$$\begin{aligned}
\langle k\sigma|n_{i\sigma}|k\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle k,-\sigma|n_{i\sigma}|k,-\sigma\rangle = 0\,, \quad (k = 1b, 1a)\,, \\
\langle 1\sigma|n_{1\sigma}|2\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle 1\sigma|n_{2\sigma}|2\sigma\rangle = -\tfrac{1}{2}\,, \qquad (85) \\
\langle k\sigma|n_{1\sigma}^2|k\sigma\rangle &= \langle k\sigma|n_{2\sigma}^2|k\sigma\rangle = \tfrac{1}{2}\,, \qquad (k = 1b, 1a)\,, \\
\langle 1\sigma|n_{1\sigma}^2|2\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle 1\sigma|n_{2\sigma}^2|2\sigma\rangle = -\tfrac{1}{2}\,, \\
\langle k\sigma|n_{1\sigma}n_{2\sigma}|k\sigma\rangle &= 0\,, \qquad (k = 1b, 1a)\,, \qquad \langle 1\sigma|n_{1\sigma}n_{2\sigma}|2\sigma\rangle = 0\,. \qquad (86)
\end{aligned}$$

Summing over spins yields:

$$\begin{aligned}
\langle k\sigma|n_i|k\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle k,-\sigma|n_i|k,-\sigma\rangle = \tfrac{1}{2}\,, \qquad (k = 1, 2; i = 1, 2)\,, \\
\langle 1\sigma|n_1|2\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle 1\sigma|n_2|2\sigma\rangle = -\tfrac{1}{2}\,, \qquad (87) \\
\langle k\sigma|n_1^2|k\sigma\rangle &= \langle k\sigma|n_2^2|k\sigma\rangle = \tfrac{1}{2}\,, \qquad (k = 1b, 1a)\,, \\
\langle 1\sigma|n_1^2|2\sigma\rangle &= \tfrac{1}{2}\,, \qquad \langle 1\sigma|n_2^2|2\sigma\rangle = -\tfrac{1}{2}\,, \\
\langle k\sigma|n_1n_2|k\sigma\rangle &= 0\,, \qquad (k = 1b, 1a)\,, \qquad \langle 1\sigma|n_1n_2|2\sigma\rangle = 0\,, \qquad (88) \\
\langle k\sigma|n_1^2n_2|k\sigma\rangle &= \langle k\sigma|n_1n_2^2|k\sigma\rangle = 0\,, \quad \langle k\sigma|n_1^3|k\sigma\rangle = 1 \quad (k = 1, 2)\,. \qquad (89)
\end{aligned}$$

$\underline{N = 2 \text{ (half filled orbital)}}$.

For the spin-resolved $n_{i\sigma}$ we have:

$$\begin{aligned}
\langle 3|n_{1\sigma}|3\rangle &= \frac{1}{2}\,, \quad \langle 3|n_{1\sigma}|5\rangle = \frac{\sin\theta}{2}\,, \quad \langle 3|n_{1\sigma}|6\rangle = 0\,, \\
\langle 3|n_{1\sigma}|4,\sigma\rangle &= 0\,, \quad \langle 3|n_{1\uparrow}|4,0\rangle = -\frac{\cos\theta}{2} \quad \langle 3|n_{1\downarrow}|4,0\rangle = \frac{\cos\theta}{2}\,, \qquad (90) \\
\langle 3|n_{2\sigma}|3\rangle &= \frac{1}{2}\,, \quad \langle 3|n_{2\sigma}|5\rangle = -\frac{\sin\theta}{2} \quad \langle 3|n_{2\sigma}|6\rangle = 0\,, \\
\langle 3|n_{2\sigma}|4,\sigma\rangle &= 0\,, \quad \langle 3|n_{2\uparrow}|4,0\rangle = \frac{\cos\theta}{2}\,, \quad \langle 3|n_{2\downarrow}|4,0\rangle = -\frac{\cos\theta}{2}\,, \qquad (91)
\end{aligned}$$

$$\langle 4,\sigma|n_{i\sigma}|4,\sigma\rangle = 1\,, \;\; \langle 4,-\sigma|n_{i\sigma}|4,-\sigma\rangle = 0\,, \;\; \langle 4,\sigma|n_{i\sigma}|5\rangle = 0 \;\; \langle 4,\sigma|n_{i\sigma}|6\rangle = 0\,, \qquad (92)$$

$$\begin{aligned}
\langle 4,0|n_{i\sigma}|4,0\rangle &= \frac{1}{2}\,, \quad \langle 4,0|n_{i\sigma}|4,\pm\sigma\rangle = 0\,,\\
\langle 4,0|n_{1\uparrow}|6\rangle &= \frac{\sin\theta}{2}\,, \quad \langle 4,0|n_{1\downarrow}|6\rangle = -\frac{\sin\theta}{2}\,,\\
\langle 4,0|n_{2\uparrow}|6\rangle &= -\frac{\sin\theta}{2}\,, \quad \langle 4,0|n_{2\downarrow}|6\rangle = \frac{\sin\theta}{2}\,,
\end{aligned} \tag{93}$$

$$\langle 5|n_{i\sigma}|5\rangle = \frac{1}{2} \quad \langle 5|n_{1\sigma}|6\rangle = \frac{\cos\theta}{2} \quad \langle 5|n_{2\sigma}|6\rangle = -\frac{\cos\theta}{2}\,.$$

For the total charges on the sites $n_i = n_{i\uparrow} + n_{i\downarrow}$ we have:

$$\langle 3|n_1|3\rangle = 1\,, \quad \langle 3|n_1|4\rangle = 0\,, \quad \langle 3|n_1|5\rangle = \sin\theta\,, \quad \langle 3|n_1|6\rangle = 0\,, \tag{94}$$

$$\langle 3|n_2|3\rangle = 1\,, \quad \langle 3|n_2|4\rangle = 0\,, \quad \langle 3|n_2|5\rangle = -\sin\theta\,, \quad \langle 3|n_2|6\rangle = 0\,, \tag{95}$$

$$\begin{aligned}
\langle 4,\sigma|n_i|4,\sigma\rangle &= 1\,, \quad \langle 4,\sigma|n_i|5\rangle = 0\,, \quad \langle 4,\sigma|n_i|6\rangle = 0\,,\\
\langle 4,0|n_i|4,0\rangle &= 1\,, \quad \langle 4,0|n_i|5\rangle = 0\,, \quad \langle 4,0|n_i|6\rangle = 0\,, \qquad (96)\\
\langle 5|n_i|5\rangle &= 1\,, \quad \langle 5|n_1|6\rangle = \cos\theta\,, \quad \langle 5|n_2|6\rangle = -\cos\theta\,. \qquad (97)
\end{aligned}$$

To evaluate the matrix elements of n_j^2 we use the decomposition of the identity, *i.e.* $\langle i|n_j^2|i\rangle \equiv \langle i|\sum_k n_j|k\rangle\langle k|n_j|i\rangle$, yielding:

$$\langle 3|n_1^2|3\rangle = 1+\sin^2\theta\,,\ \langle 3|n_1^2|4,\sigma,0\rangle = 0\,,\ \langle 3|n_1^2|5\rangle = 2\sin\theta\,,\ \langle 3|n_1^2|6\rangle = 0\,, \tag{98}$$

$$\langle 3|n_2^2|3\rangle = 1+\sin^2\theta\,,\ \langle 3|n_2^2|4,\sigma,0\rangle = 0\,,\ \langle 3|n_2^2|5\rangle = -2\sin\theta\,,\ \langle 3|n_2^2|6\rangle = 0\,, \tag{99}$$

$$\begin{aligned}
\langle 4,\sigma|n_i^2|4,\sigma\rangle &= 1\,,\ \langle 4,\sigma|n_i^2|5\rangle = 0\,,\ \langle 4,\sigma|n_i^2|6\rangle = 0\\
\langle 4,0|n_i^2|4,0\rangle &= 1\,,\ \langle 4,0|n_i^2|5\rangle = 0\,,\ \langle 4,0|n_i^2|6\rangle = 0\,, \qquad (100)\\
\langle 5|n_i^2|5\rangle &= 2\,,\ \langle 5|n_1^2|6\rangle = 2\cos\theta\,,\ \langle 5|n_2^2|6\rangle = -2\cos\theta\,. \qquad (101)
\end{aligned}$$

The correlation functions are the quantities accessible to experimental measurement. We shall show that some of them depend only on the displacement, and other ones only on the squeezing.

7.1. Correlation between site deformations

The correlation between the site deformations is a quantity depending only on the displacement parametrs. Its evaluation will show that the *complete* Lang–Firsov transformation ($\delta = 1$) leads to wrong results. To study

that problem in our general case of *incomplete* ($\delta \neq 1$) transformation, we shall evaluate

$$\langle\langle u_2(t)u_1(0)\rangle\rangle_{|k\rangle} = \langle k|\langle\Psi_{SQ}|\mathrm{e}^{R+R_s}\mathrm{e}^{iHt/\hbar}u_2\mathrm{e}^{-iHt/\hbar}u_1\mathrm{e}^{-(R+R_s)}|\Psi_{SQ}\rangle|k\rangle\,. \tag{102}$$

It is convenient to write:

$$\langle\langle u_2(t)u_1(0)\rangle\rangle_{|k\rangle} = \langle k|\sum_p \langle\Psi_{SQ}|u_2^T|\Psi_{SQ}\rangle|p\rangle\langle p|\langle\Psi_{SQ}|u_1^T|\Psi_{SQ}\rangle\mathrm{e}^{i(E_p^*-E_k^*)t/\hbar}|k\rangle\,, \tag{103}$$

where $\{|p\rangle\}$ is the set of eigenstates of H^*. By expressing u_1, u_2 in terms of $b_0^\dagger, b_0$ and $b_{\pi/a}^\dagger, b_{\pi/a}$ as:

$$u_1 = \tfrac{L}{2}(\mathrm{b}_0^\dagger + \mathrm{b}_0 + \mathrm{b}_{\pi/\mathrm{a}}^\dagger + \mathrm{b}_{\pi/\mathrm{a}}) \qquad u_2 = \tfrac{L}{2}(\mathrm{b}_0^\dagger + \mathrm{b}_0 - \mathrm{b}_{\pi/\mathrm{a}}^\dagger - \mathrm{b}_{\pi/\mathrm{a}}) \tag{104}$$

transforming $u_{1,2}$ by $\exp\left(R_0 + R_{\pi/a}\right)$ and applying the squeezing we find:

$$\begin{aligned}
\langle\Psi_{SQ}|\mathrm{e}^{\left(R_0+R_{\pi/a}\right)}u_1\mathrm{e}^{-\left(R_0+R_{\pi/a}\right)}|\Psi_{SQ}\rangle &= -L\gamma_0\left[n_1+n_2+\delta_{\pi/a}(n_1-n_2)\right]\,,\\
\langle\Psi_{SQ}|\mathrm{e}^{\left(R_0+R_{\pi/a}\right)}u_2\mathrm{e}^{-\left(R_0+R_{\pi/a}\right)}|\Psi_{SQ}\rangle &= -L\gamma_0\left[n_1+n_2-\delta_{\pi/a}(n_1-n_2)\right]
\end{aligned} \tag{105}$$

whence it follows $\langle u_1\rangle = \langle u_2\rangle$ for any $|k\rangle$ as $\langle k|n_1 - n_2|k\rangle = 0$. For $N = 1$ in the ground state $|1b\sigma\rangle$ we have:

$$\langle\langle u_2(t)u_1(0)\rangle\rangle_{|1b\sigma\rangle} = L^2\gamma_0^2\left[1-\delta_{\pi/a}^2\mathrm{e}^{-i(2t^*)t/\hbar}\right] \tag{106}$$

while for $N = 2$ and in the different eigenstates which can be the ground state, we get:

$$\begin{aligned}
\langle\langle u_2(t)u_1(0)\rangle\rangle_{|3\rangle} &= 4L^2\gamma_0^2\left(1-\delta_{\pi/a}^2\sin^2\theta\mathrm{e}^{-i(E_{CT}^*-E_{Sb}^*)t/\hbar}\right)\,,\\
\langle\langle u_2(t)u_1(0)\rangle\rangle_{|4\rangle} &= 4L^2\gamma_0^2\,,\\
\langle\langle u_2(t)u_1(0)\rangle\rangle_{|5\rangle} &= 4L^2\gamma_0^2\\
&\quad\times\left[-\delta_{\pi/a}^2\sin^2\theta\mathrm{e}^{-i(E_{Sb}^*-E_{CT}^*)t/\hbar}-\delta_{\pi/a}^2\cos^2\theta\mathrm{e}^{-i(E_{Sa}^*-E_{CT}^*)t/\hbar}\right]\,.
\end{aligned} \tag{107}$$

Notice that forcing $\delta_{\pi/a} = 1$ does not describe correctly the correlated dynamics of the site deformations. In particular, at $t = 0$, both for $N = 1$ and $N = 2$, the correlation functions, when δ-depending, either vanish, or are minimal, if $\delta_{\pi/a} = 1$.

To make more explicit the role of $\delta_{\pi/a}$ in coherently propagating the deformation between the sites, one can look at the equal-time quantity

$\langle\langle u_2(0)u_1(0)\rangle\rangle_{|k\rangle} - \langle\langle u_2(0)\rangle\rangle\langle\langle u_1(0)\rangle\rangle_{|k\rangle}$ which vanishes in the state $|4\rangle$, while in the other ones reads:

$$\begin{aligned}
\langle\langle u_2(0)u_1(0)\rangle\rangle_{|1b\rangle} - \langle\langle u_2(0)\rangle\rangle\langle\langle u_1(0)\rangle\rangle_{|1b\rangle} &= -L^2\gamma_0^2\delta_{\pi/a}^2 \\
\langle\langle u_2(0)u_1(0)\rangle\rangle_{|3\rangle} - \langle\langle u_2(0)\rangle\rangle\langle\langle u_1(0)\rangle\rangle_{|3\rangle} &= -4L^2\gamma_0^2\delta_{\pi/a}^2\sin^2\theta \\
\langle\langle u_2(0)u_1(0)\rangle\rangle_{|5\rangle} - \langle\langle u_2(0)\rangle\rangle\langle\langle u_1(0)\rangle\rangle_{|5\rangle} &= -4L^2\gamma_0^2\delta_{\pi/a}^2\,. \qquad (108)
\end{aligned}$$

7.2. Electron–phonon correlation functions

Those functions were introduced in Ref. [11] for the case of one electron in the lattice. Besides having an intuitive meaning, these CF's enter the evaluation of the optical conductivity due to charges on the i sites $\sigma_{xx} \approx \sum_i \langle\langle n_i \prod_{\boldsymbol{q}} Y(b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}})\rangle\rangle$, where $Y(b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}})$ is a function of the phonon $\boldsymbol{q}$-mode occupation numbers, whose explicit form can be found in Ref. [12]. For the dimer, the only wavevector yielding a non-vanishing contribution is $\boldsymbol{q} = \pi/a$ so that the above expression reduces to $\sigma_{xx} \approx \langle\langle n_1(b_1^\dagger b_1 - b_2^\dagger b_2\rangle\rangle$.

In our case the inter-site electron–phonon correlation function is defined as $(i, j = 1, 2)$:

$$\begin{aligned}
F_{ij|k\rangle}^{\mathrm{ep}} &\equiv \langle k|\langle\Psi_{SQ}|\mathrm{e}^R n_i b_j^\dagger b_j \mathrm{e}^{-R}|\Psi_{SQ}\rangle|k\rangle \\
&= \langle k|\langle\Psi_{SQ}|(\mathrm{e}^R n_i \mathrm{e}^{-R})(\mathrm{e}^R b_j^\dagger b_j \mathrm{e}^{-R})|\Psi_{SQ}\rangle|i\rangle\,. \qquad (109)
\end{aligned}$$

We need the phonon operators for each site, which are obtained by inverting the definitions of $b_q^\dagger, b_q$. Then

$$\begin{aligned}
b_1^\dagger b_1 &= \tfrac{1}{4}[b_0^\dagger b_0 + b_{\pi/a}^\dagger b_{\pi/a} + (b_0^\dagger b_{\pi/a} + b_{\pi/a}^\dagger b_0)] \\
b_2^\dagger b_2 &= \tfrac{1}{4}[b_0^\dagger b_0 + b_{\pi/a}^\dagger b_{\pi/a} - (b_0^\dagger b_{\pi/a} + b_{\pi/a}^\dagger b_0)]\,. \qquad (110)
\end{aligned}$$

Applying the displacement transformation yields:

$$\begin{aligned}
\mathrm{e}^{R_{\pi/a}} b_{\pi/a}^\dagger b_{\pi/a} \mathrm{e}^{-R_{\pi/a}} &= b_{\pi/a}^\dagger b_{\pi/a} - \delta_{\pi/a}\gamma_0(b_{\pi/a}^\dagger + b_{\pi/a})(n_1 - n_2) \\
&\quad + \delta_{\pi/a}^2\gamma_0^2(n_1 - n_2)^2\,, \qquad (111) \\
\mathrm{e}^{R_0} b_0^\dagger b_0 \mathrm{e}^{-R_0} &= b_0^\dagger b_0 - \gamma_0(b_0^\dagger + b_0)(n_1 + n_2) + \gamma_0^2(n_1 + n_2)^2\,, \qquad (112) \\
\mathrm{e}^{R_0} b_0^\dagger \mathrm{e}^{-R_0} \mathrm{e}^R b_{\pi/a} \mathrm{e}^{-R} &= b_0^\dagger b_{\pi/a} - \gamma_0 b_{\pi/a}(n_1 + n_2) - \delta_{\pi/a}\gamma_0 b_0^\dagger(n_1 - n_2) \\
&\quad + \delta_{\pi/a}\gamma_0^2(n_1 - n_2)^2\,, \qquad (113) \\
\mathrm{e}^{R_0} b_{\pi/a}^\dagger \mathrm{e}^{-R_0} \mathrm{e}^R b_0 \mathrm{e}^{-R} &= b_{\pi/a}^\dagger b_0 - \gamma_0 b_{\pi/a}^\dagger(n_1 + n_2) - \delta_{\pi/a}\gamma_0 b_0(n_1 - n_2) \\
&\quad + \delta_{\pi/a}\gamma_0^2(n_1 - n_2)^2\,. \qquad (114)
\end{aligned}$$

When evaluated in the squeezed state, the above results reduce to:

$$\begin{aligned}
\langle\Psi_{SQ}|\mathrm{e}^{R_{\pi/a}}b^{\dagger}_{\pi/a}b_{\pi/a}\mathrm{e}^{-R_{\pi/a}}|\Psi_{SQ}\rangle &= Sh^2(2\alpha)+\delta^2_{\pi/a}\gamma_0^2(n_1-n_2)^2\\
\langle\Psi_{SQ}|\mathrm{e}^{R_0}b^{\dagger}_{0}b_{0}\mathrm{e}^{-R_{0}}|\Psi_{SQ}\rangle &= \gamma_0^2(n_1+n_2)^2\\
\langle\Psi_{SQ}|\mathrm{e}^{R_0}\mathrm{e}^{R_{\pi/a}}(b^{\dagger}_{\pi/a}b_{\pi/a}b^{\dagger}_{0}b_{0}\mathrm{e}^{-R_{\pi/a}}\mathrm{e}^{-R_{0}}|\Psi_{SQ}\rangle &= 2\delta_{\pi/a}\gamma_0^2(n_1^2-n_2^2)\,. \qquad (115)
\end{aligned}$$

The local deformations in the squeezed state therefore result in:

$$\begin{aligned}
\langle\Psi_{SQ}|b^{\dagger}_1b_1|\Psi_{SQ}\rangle &= \frac{Sh^2(2\alpha)}{4}+\frac{\gamma_0^2}{4}\left[n_1^2(1+\delta_{\pi/a})^2+n_2^2(1-\delta_{\pi/a})^2+2n_1n_2(1-\delta^2_{\pi/a})\right],\\
\langle\Psi_{SQ}|b^{\dagger}_2b_2|\Psi_{SQ}\rangle &= \frac{Sh^2(2\alpha)}{4}+\frac{\gamma_0^2}{4}\left[n_1^2(1-\delta_{\pi/a})^2+n_2^2(1+\delta)^2+2n_1n_2(1-\delta^2_{\pi/a})\right], \qquad (116)
\end{aligned}$$

We can now evaluate the correlation function in each eigenstate $|i\rangle$.

$\underline{N=1}$

As the state $|1a\sigma\rangle$ is always higher in energy than $|1b\sigma\rangle$, we shall consider only the latter.

$$\begin{aligned}
F^{\mathrm{ep}}_{12|1b\sigma\rangle} &\equiv \frac{Sh^2(2\alpha)}{4}\langle 1b\sigma|n_1|1b\sigma\rangle\\
&\quad+\frac{\gamma_0^2}{4}\Big[(1-\delta_{\pi/a})^2\langle 1b\sigma|\sum_{i=1b,1a}\sum_{\tau}n_1|i\tau\rangle\langle i\tau|n_1^2|1b\sigma\rangle\\
&\quad+(1+\delta_{\pi/a})^2\langle 1b\sigma|\sum_{i=b1,1a}\sum_{\tau}n_1|i\tau\rangle\langle i\tau|n_2^2|1b\sigma\rangle\\
&\quad+2(1-\delta^2_{\pi/a})\langle 1b\sigma|\sum_{i=1b,1a}\sum_{\tau}n_1^2|i\tau\rangle\langle i\tau|n_2|1b\sigma\rangle\Big], \qquad (117)\\
F^{\mathrm{ep}}_{12|1b\sigma\rangle} &\equiv \frac{Sh^2(2\alpha)}{4}+\frac{\gamma_0^2}{4}(1-\delta_{\pi/a})^2\,. \qquad (118)
\end{aligned}$$

$\underline{N=2}$

In the state $|3\rangle$ we have:

$$\begin{aligned}
F^{\mathrm{ep}}_{12|3\rangle} &\equiv \frac{Sh^2(2\alpha)}{4}\langle 3|n_1|3\rangle+\frac{\gamma^2}{4}\Big[(1-\delta_{\pi/a})^2\langle 3|\sum_{i=3,5}n_1|i\rangle\langle i|n_1^2|3\rangle\\
&+(1+\delta_{\pi/a})^2\langle 3|\sum_{i=3,5}n_1|i\rangle\langle i|n_2^2|3\rangle+2(1-\delta^2_{\pi/a})\langle 3|\sum_{i=3,5}n_1^2|i\rangle\langle i|n_2|3\rangle\Big]. \qquad (119)
\end{aligned}$$

Only the states $|3\rangle$ and $|5\rangle$ appear in the decomposition of the identity because $|4,\sigma\rangle$, $|4,0\rangle$ and $|6\rangle$ have vanishing matrix elements with $|3\rangle$. By

using the matrix elements as evaluated above we obtain:

$$\begin{aligned} F^{\rm ep}_{12|3\rangle} &= \frac{Sh^2(2\alpha)}{4} + \frac{\gamma^2}{4}\Big[(1-\delta_{\pi/a})^2(1+3\sin^2\theta) \\ &\quad +(1+\delta_{\pi/a})^2(1-\sin^2\theta) + 2(1-\delta^2_{\pi/a})(1-\sin^2\theta)\Big]\,, \\ F^{\rm ep}_{12|3\rangle} &= \frac{Sh^2(2\alpha)}{4} + \gamma^2\left[1-\delta_{\pi/a}(2-\delta_{\pi/a})\sin^2\theta\right]\,. \end{aligned} \tag{120}$$

One can verify that $F^{\rm ep}_{21|3\rangle} = F^{\rm ep}_{12|3\rangle}$, so that one can drop the site indexes.

By analogous calculations one finds for the degenerate $|4\rangle$ eigenstates:

$$F^{\rm ep}_{12|4,\sigma\rangle} = F^{\rm ep}_{12|4,0\rangle} = \frac{Sh^2(2\alpha)}{4} + \gamma^2 \tag{121}$$

while for the state $|5\rangle$ one has to evaluate:

$$\begin{aligned} F^{\rm ep}_{12|5\rangle} &\equiv \frac{Sh^2(2\alpha)}{4}\langle 5|n_1|5\rangle \\ &\quad +\frac{\gamma^2}{4}\Big[(1-\delta_{\pi/a})^2\langle 5|\sum_{i=3,5,6} n_1|i\rangle\langle i|n_1^2|5\rangle \\ &\quad +(1+\delta_{\pi/a})^2\langle 5|\sum_{i=3,5,6} n_1|i\rangle\langle i|n_2^2|5\rangle \\ &\quad +2(1-\delta^2_{\pi/a})\langle 5|\sum_{i=3,5,6} n_1^2|i\rangle\langle i|n_2|5\rangle\Big] \end{aligned} \tag{122}$$

yielding

$$F^{\rm ep}_{12|5\rangle} = \frac{Sh^2(2\alpha)}{4} + \gamma^2(1-\delta_{\pi/a})^2\,. \tag{123}$$

Notice that, in evaluating $F^{\rm ep}_{12|5\rangle}$ one must include in the decomposition of the identity also the states $|6\rangle$, because $|5\rangle$, differently from $|3\rangle$, is connected to $|6\rangle$ by n_i, n_i^2.

The on-site electron–phonon CF $F^{\rm ep}_{11|k\rangle} \equiv \langle n_1 b_1^\dagger b_1\rangle$ is evaluated in the same way, with the site-independent results:

$\underline{N=1}$

$$F^{\rm ep}_{11|1b\sigma\rangle} = \frac{Sh^2(2\alpha)}{4} + \frac{\gamma_0^2}{4}(1+\delta_{\pi/a})^2 \tag{124}$$

$\underline{N=2}$

$$F^{\rm ep}_{11|3\rangle} = \frac{Sh^2(2\alpha)}{4} + \gamma_0^2\left[1+\delta_{\pi/a}(2+\delta_{\pi/a})\sin^2\theta\right], \tag{125}$$

$$F^{\rm ep}_{11|4,\sigma\rangle} = F^{\rm ep}_{11|4,0\rangle} = \frac{Sh^2(2\alpha)}{4} + \gamma_0^2, \tag{126}$$

$$F^{\rm ep}_{11|5\rangle} = \frac{Sh^2(2\alpha)}{4} + \gamma_0^2(1+\delta^2_{\pi/a}). \tag{127}$$

From the results above, the optical conductivity is linear in $\delta_{\pi/a}$ and independent from squeezing.

7.3. The Debye–Waller factor

Let us now consider an important quantity depending only on the squeezing. Following Ref. [13] we define the Debye–Waller factor $F^{\rm DW}$ as $F^{\rm DW} \equiv \langle\langle u_i^2\rangle\rangle - \langle\langle u_i\rangle\rangle^2$. It is actually a site-independent quantity, as we shall show. We shall define for short the characteristic length $L \equiv \sqrt{\hbar/2M\Omega}$ so that:

$$u_i = (L/2)\left[b_0^\dagger + b_0 + (-1)^{i+1}(b^\dagger_{\pi/a} + b_{\pi/a})\right], \quad (i=1,2). \tag{128}$$

Then one finds:

$$\begin{aligned}\langle\langle u_1\rangle\rangle &= -\gamma_0 L\Big[(1+\delta_{\pi/a})\langle\sum_s n_{1\sigma}\rangle + (1-\delta_{\pi/a})\langle\sum_s n_{2\sigma}\rangle\Big]\\ \langle\langle u_2\rangle\rangle &= -\gamma_0 L\Big[(1-\delta_{\pi/a})\langle\sum_s n_{1\sigma}\rangle + (1+\delta_{\pi/a})\langle\sum_s n_{2\sigma}\rangle\Big].\end{aligned} \tag{129}$$

The expression of $\langle\langle u_i^2\rangle\rangle$ can be worked out by noting that

$$\langle\Psi_{SQ}|b^\dagger b^\dagger|\Psi_{SQ}\rangle = \langle\Psi_{SQ}|bb|\Psi_{SQ}\rangle = Sh(4\alpha)/2$$

yielding, for $i=1,2$:

$$\begin{aligned}&\langle\Psi_{SQ}|u_i^2|\Psi_{SQ}\rangle = L^2[Sh(4\alpha)+Sh^2(2\alpha)+1]/2\\ &+L^2\gamma^2\left[\Big\langle\sum_\sigma(n_{1\sigma}+n_{2\sigma})\Big\rangle^2 + \delta^2_{\pi/a}\Big\langle\sum_\sigma(n_{1\sigma}-n_{2\sigma})\Big\rangle^2\right]\end{aligned} \tag{130}$$

so that:

$$\begin{aligned}&\langle\langle u_1^2\rangle\rangle_{|k\rangle} - \langle\langle u_i\rangle\rangle^2_{|k\rangle} = \frac{L^2}{2}\left[{\rm e}^{2\alpha}Sh(2\alpha)+1\right]\\ &+(-1)^i L^2\left[\langle k|\sum_s(n_{1\sigma}-n_{2\sigma})|k\rangle\langle k|\sum_s(n_{1\sigma}+n_{2\sigma})|k\rangle\right],\end{aligned} \tag{131}$$

where $|k\rangle$ is an eigenstate of H^*. As $\langle k|\sum_s(n_{1\sigma}-n_{2\sigma})|k\rangle$ vanishes identically, we finally obtain the site-independent result:

$$F^{\mathrm{DW}} = \frac{L^2}{4}[1+\mathrm{e}^{4\alpha}]\,. \tag{132}$$

7.4. Average vibrational energy

The average vibrational energy $\langle E_\Omega\rangle$ is related to the Debye–Waller factor, and, following [13] can be defined as:

$$\langle E_\Omega\rangle \equiv \frac{M}{2}\left\langle\left\langle\left(\frac{du_{H_i}(t)}{dt}\right)^2\right\rangle\right\rangle, \tag{133}$$

where $u_i(t) = \mathrm{e}^{iHt/\hbar}u_i\mathrm{e}^{-iHt/\hbar}$ is the Heisenberg representation of the local deformation. Its equation of motion is actually governed by only the phononic part $H_{\mathrm{ph}} + H_{\mathrm{el-ph}}$ of the total bare Hamiltonian of Eq. (1)

$$i\hbar\frac{du_i(t)}{dt} = [u_i(t), H] = [u_i(t), H_{\mathrm{ph}} + H_{\mathrm{el-ph}}]\,. \tag{134}$$

By writing u_i as in Eq. (128) one finds:

$$\left[\frac{du_i(t)}{dt}\right]^2 = \left(\frac{L\Omega}{2}\right)^2\left[\mathrm{e}^{-iHt/\hbar}(b_0^\dagger - b_0 + b_{\pi/a}^\dagger - b_{\pi/a})^2\mathrm{e}^{-iHt/\hbar}\right]. \tag{135}$$

The transformation $\exp(R_0+R_{\pi/a})$ changes H into H^T with displaced Bose operators, so that the Eq. (135) reads:

$$\begin{aligned}&\left(\frac{2}{L\Omega}\right)^2\mathrm{e}^{(R_0+R_{\pi/a})}\left[\frac{du_i(t)}{dt}\right]^2\mathrm{e}^{-(R_0+R_{\pi/a})}\\ &= \mathrm{e}^{-iH^Tt/\hbar}\,[\,b_0^\dagger b_0^\dagger + b_0b_0 - 2b_0^\dagger b_0 - 1 + b_{\pi/a}^\dagger b_{\pi/a}^\dagger + b_{\pi/a}b_{\pi/a}\\ &-2b_{\pi/a}^\dagger b_{\pi/a} - 1 + 2(b_0^\dagger - b_0)(b_{\pi/a}^\dagger - b_{\pi/a})\,]\,\mathrm{e}^{-iH^Tt/\hbar}\,.\end{aligned} \tag{136}$$

Finally, when evaluated over the combined squeezed- phonon and electronic state defined by $H^T|\Psi_{SQ}\rangle|k\rangle = E_k^*|\Psi_{SQ}\rangle|k\rangle$ the Eq. (136) yields, after explicitating L:

$$\langle \mathrm{E}_\Omega\rangle = \frac{\hbar\Omega}{16}\left[1+\mathrm{e}^{4\alpha}\right] \tag{137}$$

which is proportional to the Debye–Waller factor.

Let us now consider quantities depending on both the displacement and the squeezing.

7.5. The longitudinal and transverse magnetic correlation functions

The longitudinal magnetic CF $\langle\langle S_1^z S_2^z\rangle\rangle$ vanishes for $N = 1$, while for $N = 2$ by writing $S_i^z = (n_{i\uparrow} - n_{i\downarrow})/2$ we get, for the state $|3\rangle$

$$\langle\langle S_1^z S_2^z\rangle\rangle_{|3\rangle} = \frac{1}{4}\langle 3|\,(n_{1\uparrow} - n_{1\downarrow})\,|4,0\rangle\langle 4,0|\,(n_{2\uparrow} - n_{2\downarrow})\,|3\rangle = -\frac{\cos^2\theta}{4} \quad (138)$$

while

$$\langle\langle S_1^z S_2^z\rangle\rangle_{|4\sigma\rangle} = \frac{1}{4}\,, \qquad \langle\langle S_1^z S_2^z\rangle\rangle_{|40\rangle} = -\frac{\cos^2\theta}{4}\,, \qquad \langle\langle S_1^z S_2^z\rangle\rangle_{|5\rangle} = 0\,. \quad (139)$$

The transverse magnetic CF $\langle\langle S_1^- S_2^+\rangle\rangle$for $N = 1$ vanishes. For $N = 2$ it also vanishes in the states $|4,\sigma\rangle$ and $|5\rangle$ while

$$\langle 3|S_1^- S_2^+|3\rangle = -\frac{\cos^2\theta}{2}\,, \qquad \langle 4,0|S_1^- S_2^+|4,0\rangle = \frac{1}{2}\,.$$

Those functions depend on the combined effect of displacement and squeezing, which is contained in the parameter θ, defined as in Table I.

7.6. The charge transfer correlation function

Following Ref. [8] the charge transfer CF is conveniently defined as:

$$F_{|i\rangle}^{\mathrm{ct}} \equiv \frac{\langle i|\langle\Psi_{SQ}|e^R(n_1 - n_2)(\boldsymbol{u}_1 - \boldsymbol{u}_2)\mathrm{e}^{-R}|\Psi_{SQ}\rangle|i\rangle}{\sqrt{\langle i|\langle\Psi_{SQ}|\mathrm{e}^R(\boldsymbol{u}_1 - \boldsymbol{u}_2)^2\mathrm{e}^{-R}|\Psi_{SQ}\rangle|i\rangle}} \quad (140)$$

or, expressing $u_1 - u_2$ throughthe $b_{\pi/a}^\dagger, b_{\pi/a}$ operators :

$$F_{|i\rangle}^{\mathrm{ct}} \equiv \frac{\langle i|\langle\Psi_{SQ}|\mathrm{e}^{R_{\pi/a}}(n_1 - n_2)(b_{\pi/a}^\dagger + b_{\pi/a})\mathrm{e}^{-R_{\pi/a}}|\Psi_{SQ}\rangle|i\rangle}{\sqrt{\langle i|\langle\Psi_{SQ}|\mathrm{e}^{R_{\pi/a}}(b_{\pi/a}^\dagger + b_{\pi/a})^2\mathrm{e}^{-R_{\pi/a}}|\Psi_{SQ}\rangle|i\rangle}}\,. \quad (141)$$

Substituting $\mathrm{e}^{R_{\pi/a}}(b_{\pi/a}^\dagger + b_{\pi/a})\mathrm{e}^{-R_{\pi/a}} = b_{\pi/a}^\dagger + b_{\pi/a} - 2\delta_{\pi/a}\gamma\,(n_1 - n_2)$in the numerator of F^{ct} we have:

$$\langle\Psi_{SQ}|(n_1 - n_2)[\mathrm{e}^{R_{\pi/a}}(b_{\pi/a}^\dagger + b_{\pi/a})\mathrm{e}^{-R_{\pi/a}}]|\Psi_{SQ}\rangle = -2\delta_{\pi/a}\gamma_0(n_1 - n_2)^2\,. \quad (142)$$

In the denominator we develop $(b^\dagger + b)^2 = (b^\dagger)^2 + (b)^2 + 2b^\dagger b + 1$, so that:

$$\mathrm{e}^{R_{\pi/a}}(b_{\pi/a}^\dagger + b_{\pi/a})^2\mathrm{e}^{-R_{\pi/a}} = (b_{\pi/a}^\dagger + b_{\pi/a})^2 - 4\delta_{\pi/a}G(b_{\pi/a}^\dagger + b_{\pi/a}) + 4\delta_{\pi/a}^2 G^2\,. \quad (143)$$

In the squeezed state Eq. (143) yields

$$\langle \Psi_{SQ}|\mathrm{e}^{R_{\pi/a}}(b^{\dagger}_{\pi/a}+b_{\pi/a})^2\mathrm{e}^{-R_{\pi/a}}|\Psi_{SQ}\rangle = 2Sh^2(2\alpha)+1+4\delta^2_{\pi/a}G^2\,. \quad (144)$$

Now we can re- write the CF of Eq. (141) as

$$F^{\mathrm{ct}}_{|i\rangle} \equiv \frac{-\sqrt{2}\delta_{\pi/a}\gamma_0\langle i|(n_1-n_2)^2|i\rangle}{\sqrt{Sh^2(2\alpha)+1/2+2\delta^2_{\pi/a}\gamma_0^2\langle i|(n_1-n_2)^2|i\rangle}}\,. \quad (145)$$

The evaluation of F^{ct} requires therefore the knowledge of the matrix elements of $(n_1-n_2)^2$. By the usual decomposition of the identity one obtains:

for $N=1$

$$\langle i\sigma|(n_1-n_2)^2|i\sigma\rangle = 1 \qquad (i=1,2) \quad (146)$$

so that

$$F^{\mathrm{ct}}_{|1\sigma\rangle} \equiv \frac{-\sqrt{2}\delta_{\pi/a}\gamma}{\sqrt{Sh^2(2\alpha)+1/2+2\delta^2_{\pi/a}\gamma^2}} = \frac{-2\delta_{\pi/a}\gamma}{\sqrt{Ch(4\alpha)+4\delta^2_{\pi/a}\gamma^2}}\,. \quad (147)$$

for $N=2$

$$\langle 3|(n_1-n_2)^2|3\rangle = 4\sin^2\theta\,, \qquad \langle 4|(n_1-n_2)^2|4\rangle = 0\,, \qquad \langle 5|(n_1-n_2)^2|5\rangle = 4\,. \quad (148)$$

Finally we obtain the explicit form of the charge transfer CF:

$$\begin{aligned} F^{\mathrm{ct}}_{|3\rangle} &\equiv -4\sqrt{2}\delta_{\pi/a}\gamma_0\frac{\sin^2\theta}{\sqrt{Sh^2(2\alpha)+1/2+8\delta^2_{\pi/a}\gamma_0^2\sin^2\theta}} \\ &= -\frac{16\delta_{\pi/a}\gamma_0\sin^2\theta}{\sqrt{Ch(4\alpha)+(4\delta_{\pi/a}\gamma_0\sin\theta)^2}}\,, \end{aligned} \quad (149)$$

$$\begin{aligned} F^{\mathrm{ct}}_{|5\rangle} &\equiv -4\sqrt{2}\delta_{\pi/a}\gamma_0\frac{1}{\sqrt{Sh^2(2\alpha)+1/2+8\delta^2_{\pi/a}\gamma_0^2}} \\ &= -\frac{16\delta_{\pi/a}\gamma_0}{\sqrt{Ch(4\alpha)+(4\delta_{\pi/a}\gamma_0)^2}} \end{aligned} \quad (150)$$

while $F^{\mathrm{ct}}_{|4\rangle}=0$. Once more, this quantity depends on both displacement and squeezing through ϑ.

The quantitative behaviour of the CF's evaluated above is discussed in Ref. [2].

8. Summary of phonon polaron discussion and introduction to the spin polarons

Let us summarize the main points of this first part of the Lectures. We have introduced a sequence of displacement and squeezing transformations (in this order) as a general non-perturbative way to transform an interacting boson-fermion Hamiltonian into an effective one with only fermionic operators. The effect of the bosons results in a renormalization of the electronic interactions, and possibly in the presence of electronic terms which where absent in the electron–only part of the original Hamiltonian. From the formal point of view we have stressed two points: first, the dependance of the parameters characterizing the transformations on the wavevectors of the bosonic modes is a basic feature of the physics of the problem, and its neglect is likely to lead to questionable results. Second, whenever feasible, the parameters values have to be determined variationally, instead of being set by some diagonalization requirement. By way of application we have considered the case where the bosons are phonons. We have produced an effective polaronic Hamiltonian, containing a long range Coulomb interaction term which was absent from electronic part of the original Hamiltonian. Finally, we have taken the dimer and the four-site chain as simple concrete systems where to apply the general formalism, showing how one gets quantities which can be experimentally tested.

Besides the phonons, electrons in solids can couple to other bosonic excitations: we shall now consider the case of coupling to magnetic fluctuations, which, in the spin wave formalism, can be described as a special kind of boson. If the magnetic properties can be described by a Heisenberg term $J_H \sum_{i,\langle j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j = J_H \sum_{i,\langle j\rangle} \left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+ \right) \right]$ one calls *longitudinal* the fluctuations related to $S_i^z S_j^z$ and *transverse* those related to $S_i^+ S_j^-$. Spin polarons due to longitudinal fluctuations have been considered in the *Spin Bag* model [14] in connection with the high T_c superconductors, but we shall not discuss them. Our interest will be centred on the spin polarons due to transverse fluctuations. There are two main families of models, *i.e.* double band and single band ones, and we shall deal with them in turn.

9. Two-band (Kondo–Heisenberg) model for spin polarons

This model is based on the electronic structure of the *High-T_c Superconductors (HTS)* but it applies also to other systems, *e.g.* the *Heavy Fermion (HF)* and the *Colossal Magnetoresistance (CMR) Systems.* In all those materials, there are moment-bearing ions (respectively, Cu^{2+}, rare earth ions, and Mn^{3+}) and itinerant electrons hopping in hybridized bands. The dynamics of the electrons is conditioned by the magnetic excitations, which, if the local moments have long range order, are spin waves. In the case of CMR there are also very important phononic interactions, which by themselves may create phononic polarons, but we shall consider here only the magnetic polarons for sake of simplicity.

Two are the basic ingredients for the Heisenberg–Kondo Hamiltonian: first, a set of magnetic ions whose local moments, of length S, interacting between themselves through a Heisenberg term and, second, itinerant fermions (represented by $c^\dagger_{i\sigma}, c_{i\sigma}$ operators) whose spin $\boldsymbol{s}_i = [c^\dagger_{i\uparrow}c_{i\downarrow}, c^\dagger_{i\downarrow}c_{i\uparrow}, (n_{i\uparrow} - n_{i\downarrow})/2]$ interacts with a local moment through a Kondo-type term $J_K \sum_i \boldsymbol{s}_i \cdot S_i$. The Heisenberg term is due to superexchange involving bridging Oxygen anions in HTS and CMR , and due to the indirect RKKY interaction in HF. The fermion band arises through hybridization of cation $3d$ with anion $2p$ orbitals (in the case of HTS and CMR) or of $3d$ and $4f$ or $5f$ orbitals (for HF). The total Kondo–Heisenberg (or two-band) Hamiltonian is:

$$\begin{aligned} H \;=\; & \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_{i,\langle j\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ & + \sum_{i,\langle j\rangle} V_{i,j} n_i n_i + J_K \sum_i \boldsymbol{s}_i \cdot \boldsymbol{S}_i + J_H \sum_{i,\langle j\rangle} \boldsymbol{S}_i \cdot S_j \,, \end{aligned} \tag{151}$$

where $\sum_{i,\langle j\rangle}$ means summing over the z sites labelled by j which are nearest neighbours of i, and then summing over all i's. The spin polaron physics comes from the Kondo term. The type of coupling can be either antiferromagnetic (AF), as in HTSC and HF, or ferromagnetic, as in CMR. In both cases, this term forces the electron spin $\boldsymbol{s}_i$ to have a well defined direction with respect to the local moment $\boldsymbol{S}_i$. Consider now the case where the local moments have a long range antiferromagnetic (AF) order of the Ne'el type, *i.e.* such that up and down moments occupy two interpenetrating sublattices, each up moment on sublattice A having as nearest neighbours only down moments on sublattice B. Here "long range" includes also the situation of finite size, long lived AF fluctuation where the order extends over many lattice spacings, and the lifetime of such an "AF droplet" is long compared with the bare electron hopping time $\approx t_{ij}^{-1}$. If the moments are frozen, an electron on site i, where local moments are up, can hop to site j, where they

are down, only if allowed by the Kondo term on j $E_j^K = J_K \boldsymbol{s}_j \cdot \boldsymbol{S}_j$, which implies reversing $\boldsymbol{S}_j$ at the cost of the Heisenberg energy $J_H \boldsymbol{S}_i \cdot S_j$. If the magnetic energy cost exceeds the energy gain on delocalization, the electron is trapped at site i. Conversely, if the amplitude of the local moment on j is reduced, at least partially, by effect of a spin wave, the magnetic energy cost decreases and the hopping may become allowed. The reciprocal picture, emphasizing the itineracy of the fermions, is that the electron, on moving, forces the local moments to assume, with respect to its spin $\boldsymbol{s}_i$, the direction imposed by the Kondo term, thereby frustrating the AF arrangement at the price of the Heisenberg energy. In both cases, the fermion motion, if any, happens by creating a stream of spin waves, in close analogy to the phonon case, where the fermion creates a stream of phonons when hopping around in a deformable lattice.

The case of the Kondo-Heisenberg Hamiltonian in the absence of long range magnetic order is very interesting, giving rise to much of the HF and CMR physics but we shall not discuss it.

As a first step to formalize the spin polarons in the case of AF order of the local moments, let us diagonalize the Heisenberg term, by representing the local moments operators in the Holstein–Primakoff approximation. We have to distinguish between up (i-sites) and down (j-sites) sublattice, so that the operators $b_{i,(j)} b_{i,(j)}^\dagger$ are then defined through:

$$\begin{aligned} S_i^+ &\equiv \sqrt{2S}\sqrt{1 - b_i^\dagger b_i} b_i \sim \sqrt{2S} b_i \,, \qquad & S_j^+ &\equiv \sqrt{2S} b_j^\dagger \sqrt{1 - b_j^\dagger b_j} \sim \sqrt{2S} b_j^\dagger \,, \\ S_i^- &\equiv \sqrt{2S} b_i^\dagger \sqrt{1 - b_i^\dagger b_i} \sim \sqrt{2S} b_i^\dagger \,, \qquad & S_j^- &\equiv \sqrt{2S}\sqrt{1 - b_j^\dagger b_j} b_j \sim \sqrt{2S} b_j \,, \\ S_i^z &= S - b_i^\dagger b_i \,, & S_j^z &= -(S - b_j^\dagger b_j) \,. \end{aligned} \tag{152}$$

We then write $S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$ in terms of $b_{i,(j)} b_{i,(j)}^\dagger$, yielding:

$$\boldsymbol{S}_i \cdot S_j = -S^2 + S\left(b_i^\dagger b_i + b_j^\dagger b_j\right) + S\left(b_i b_j + b_i^\dagger b_j^\dagger\right) - b_i^\dagger b_i b_j^\dagger b_j \,. \tag{153}$$

The last term represents interactions of moment deviations on different sites, and will be neglected. Passing to the spin wave operators in the reciprocal space through $b_j = N^{-1/2} \sum_q b_q \mathrm{e}^{iqR_j}$ and $b_j^\dagger = N^{-1/2} \sum_q b_q^\dagger \mathrm{e}^{-iqR_j}$ yields:

$$\sum_{i\langle j\rangle} \boldsymbol{S}_i \cdot S_j = -NzS^2 + \frac{S}{2} \sum_q \left(b_q^\dagger b_q + b_{-q}^\dagger b_{-q}\right) + Sz \sum_q \left(b_q^\dagger b_{-q}^\dagger + b_q b_{-q}\right) \cos\left(q\delta\right) , \tag{154}$$

where z is the number of nearest neighbours, and $\boldsymbol{\delta} = |\boldsymbol{R}_i - \boldsymbol{R}_j|$ is the lattice parameter. The last term in Eq. (154) is an old friend, *i.e.* the type of

non-linear boson interaction which is diagonalized by a squeezing transformation (see Eq. (75)). Let us then follow the squeezing formalism, which is of course equivalent to the textbook Bogolyubov transformation. The appropriate squeezing operator is $\exp(T) = \exp\left[\sum_q \vartheta_q \left(b_q^\dagger b_{-q}^\dagger - b_q b_{-q}\right)\right]$ assuming $\vartheta_q \geq 0$. Notice the positive sign in the exponent, opposite to the one in the phonon case. The reason is that the spin wave operators are not true boson operators: the number of bosons which can "condense" is limited by the length of the local moment, because the maximum number of spin deviations on a site is such to reverse the local magnetic moment. Therefore the squeezing can not expand the indeterminacy on the moment amplitude indefinitely (as, at least in principle, can be done for deformations). The present choice of sign for T enhances the indeterminacy on the conjugated momentum $b_q^\dagger - b_{-q}$, which has no intrinsic limitations. The squeezed spin wave operators $a_q^{(\dagger)} = \mathrm{e}^T b_q^{(\dagger)} \mathrm{e}^{-T}$ can be evaluated by the equation of motion technique, yielding:.

$$\begin{aligned} a_q^\dagger &= b_q^\dagger \cosh(\vartheta_q) - b_{-q} \sinh(\vartheta_q) \ , \quad a_q = b_q \cosh(\vartheta_q) - b_{-q}^\dagger \sinh(\vartheta_q) \ , \\ b_q^\dagger &= a_q^\dagger \cosh(\vartheta_q) + a_{-q} \sinh(\vartheta_q) \ , \quad b_q = a_q \cosh(\vartheta_q) + a_{-q}^\dagger \sinh(\vartheta_q) \ . \end{aligned} \tag{155}$$

Imposing the vanishing of all the anharmonic terms in the squeezed Hamiltonian, one arrives at the diagonalization condition $\tanh(2\vartheta_q) = -2z\cos(q\delta)$. The AF Heisenberg Hamiltonian diagonalized by squeezing reads:

$$\begin{aligned} J_H \sum_{i,\langle j\rangle} \mathrm{e}^T \boldsymbol{S}_i \cdot S_j \mathrm{e}^{-T} &= -J_H S N \left(\tfrac{1}{2} + Sz\right) \\ + J_H S \sum_q \sqrt{1 - 4z^2 \cos^2(q\delta)} \left(a_q^\dagger a_q + \tfrac{1}{2}\right) \ . \end{aligned} \tag{156}$$

Eq. (156) identifies the AF spin wave frequency $\hbar\Omega_q = J_H S \sqrt{1-4z^2\cos^2(q\delta)}$.

The diagonalization of the Heisenberg term in the reciprocal space suggests to Fourier transform also the bosonic contributions in the Kondo term. We first distinguish the parts referring to the up (A) and down (B) sublattices: $J_K \sum_m \boldsymbol{s}_m \cdot \boldsymbol{S}_m = J_K \sum_{i\in A} \boldsymbol{s}_i \cdot \boldsymbol{S}_i + J_K \sum_{j\in B} \boldsymbol{s}_j \cdot \boldsymbol{S}_j$ and then use the Holstein–Primakoff representation for the local moments, yielding:

$$\begin{aligned} \boldsymbol{s}_i \cdot \boldsymbol{S}_i &= \tfrac{1}{2}\left(S - b_i^\dagger b_i\right)(n_{i\uparrow} - n_{i\downarrow}) + \tfrac{1}{2}\left(b_i c_{i\downarrow}^\dagger c_{i\uparrow} + b_i^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}\right) \ , \\ \boldsymbol{s}_j \cdot \boldsymbol{S}_j &= -\tfrac{1}{2}\left(S - b_j^\dagger b_j\right)(n_{j\uparrow} - n_{j\downarrow}) + \tfrac{1}{2}\left(b_j^\dagger c_{j\downarrow}^\dagger c_{j\uparrow} + b_j c_{j\uparrow}^\dagger c_{j\downarrow}\right) \ . \end{aligned} \tag{157}$$

We have now to go to the *reduced* Brillouin zone (RBZ) in reciprocal space, because each sublattice has only $N/2$ sites. If not explicitly stated otherwise,

from now on the spin wave wavevectors will be restricted to the RBZ. Let us consider first the longitudinal terms on A, yielding (with $n_{i\uparrow} - n_{i\downarrow} = 2s_i^z$):

$$\sum_{i\in A}\left(S - b_i^\dagger b_i\right) s_i^z = S\sum_{i\in A} s_i^z - \left(\frac{2}{N}\right)\sum_{p,q\in RBZ} b_q^\dagger b_p \mathrm{e}^{-i(q-p)R_i} s_i^z \,. \tag{158}$$

Now, it is reasonable to assume that the itinerant particles do not create a magnetic sublattice with a periodicity different from the one imposed by the AF order of the local moments, so that one can approximate on the up (A) sublattice $s_i^z = \langle s\rangle$ independently of $\boldsymbol{R}_i$. Then:

$$\sum_i \left(S - b_i^\dagger b_i\right) s_i^z = \frac{N}{2} S\langle s\rangle - \langle s\rangle \sum_q b_q^\dagger b_q \,. \tag{159}$$

The evaluation of $\sum_j \left(S - b_j^\dagger b_j\right) s_j^z$ yields the same result because on the down (B) sublattice $s_j^z = -\langle s\rangle$. We get an additional contribution to the local moment AF Hamiltonian, which modifies the diagonalization condition and the effective frequency into:

$$\begin{aligned} \tanh\left(2\vartheta_q\right) &= -\frac{2J_H S z\cos\left(q\delta\right)}{J_H S - J_K\langle s\rangle}\,, \\ \hbar\Omega_q &= \left(J_H S - J_K\langle s\rangle\right)\sqrt{1 - \left[\frac{2J_H S z\cos\left(q\delta\right)}{J_H S - J_K\langle s\rangle}\right]^2}\,. \end{aligned} \tag{160}$$

One might also treat the term $b_q^\dagger b_q s_i^z$ of Eq. (158) in mean field approximation, *i.e.* introducing a reciprocal influence of the local moment deviation and s_i^z . We are not interested here in developing this aspect of the problem.

Introducing the spin flip operators for the itinerant particles $s_i^\sigma \equiv c_{i\sigma}^\dagger c_{i-\sigma}$ ($\sigma = \pm$ when used as in s_i^σ) we write the transverse part of the Kondo term on the two sublattices as:

$$\frac{1}{2}\sum_{i\in A,\sigma=\pm} s_i^\sigma S_i^{-\sigma} = \frac{1}{2}\sqrt{\frac{2}{N}}\sum_q \left[b_q^\dagger \sum_i s_i^+ \mathrm{e}^{-iqR_i} + b_{-q}\sum_i s_i^- \mathrm{e}^{-iqR_i}\right], \tag{161}$$

$$\frac{1}{2}\sum_{j\in B,\sigma=\pm} s_j^\sigma S_j^{-\sigma} = \frac{1}{2}\sqrt{\frac{2}{N}}\sum_q \left[b_q^\dagger \sum_j s_j^- \mathrm{e}^{-iqR_j} + b_{-q}\sum_j s_j^+ \mathrm{e}^{-iqR_j}\right]. \tag{162}$$

Introducing the AF spin wave operators and rearranging yields:

$$\frac{1}{2}\sum_{i\in A,\sigma=\pm} s_i^\sigma S_i^{-\sigma} = \frac{1}{2}\sqrt{\frac{2}{N}}\sum_q a_q^\dagger \sum_i \left[\cosh\left(\vartheta_q\right) s_i^+ + \sinh\left(\vartheta_q\right) s_i^-\right]\mathrm{e}^{-iqR_i}$$

$$+\frac{1}{2}\sqrt{\frac{2}{N}}\sum_q a_{-q}\sum_i\left[\sinh\left(\vartheta_q\right)s_i^+ + \cosh\left(\vartheta_q\right)s_i^-\right]\mathrm{e}^{-iqR_i}\,, \tag{163}$$

$$\frac{1}{2}\sum_{j\in B,\sigma=\pm} s_j^\sigma S_j^{-\sigma} = \frac{1}{2}\sqrt{\frac{2}{N}}\sum_q a_q^\dagger\sum_j\left[\sinh\left(\vartheta_q\right)s_j^+ + \cosh\left(\vartheta_q\right)s_j^-\right]\mathrm{e}^{-iqR_j}$$

$$+\frac{1}{2}\sqrt{\frac{2}{N}}\sum_q a_{-q}\sum_j\left[\cosh\left(\vartheta_q\right)s_j^+ + \sinh\left(\vartheta_q\right)s_j^-\right]\mathrm{e}^{-iqR_j}\,. \tag{164}$$

Physically, these are the terms which we expect to control the dynamics of the carriers. In analogy to what we did for the phonon case, we shall try to get rid of this fermion- boson coupling terms by mean of a "displacement" transformation, in principle different on each sublattice, but formally identical. Let us introduce two generators $D^L(L = A, B \text{ and } l \in L)$:

$$D^L = \sqrt{\frac{2}{N}}\sum_q \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\left(a_q^\dagger - a_{-q}\right)\sum_l\left(s_l^+ + s_l^-\right)\mathrm{e}^{-iqR_l}\,. \tag{165}$$

The displacement parameters $\{\delta_q\}$ should not to be confused with the lattice parameter $\delta = |\boldsymbol{R}_i - \boldsymbol{R}_j|$. The displaced Bose operators on each sublattice $\mathcal{A}_{qL}^{(\dagger)} = \mathrm{e}^{D^L}a_q^{(\dagger)}\mathrm{e}^{-D^L}$ $(l = A, B)$ are obtained from the commutators

$$\begin{aligned}\left[D^L, a_q^\dagger\right] &= -\delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_l\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\,,\\ \left[D^L, a_q\right] &= -\delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_l\left(s_l^+ + s_l^-\right)\mathrm{e}^{-iqR_l}\end{aligned} \tag{166}$$

in the form:

$$\begin{aligned}\mathcal{A}_{qL}^\dagger &= a_q^\dagger - \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_{l\in L}\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\,,\\ \mathcal{A}_{-qL} &= a_{-q} - \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_{l\in L}\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\,.\end{aligned} \tag{167}$$

We can now obtain the displaced free oscillator term:

$$\mathrm{e}^{D^L}\left[\sum_q\hbar\Omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)\right]\mathrm{e}^{-D^L} = \sum_q\hbar\Omega_q\left(\mathcal{A}_q^\dagger\mathcal{A}_q + \frac{1}{2}\right) = \sum_q\hbar\Omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)$$

$$-\sum_q\hbar\Omega_q\delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_l\left(s_l^+ + s_l^-\right)\left[a_q^\dagger\mathrm{e}^{iqR_l} + a_q\mathrm{e}^{-iqR_l}\right]$$

$$+\sum_q\hbar\Omega_q\delta_q^2\left(\frac{J_K}{\hbar\Omega_q}\right)^2\left(\frac{2}{N}\right)\sum_{l,m}\left(s_l^+ + s_l^-\right)\left(s_m^+ + s_m^-\right)\mathrm{e}^{iq(R_l - R_m)}\,. \tag{168}$$

Notice that R_l, R_m both belong to the *same* sublattice so that, if $R_l \neq R_m$, they are next nearest, or more distant, neighbours. In the last line of Eq. (168) the terms with $l \neq m$ yield contributions like $s_l^{\pm}\ s_m^{\pm}$, which we shall neglect, and terms $s_l^+ s_m^- + \text{h.c.} = (c_{l\uparrow}^\dagger c_{m\downarrow}^\dagger)(c_{m\uparrow} c_{l\downarrow}) + \text{h.c.}$, which correspond to inter-site, intra-sublattice singlets, possibly of interest for high temperature superconductors. After those simplifications we can write:

$$\mathrm{e}^{D^L}\left[\sum_q \hbar\Omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)\right]\mathrm{e}^{-D^L} \Longrightarrow \sum_q \hbar\Omega_q\left(a_q^\dagger a_q + \frac{1}{2}\right)$$
$$+\sum_q \hbar\Omega_q \delta_q^2 \left(\frac{J_K}{\hbar\Omega_q}\right)^2 \left(\frac{1}{N}\right)\sum_{l,m} c_{l\uparrow}^\dagger c_{m\downarrow}^\dagger c_{m\uparrow} c_{l\downarrow} \cos\left[q\left(R_l - R_m\right)\right] . \quad (169)$$

Notice that once more we find a long range interaction produced by the displacement transformation connected to a local interaction, just as it happened for the long range intersite charge interaction in the case of electrons and phonons coupled by the Holstein term.

The terms with $l = m$ yield:

$$\sum_q \hbar\Omega_q \delta_q^2 \left(\frac{J_K}{\hbar\Omega_q}\right)^2 \left(\frac{2}{N}\right)\sum_l \left(s_l^+ + s_l^-\right)^2$$
$$= \sum_q \delta_q^2 \left(\frac{J_K^2}{\hbar\Omega_q}\right)\left(\frac{2}{N}\right)\sum_l \left[-2n_{l\uparrow}n_{l\downarrow} + n_{l\uparrow} + n_{l\downarrow}\right] . \quad (170)$$

We recognize contributions to the Hubbard and the atomic terms, in close analogy to the phonon case. Summarizing our findings, by transforming the free oscillator term we obtain not only a renormalization of the Hubbard and atomic energy terms, but also a long range interaction between sites of the same magnetic sublattice, which was absent in the starting electronic Hamiltonian.

To transform the Fermi operators, we note that, for $m = i, j$, the relevant commutators are:

$$\left[\sum_l s_l^+, c_{m\sigma}^\dagger\right] = c_{m-\sigma}^\dagger \delta_{\sigma\downarrow} , \qquad \left[\sum_l s_l^-, c_{m\sigma}^\dagger\right] = c_{m-\sigma}^\dagger \delta_{\sigma\uparrow} ,$$
$$\left[\sum_l s_l^+, c_{m\sigma}\right] = -c_{m-\sigma}\delta_{\sigma\uparrow} , \qquad \left[\sum_l s_l^-, c_{m\sigma}\right] = -c_{m-\sigma}\delta_{\sigma\downarrow} . \quad (171)$$

Defining for short:

$$\Delta_l = \sqrt{\frac{2}{N}}\sum_q \delta_q \left(\frac{J_K}{\hbar\Omega_q}\right)\mathrm{e}^{-iqR_l}\left(a_q^\dagger - a_{-q}\right) \quad (172)$$

it follows that in the series development of $f^\dagger_{l\sigma} = \mathrm{e}^{D^L} c^\dagger_{l\sigma} \mathrm{e}^{-D^L}$ the even-order $(2n)$ nested commutators of D^L and $c^\dagger_{l\sigma}$ yield $c^\dagger_{l\sigma}\Delta_l^{2n}$, while those of odd order $(2n{+}1)$ yield $c^\dagger_{l-\sigma}\Delta_l^{2n+1}$. For the destruction operator $f_{l\sigma} = \mathrm{e}^{D^L} c_{l\sigma} \mathrm{e}^{-D^L}$ one has the even-order nested commutators yielding $c_{l\sigma}\Delta_l^{2n}$ and the odd-order ones $-c_{l-\sigma}\Delta_l^{2n+1}$. Summing the series then yields:

$$f^\dagger_{l\sigma} = c^\dagger_{l\sigma}\cosh(\Delta_l) + c^\dagger_{l-\sigma}\sinh(\Delta_l)\ , \quad f_{l\sigma} = c_{l\sigma}\cosh(\Delta_l) - c_{l-\sigma}\sinh(\Delta_l)\ . \tag{173}$$

Now we can transform the whole Kondo–Heisenberg Hamiltonian. The number operator transforms into:

$$f^\dagger_{l\sigma} f_{l\sigma} = n_{l\sigma}\cosh^2(\Delta_l) - n_{l-\sigma}\sinh^2(\Delta_l) - \sigma\frac{\left(s^+_l - s^-_l\right)}{2}\sinh(2\Delta_l) \tag{174}$$

so that the total charge on each site $\sum_\sigma f^\dagger_{l\sigma} f_{l\sigma}$ is unaffected .

The Hubbard term, dropping terms odd in $\sinh(2\Delta_l)$ (which will not survive the average over the squeezed state to be introduced later on) is not modified: $f^\dagger_{l\uparrow} f_{l\uparrow} f^\dagger_{l\downarrow} f_{l\downarrow} = n_{l\uparrow} n_{l\downarrow}$.

The hopping term has to be split into

$$\sum_{i_A\langle j_B\rangle\sigma} t f^\dagger_{i_A\sigma} f_{j_B\sigma} + \sum_{j_B\langle i_A\rangle\sigma} t f^\dagger_{j_B\sigma} f_{i_A\sigma}$$

yielding:

$$\begin{aligned}
\sum_{i_A\langle j_B\rangle\sigma} t f^\dagger_{i_A\sigma} f_{j_B\sigma} &= \sum_{i_A\langle j_B\rangle\sigma} t c^\dagger_{i_A\sigma} c_{j_B\sigma}\left[\cosh(\Delta_i)\cosh(\Delta_j) - \sinh(\Delta_i)\sinh(\Delta_j)\right] \\
&+ \sum_{i_A\langle j_B\rangle\sigma} t c^\dagger_{i_A\sigma} c_{j_B-\sigma}\left[\sinh(\Delta_i)\cosh(\Delta_j) - \cosh(\Delta_i)\sinh(\Delta_j)\right] \\
&\Longrightarrow \sum_{i_A\langle j_B\rangle\sigma} t c^\dagger_{i_A\sigma} c_{j_B\sigma}\cosh(\Delta_i)\cosh(\Delta_j)\ , \qquad (175) \\
\sum_{j_B\langle i_A\rangle\sigma} t f^\dagger_{j_B\sigma} f_{i_A\sigma} &= \sum_{j_B\langle i_A\rangle\sigma} t c^\dagger_{j_B\sigma} c_{i_A\sigma}\left[\cosh(\Delta_i)\cosh(\Delta_j) - \sinh(\Delta_i)\sinh(\Delta_j)\right] \\
&- \sum_{j_B\langle i_A\rangle\sigma} t c^\dagger_{j_B\sigma} c_{i_A-\sigma}\left[\sinh(\Delta_i)\cosh(\Delta_j) - \cosh(\Delta_i)\sinh(\Delta_j)\right] \\
&\Longrightarrow \sum_{j_B\langle i_A\rangle\sigma} t c^\dagger_{j_B\sigma} c_{i_A\sigma}\cosh(\Delta_i)\cosh(\Delta_j)\ , \qquad (176)
\end{aligned}$$

where the double arrow indicates the terms which will survive the squeezed average.

Let us now consider the itinerant electron moment. By using the number operators its z- component transforms as:

$$\mathrm{e}^{D^L} s_l^z \mathrm{e}^{-D^L} = \frac{1}{2} s_l^z \cosh(2\Delta_l) - \frac{1}{2}\left(s_l^+ - s_l^-\right)\sinh(2\Delta_l) \Longrightarrow \frac{1}{2} s_l^z \cosh(2\Delta_l) \ . \tag{177}$$

The other components, the spin flip operators, are ($l = i \in A$ or $j \in B$):

$$f_{l\uparrow}^\dagger f_{l\downarrow} = s_l^+ \cosh^2(\Delta_l) - s_l^- \sinh^2(\Delta_l) - \frac{s_l^z}{4}\sinh(2\Delta_l) \ ,$$

$$f_{l\downarrow}^\dagger f_{l\uparrow} = s_l^- \cosh^2(\Delta_l) - s_l^+ \sinh^2(\Delta_l) + \frac{s_l^z}{4}\sinh(2\Delta_l) \ . \tag{178}$$

Introducing the displaced spin-wave operators and Eq. (178), we have for the A sublattice:

$$\begin{aligned}
&\mathrm{e}^{D^A}\left[\frac{J_K}{2}\sum_{i\in A,\sigma} s_i^\sigma S_i^{-\sigma}\right]\mathrm{e}^{-D^A} \\
&= \frac{J_K}{2}\sqrt{\frac{2}{N}}\sum_q\left[a_q^\dagger - \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_{l\in A}\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\right]\mathcal{C}_q \\
&+ \frac{J_K}{2}\sqrt{\frac{2}{N}}\sum_q\left[a_{-q} - \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sqrt{\frac{2}{N}}\sum_{l\in A}\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\right]\mathcal{D}_q \ ,
\end{aligned} \tag{179}$$

where:

$$\begin{aligned}
\mathcal{C}_q \ = \ &\sum_{i\in A}\mathrm{e}^{-iqR_i}\Big\{s_i^-\cosh(\vartheta_q) + s_i^+\sinh(\vartheta_q) + \left(s_i^+ - s_i^-\right)\cosh^2(\Delta_i)\,\mathrm{e}^{-\vartheta_q} \\
&- \frac{s_i^z}{4}\sinh(2\Delta_i)\,\mathrm{e}^{-\vartheta_q}\Big\} ,
\end{aligned} \tag{180}$$

$$\begin{aligned}
\mathcal{D}_q \ = \ &\sum_{i\in A}\mathrm{e}^{-iqR_i}\Big\{s_i^-\sinh(\vartheta_q) + s_i^+\cosh(\vartheta_q) - \left(s_i^+ - s_i^-\right)\cosh^2(\Delta_i)\,\mathrm{e}^{-\vartheta_q} \\
&+ \frac{s_i^z}{4}\sinh(2\Delta_i)\,\mathrm{e}^{-\vartheta_q}\Big\} .
\end{aligned} \tag{181}$$

When developing the products in Eq. (179) the terms linear in $a_q^\dagger, a_q$ can be dropped, as they yield vanishing expectation values in the squeezed state. The terms containing only the spin flip operators sum up to:

$$-\frac{J_K}{N}\sum_q \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\sum_{l\in A}\left(s_l^+ + s_l^-\right)\mathrm{e}^{iqR_l}\sum_{i\in A}\mathrm{e}^{-iqR_i}\left(s_i^+ + s_i^-\right)\mathrm{e}^{\vartheta_q} \ . \tag{182}$$

The calculation for the B sublattice is analogous, but for interchanging spin raising and lowering operators, which leaves the above result unaffected. Therefore, on both sublattices, the terms surviving the squeezing yield:

$$\begin{aligned}&\mathrm{e}^{D^L}\left[\frac{J_K}{2}\sum_{l\in L}\left(s_l^+S_l^- + \mathrm{h.c.}\right)\right]\mathrm{e}^{-D^L}\\&\Longrightarrow -\frac{J_K}{N}\sum_q \delta_q\left(\frac{J_K}{\hbar\Omega_q}\right)\mathrm{e}^{\vartheta_q}\sum_{l,m\in L}\left(s_l^+ + s_l^-\right)\left(s_m^+ + s_m^-\right)\mathrm{e}^{iq(R_l-R_m)}\,. \quad (183)\end{aligned}$$

Proceeding as we did in the transformation of the free oscillator term, if $l \neq m$ we have:

$$\begin{aligned}&\sum_{l,m}\left(s_l^+ + s_l^-\right)\left(s_m^+ + s_m^-\right)\mathrm{e}^{iq(R_l-R_m)} \Longrightarrow \sum_{l,m}\left(s_l^+ s_m^- + s_l^- s_m^+\right)\mathrm{e}^{iq(R_l-R_m)}\\&= \sum_{l,m} c_{l\uparrow}^\dagger c_{m\downarrow}^\dagger c_{m\uparrow}c_{l\downarrow}\left\{2\cos\left[q\left(R_l - R_m\right)\right]\right\} \quad (184)\end{aligned}$$

while if $l = m$ then $\sum_l \left(s_l^+ + s_l^-\right)^2 = \sum_l \left(-2n_{l\uparrow}n_{l\downarrow} + n_{l\uparrow} + n_{l\downarrow}\right)$ and we obtain a renormalization of the Hubbard and of the atomic terms. Therefore:

$$\begin{aligned}&\mathrm{e}^{D^L}\left[\frac{J_K}{2}\sum_{l}\left(s_l^+ S_l^- + \mathrm{h.c.}\right)\right]\mathrm{e}^{-D^L}\\&\Longrightarrow -\frac{1}{N}\sum_q \delta_q\left(\frac{J_K^2}{\hbar\Omega_q}\right)\mathrm{e}^{\vartheta_q}\sum_l\left(-2n_{l\uparrow}n_{l\downarrow} + n_{l\uparrow} + n_{l\downarrow}\right)\\&-\frac{2}{N}\sum_q \delta_q\left(\frac{J_K^2}{\hbar\Omega_q}\right)\mathrm{e}^{\vartheta_q}\sum_{l,m} c_{l\uparrow}^\dagger c_{m\downarrow}^\dagger c_{m\uparrow}c_{l\downarrow}\left\{2\cos\left[q\left(R_l - R_m\right)\right]\right\} \quad (185)\end{aligned}$$

which is the same type of contributions produced by transforming the free oscillator term. On the B sublattice the contributions turn out to be the same as on A.

Written out in all its glory, the displaced Hamiltonian, dropping the terms linear either in $a_{q,}^\dagger a_{-q}$ or in $\sinh\left(n\Delta_l\right)$, which would not survive the squeezed average to be performed next, reads:

$$\begin{aligned}&\mathrm{e}^{D^i}\mathrm{e}^{D^j}H\mathrm{e}^{-D^j}\mathrm{e}^{-D^i} \Longrightarrow \sum_l n_l\left[\varepsilon_l + \frac{J_K}{N}\sum_q\left(\frac{J_K}{\hbar\Omega_q}\right)\delta_q\left(2\delta_q - \mathrm{e}^{\vartheta_q}\right)\right]\\&+\sum_{i\langle j\rangle\sigma} t c_{i\sigma}^\dagger c_{j\sigma}\cosh\left(\Delta_i\right)\cosh\left(\Delta_j\right) + V\sum_{i\langle j\rangle} n_i n_j\end{aligned}$$

$$+\sum_{l} n_{l\uparrow} n_{l\downarrow} \left[U - \frac{2J_K}{N} \sum_{q} \left(\frac{J_K}{\hbar\Omega_q} \right) \delta_q \left(2\delta_q - \mathrm{e}^{\vartheta_q} \right) \right]$$
$$+\frac{2}{N} \sum_{q} \left(\frac{J_K^2}{\hbar\Omega_q} \right) \delta_q \left(2\delta_q - \mathrm{e}^{\vartheta_q} \right) \sum_{l,m\in A} c_{l\uparrow}^{\dagger} c_{m\downarrow}^{\dagger} c_{m\uparrow} c_{l\downarrow} \cos\left[q \left(R_l - R_m \right) \right]$$
$$+\frac{2}{N} \sum_{q} \left(\frac{J_K^2}{\hbar\Omega_q} \right) \delta_q \left(2\delta_q - \mathrm{e}^{\vartheta_q} \right) \sum_{l,m\in B} c_{l\uparrow}^{\dagger} c_{m\downarrow}^{\dagger} c_{m\uparrow} c_{l\downarrow} \cos\left[q \left(R_l - R_m \right) \right]$$
$$+\sum_{q} \hbar\Omega_q \left(a_q^{\dagger} a_{-q} + \frac{1}{2} \right) - J_H S N \left(\frac{1}{2} + Sz \right) + NS \left\langle s \right\rangle J_K \,. \tag{186}$$

Of the electronic terms, only the hopping term contains non-linear functions of spin wave operators.

We shall now proceed to evaluating the average of Eq. (186) over a squeezed magnon wavefunction. By defining a squeezing operator:

$$\mathrm{e}^{S} = \exp\left[- \sum_{q} \eta_q \left(a_q^{\dagger} a_{-q}^{\dagger} - a_q a_{-q} \right) \right] \tag{187}$$

we obtain

$$\left\langle 0 | \mathrm{e}^{S} \cosh\left(\Delta_l \right) \mathrm{e}^{-S} | 0 \right\rangle = \exp\left[-\frac{1}{2} \sum_{q} \mathrm{e}^{-2\eta_q} \delta_q^2 \left(\frac{J_K}{\hbar\Omega_q} \right)^2 \right] ,$$
$$\left\langle 0 | \mathrm{e}^{S} \sinh\left(\Delta_l \right) \mathrm{e}^{-S} | 0 \right\rangle = 0 \tag{188}$$

which justifies the simplifications introduced in transforming the Hubbard term. In the hopping terms we have to squeeze products like $\cosh\left(\Delta_i\right) \cosh\left(\Delta_j\right)$, which imply products of the form $\mathrm{e}^{\pm\Delta_i} \mathrm{e}^{\pm\Delta_j}$. Due to $[\Delta_i, \Delta_j] = 0$ one has:

$$\left\langle \Psi_{SQ} | \mathrm{e}^{\pm\Delta_i} \mathrm{e}^{\pm\Delta_j} | \Psi_{SQ} \right\rangle = \left\langle 0 | \mathrm{e}^{S} \mathrm{e}^{\pm\Delta_i \pm\Delta_j} \mathrm{e}^{-S} | 0 \right\rangle$$
$$= \left\langle 0 \right| \exp\left[\mathrm{e}^{S} \left(\pm\Delta_i \pm \Delta_j \right) \mathrm{e}^{-S} \right] \left| 0 \right\rangle$$
$$= \left\langle 0 \right| \exp\left[\sum_{q} \mathrm{e}^{-\eta_q} \delta_q \left(\frac{J_K}{\hbar\Omega_q} \right) \left(a_q^{\dagger} - a_{-q} \right) \left(\mathrm{e}^{-iqR_i} + \mathrm{e}^{-iqR_j} \right) \right] \left| 0 \right\rangle \tag{189}$$

which is a standard form we have already evaluated in the phonon case. By setting as usual $|\boldsymbol{R}_j - \boldsymbol{R}_i| = \delta$ the final result can be written as:

$$\left\langle 0 | \mathrm{e}^{S} \cosh\left(\Delta_i \right) \cosh\left(\Delta_j \right) \mathrm{e}^{-S} | 0 \right\rangle = \exp\left[-2 \sum_{q} \mathrm{e}^{-2\eta_q} \delta_q^2 \left(\frac{J_K}{\hbar\Omega_q} \right)^2 \cos^2\left(\frac{q\delta}{2} \right) \right] \tag{190}$$

Notice that the above quantity, which we shall indicate by τ, is independent of both site indexes. Squeezing $\sinh(\Delta_i)\sinh(\Delta_j)$ yields zero. After squeezing, the terms of the displaced Hamiltonian linear in the Bose operators disappear, and we finally obtain the effective Kondo–Heisenberg spin polaron Hamiltonian:

$$\begin{aligned}
&\left\langle 0|\mathrm{e}^{S}\mathrm{e}^{D^A}\mathrm{e}^{D^B}H\mathrm{e}^{-D^B}\mathrm{e}^{-D^A}\mathrm{e}^{-S}|0\right\rangle \\
&= \sum_l \varepsilon^* n_l + \sum_{i\langle j\rangle\sigma} t^* c^\dagger_{i\sigma}c_{j\sigma} + \sum_l U^* n_{l\uparrow}n_{l\downarrow} + V\sum_{i\langle j\rangle} n_i n_j \\
&+ \left(\frac{2}{N}\right)\sum_q \left\{ \sum_{l,m\in A} \Gamma^A_{lmq} c^\dagger_{l\uparrow}c^\dagger_{m\downarrow}c_{m\uparrow}c_{l\downarrow} + \sum_{l,m\in B} \Gamma^B_{lmq} c^\dagger_{l\uparrow}c^\dagger_{m\downarrow}c_{m\uparrow}c_{l\downarrow} \right\} \\
&+ \sum_q \hbar\Omega_q \left[\sinh^2(\eta_q) + \frac{1}{2}\right] - J_H SN\left(\frac{1}{2} + Sz\right) + NS\langle s\rangle J_K\,, \qquad (191)
\end{aligned}$$

where the renormalized interactions are:

$$\varepsilon^* = \varepsilon_l + \frac{J_K}{N}\sum_q \left(\frac{J_K}{\hbar\Omega_q}\right)\delta_q\left(2\delta_q - \mathrm{e}^{\vartheta_q}\right), \qquad (192)$$

$$t^* = t\exp\left[-\frac{2}{N}\sum_q \mathrm{e}^{-2\eta_q}\delta_q^2\left(\frac{J_K}{\hbar\Omega_q}\right)^2\cos^2\left(\frac{q\delta}{2}\right)\right], \qquad (193)$$

$$U^* = U - \frac{2J_K}{N}\sum_q \left(\frac{J_K}{\hbar\Omega_q}\right)\delta_q\left(2\delta_q - \mathrm{e}^{\vartheta_q}\right), \qquad (194)$$

$$\Gamma^L_{lmq} = J_K\left(\frac{J_K}{\hbar\Omega_q}\right)\delta_q\left(2\delta_q - \mathrm{e}^{\vartheta_q}\right)\cos\left[q\left(R_l - R_m\right)\right]. \qquad (195)$$

Besides the reduction of the hopping amplitude, the new physics evidenced by the displacement transformation depends crucially on the sign of $2\delta_q - \mathrm{e}^{\vartheta_q}$. If positive, then the "spin polaron shift" is positive and the Hubbard repulsion is reduced, while the sign of the intra-sublattice, long range singlet-producing term depends on the product $\left(2\delta_q - \mathrm{e}^{\vartheta_q}\right)\cos\left[q\left(R_l - R_m\right)\right]$. From the diagonalization condition $\mathrm{Th}(2\vartheta_q) = -2z\cos(q\delta)$ the value of e^{ϑ_q} can be easily worked out as:

$$\mathrm{e}^{\vartheta_q} = \sqrt[4]{1 - \frac{4z\cos(q\delta)}{1 - \frac{J_K\langle s\rangle}{J_H S} + 2z\cos(q\delta)}}\,. \qquad (196)$$

We have succeeded in reducing the problem of the itinerant charges interacting with local magnetic moments in AF order, to a model of fermions dressed by spin waves in strict analogy to what we did for the electron-phonon problem. The way the spin waves renormalize the electronic interactions is different from the phonon case, as one can see by noting the opposite effects on the local energy ε_l and on the Hubbard interaction U, and the insensitivity of the inter-site interaction V, but the conceptual picture is the same.

10. Single-band (t–J) model for spin polarons

As Zhang and Rice [15] have shown, in the case of the HTS the low-energy properties can still be well described if one reduces the many-band model to a single-band one, where the latttice sites are substituted by the CuO_4 plaquettes, and the charge carriers are of two types. One, to be associated to a plaquette (called the Zhang-Rice singlet) is composed by the spin 1/2 hole on the central Cu^{2+} ion, and the doped hole residing essentially on the four surrounding Oxygen ions. The carrier on the doped plaquette has zero total spin (because the Kondo interaction of the two-band model is AF in this case). To the undoped plaquettes we associate the local Cu^{2+} hole, carrying a moment. Then we have spin zero entities surrounded by local moments, which we assume to retain the AF Neel order, even in the presence of the doping, at least over distances long with respect to the lattice spacing, and times long with respect to the hole hopping time. Experimental data show that this assumption is valid for doping smaller than 10%. As in the Kondo–Heisenberg picture, the motion of the singlet requires frustrating the AF pattern. Now a single hop of the singlet is represented as an exchange of site between the singlet and a neighbouring Cu^{2+} hole, carrying its moment. This can be explained more clearly in terms of the two-band language. Indeed, to hop from site i (spin up) to j (spin down), the doped hole must either reverse the moment on j, or its own spin while still on i. It is this second way which underlies the present picture: before hopping, the doped hole reverses both its spin and the local moment on i. Then it moves to j, where the singlet is rebuilt, leaving behind the reversed Cu^{2+} moment on i.

Whatever the picture, after the singlet has moved, the situation is as if it were the Cu^{2+}on site j which has moved to site i, bodily carrying its spin, which now points in the wrong direction. One can say that the Kondo–Heisenberg model associates the frustration of the AF order to the site where the hole goes (j), while the t–J model with the site from where it starts (i). The overall physics is clearly the same, namely the itineracy of the fermion is conditioned by the spin waves of the local moments lattice. To discuss

in formal terms this model, Zhang and Rice have proved [15] that one can describe the dynamics of the system composed of singlets and Cu^{2+} holes by an effective Hamiltonian for Cu^{2+} holes only, where the singlets do not appear explicitly. The motion of the Cu^{2+} holes is described by the t–J model, *i.e.* the single-band Hubbard Hamiltonian in the $U/t \to \infty$ limit. In its simplest version it reads:

$$H_{t-J} = \sum_{i\langle j\rangle\sigma} t c_{i\sigma}^{\dagger} \left(1 - n_{i-\sigma}\right) c_{j\sigma} \left(1 - n_{j-\sigma}\right) + \sum_{i\langle j\rangle} \frac{J}{2} \left(\boldsymbol{S}_i \cdot S_j - \frac{\nu_i \nu_j}{4} \right) . \quad (197)$$

The operators $c_{i\sigma}^{\dagger}, c_{i\sigma}$ describe the Cu^{2+} holes, $J = 4t^2/U$ is the effective AF exchange, and $\nu_i = \sum_{\sigma} n_{i\sigma} \left(1 - n_{i-\sigma}\right)$ is non-vanishing only if the site i is singly occupied. As before, the label i corresponds to sites with up local moment $\boldsymbol{S}_i = \left(c_{i\uparrow}^{\dagger} c_{i\downarrow}, c_{i\downarrow}^{\dagger} c_{i\uparrow}, 1/2(n_{i\uparrow} - n_{i\downarrow}) \right)$ in the ground state, and the label j to its down moment counterpart.

First of all we shall show that spin polarons are, in a sense, intrinsic to the t–J model. If, from $\left[c_{l\sigma}^{\dagger}, c_{l\sigma} \right]_{+} = 1$, we derive $1 - n_{l-\sigma} = c_{l-\sigma} c_{l-\sigma}^{\dagger}$ and define the spin deviation operators $S_l^{\sigma} = c_{l\sigma}^{\dagger}\, c_{l-\sigma}$ (with $\sigma = \pm$ when in S_l^{σ}) then

$$\sum_{i\langle j\rangle\sigma} c_{i\sigma}^{\dagger} \left(1 - n_{i-\sigma}\right) c_{j\sigma} \left(1 - n_{j-\sigma}\right) = \sum_{i\langle j\rangle\sigma} S_i^{-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} S_j^{\sigma} ,$$

$$\nu_i \nu_j = \sum_{\sigma\tau} S_i^{\sigma} S_i^{-\sigma} S_j^{\tau} S_j^{-\tau} . \quad (198)$$

We can then conclude that the projected operators $p_{l\sigma}^{(\dagger)} = c_{l\sigma}^{\dagger} \left(1 - n_{l-\sigma}\right)$ characterizing the t–J model are the product of a Fermi operator times a spin deviation, namely:

$$p_{l\uparrow}^{\dagger} = S_l^{+} c_{l\downarrow} , \qquad p_{l\downarrow}^{\dagger} = S_l^{-} c_{l\uparrow} , \qquad p_{l\uparrow} = c_{l\downarrow} S_l^{-} , \qquad p_{l\downarrow} = c_{l\uparrow} S_l^{+} . \quad (199)$$

We can go further, if we decouple Eq. (198) in mean field approximation:

$$S_i^{-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} S_j^{\sigma} = \left\langle S_i^{-\sigma} S_j^{\sigma} \right\rangle c_{i\sigma}^{\dagger} c_{j\sigma} + \left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle S_i^{-\sigma} S_j^{\sigma} - \left\langle S_i^{-\sigma} S_j^{\sigma} \right\rangle \left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle , \quad (200)$$

$$\sum_{\sigma\tau} S_i^{\sigma} S_i^{-\sigma} S_j^{\tau} S_j^{-\tau} = 4 \left[\sum_{\sigma} \left\langle S_i^{-\sigma} S_j^{\sigma} \right\rangle S_i^{\sigma} S_j^{-\sigma} - \sum_{\sigma} \left\langle S_i^{-\sigma} S_j^{\sigma} \right\rangle \left\langle S_i^{\sigma} S_j^{-\sigma} \right\rangle \right] . \quad (201)$$

Substituting into Eq. (197) and reordering yields:

$$H_{t-J} \;=\; t \sum_{i\langle j\rangle\sigma} \left\langle S_i^{-\sigma} S_j^{\sigma} \right\rangle c_{i\sigma}^{\dagger} c_{j\sigma} + J \sum_{i\langle j\rangle} S_i^{z} S_j^{z}$$

$$+\frac{J}{2}\sum_{i\langle j\rangle\sigma}\left[1+\frac{2t}{J}\left\langle c^{\dagger}_{i\sigma}c_{j\sigma}\right\rangle-\left\langle S^{-\sigma}_{i}S^{\sigma}_{j}\right\rangle\right]S^{-\sigma}_{i}S^{\sigma}_{j}$$

$$-\frac{J}{2}\sum_{i\langle j\rangle\sigma}\left\langle S^{-\sigma}_{i}S^{\sigma}_{j}\right\rangle\left\langle S^{\sigma}_{i}S^{-\sigma}_{j}\right\rangle-t\sum_{i\langle j\rangle\sigma}\left\langle c^{\dagger}_{i\sigma}c_{j\sigma}\right\rangle\left\langle S^{-\sigma}_{i}S^{\sigma}_{j}\right\rangle\,. \quad (202)$$

It is evident that the hopping is renormalized by the spin deviations and, at the same time, the transverse exchange is renormalized by the hopping.

To make things more quantitative, let us introduce the spin deviation operators for the local moments on the two magnetic sublattices as we did for the Kondo–Heisenberg case, by Eq. (152). Following Ref. [16], let us define spin independent Cu^{2+} hole operators h_l on the two sublattices as follows:

$$h^{\dagger}_{i}=c_{i\uparrow}\,,\qquad h_{i}=c^{\dagger}_{i\uparrow}\,,\qquad h^{\dagger}_{j}=c_{j\downarrow}\,,\qquad h_{j}=c^{\dagger}_{j\downarrow}\,. \quad (203)$$

Actually, the hole operators have a hidden spin label, which depends on the sublattice (up or down) to whose sites (i or j) they refer. One can also think of them as describing not the Cu^{2+} holes , but the doped ones composing the spinless Zhang–Rice singlet. Indeed, creating (destroying) a hole on either sublattice eliminates (restores) the local moment, reproducing the effect of the doped holes.

To express the projected operators in terms of hole operators we shall now introduce two approximations. The first one is that the projected operators for the majority- spin particles on each sublattice will be identified with the non- projected ones: $p^{(\dagger)}_{i\uparrow}\Longrightarrow c^{(\dagger)}_{i\uparrow}$ and $p^{(\dagger)}_{j\downarrow}\Longrightarrow c^{(\dagger)}_{j\downarrow}$. This amounts to neglecting the itineracy-limiting effect that minority-spin particles, supposedly very scarce because the AF order with almost saturated moments is assumed, have on the majority- spin ones. The second approximation is that, in the projected operators for the minority-spin particles, the spin deviation operators are represented in the Holstein–Primakoff approximation, namely:

$$p^{\dagger}_{i\downarrow}=S^{-}_{i}c^{\dagger}_{i\uparrow}\Longrightarrow b^{\dagger}_{i}h_{i}\,,\quad p_{i\downarrow}=c_{i\uparrow}S^{+}_{i}\Longrightarrow b_{i}h^{\dagger}_{i}\,,\quad p^{\dagger}_{j\uparrow}\Longrightarrow b^{\dagger}_{j}h_{j}\,,\quad p_{j\uparrow}\Longrightarrow h^{\dagger}_{j}b_{j}\,. \quad (204)$$

Before substituting the projected operators through the relations just obtained, we have to make sure that we are not violating the no-double-occupancy constraint inherent to the t–J model. To that aim, we write $\langle n_{l\uparrow}n_{l\downarrow}\rangle=0$ by using the identity $n_{l\downarrow}=n_{l\uparrow}-2S^{z}_{l}=n_{l\uparrow}-1+2b^{\dagger}_{l}b_{l}$ from which it follows:

$$n_{l\uparrow}n_{l\downarrow}=n^{2}_{l\uparrow}-n_{l\uparrow}+2n_{l\uparrow}b^{\dagger}_{l}b_{l}=2n_{l\uparrow}b^{\dagger}_{l}b_{l}=2\left(1-h^{\dagger}_{l}h_{l}\right)b^{\dagger}_{l}b_{l}=2h_{l}h^{\dagger}_{l}b^{\dagger}_{l}b_{l}\Longrightarrow 0\,. \quad (205)$$

Therefore we shall discard all terms containing the product $h_l h_l^\dagger b_l^\dagger b_l$. The physical meaning is that there can be either a hole or a spin deviation on a site, not both. Now we can rewrite the t–J Hamiltonian in the new representation. The hopping term yields:

$$\sum_{i\langle j\rangle\sigma} t c_{i\sigma}^\dagger \left(1-n_{i-\sigma}\right) c_{j\sigma} \left(1-n_{j-\sigma}\right) \Longrightarrow \sum_{i\langle j\rangle} t \left(h_i h_j^\dagger + h_j h_i^\dagger\right)\left(b_i^\dagger + b_j\right) \quad (206)$$

expressing the possibilty of hopping conditioned to the presence of a spin deviation on either i or j sites. The longitudinal part of the Heisenberg term , by expressing $\nu_{i\uparrow} = n_{i\uparrow}\left(1-n_{i\downarrow}\right) = n_{i\uparrow}\left(1-2S_i^z\right)$ *etc.* so that $\nu_i = 2S_i^z\left(1-2h_i^\dagger h_i\right)$ and $\nu_j = -2S_j^z\left(1-2h_j^\dagger h_j\right)$ and taking into account the condition of Eq. (205), becomes

$$\begin{aligned} S_i^z S_j^z - \frac{\nu_i\nu_j}{4} \;=\; & -\frac{1}{2}\left[1-h_i^\dagger h_i - h_j^\dagger h_j + 2h_i^\dagger h_i h_j^\dagger h_j\right] \\ & + b_i^\dagger b_i\left(1-h_j^\dagger h_j\right) + b_j^\dagger b_j\left(1-h_i^\dagger h_i\right) - 2b_j^\dagger b_j b_i^\dagger b_i \,. \quad (207) \end{aligned}$$

The last term is the interaction of spin deviations, and will be discarded. Let us consider the purely fermionic part of the expression above, where we treat the four-operator term in mean field, obtaining, with the definition of the hole concentration $\Delta = \left\langle h_l^\dagger h_l\right\rangle$ for $l = i$ or j:

$$\begin{aligned} & -\frac{1}{2}\sum_{i\langle j\rangle}\left[1-h_i^\dagger h_i - h_j^\dagger h_j + 2h_i^\dagger h_i h_j^\dagger h_j\right] \\ & \Longrightarrow -\frac{Nz}{2}\left[1-2\Delta^2\right] + z\left(1-2\Delta\right)\sum_l h_l^\dagger h_l \,. \quad (208) \end{aligned}$$

The last term is analogous to the "polaron shift" we met when dealing with phonon polarons. The terms $b_j^\dagger b_j\left(1-h_i^\dagger h_i\right)$ create a spin deviation on j provided no hole resides on j. Each site j over which the moment has been reversed is a bridge to its $z-1$ neighbours, distinct from i, but belonging to the same sublattice as i. On the whole such terms create a "ferromagnetic drop" of $z+1$ sites, freely accessible to the doped hole residing on i.

The tranverse part is simple:

$$\begin{aligned} & \frac{1}{2}\sum_{i\langle j\rangle,\sigma=\pm} S_i^\sigma S_j^{-\sigma} = \frac{1}{2}\sum_{i\langle j\rangle}\left(b_i b_j + b_i^\dagger b_j^\dagger\right) \\ & \Longrightarrow \frac{1}{2}\sum_{i\langle j\rangle}\left(1-h_i^\dagger h_i\right)\left(b_i b_j + b_i^\dagger b_j^\dagger\right)\left(1-h_j^\dagger h_j\right) \,. \quad (209) \end{aligned}$$

In the last expression the factors $\left(1-h^{\dagger}_{i(j)}h_{i(j)}\right)\approx 1-\Delta$ enforce the condition that both i and j have to be free of holes to allow for a spin deviation on both sites. The resulting approximated Hamiltonian in the real space reads ($l=i$ or j):

$$H = t\sum_{i\langle j\rangle}\left(h_ih^{\dagger}_j+h_jh^{\dagger}_i\right)\left(b^{\dagger}_i+b_j\right)-\frac{JNz}{4}\left[1-2\Delta^2\right]+z\frac{J}{2}\left(1-2\Delta\right)\sum_l h^{\dagger}_lh_l$$
$$+\frac{J}{2}\left(1-\Delta\right)\sum_l b^{\dagger}_lb_l+\frac{J}{4}\left(1-\Delta\right)^2\sum_{i\langle j\rangle}\left(b_ib_j+b^{\dagger}_ib^{\dagger}_j\right). \tag{210}$$

Let us Fourier transform to the reciprocal space, taking care that, due to the assumed AF ordering, we have to limit the wavevectors summations to the reduced Brillouin zone, *i.e.* $b^{\dagger}_l=(2/N)^{1/2}\sum_q{}' b^{\dagger}_q\mathrm{e}^{-iqR_l}$. The final result, by defining $\delta=|\boldsymbol{R}_i-\boldsymbol{R}_j|$ is the Spin Polaron Hamiltonian H^{SP}

$$H^{\mathrm{SP}}=-\left(\frac{NzJ}{4}\right)\left[1-2\Delta^2\right]+\frac{zJ}{2}\left(1-2\Delta\right)\sum_k h^{\dagger}_kh_k$$
$$-\sqrt{\frac{2}{N}}\left(2zt\right)\sum_{kq}\cos\left[(k-q)\delta\right]\left[b^{\dagger}_qh^{\dagger}_{k-q}h_k+h^{\dagger}_kh_{k-q}b_q\right]$$
$$+zJ\left(1-\Delta\right)\sum_q b^{\dagger}_qb_q+\frac{zJ}{4}\left(1-\Delta\right)^2\sum_q\cos(q\delta)\left(b^{\dagger}_qb^{\dagger}_{-q}+b_qb_{-q}\right). \tag{211}$$

The last line of H^{SP} is the by now familiar Hamiltonian for spin waves in an antiferromagnet, which can be diagonalized by transforming from $b^{(\dagger)}_q$ to $\beta^{(\dagger)}_q$as in Eq. (155), only now with the doping-dependent diagonalization condition $\tanh\left(2\vartheta_q\right)=-\left(1-\Delta\right)\cos(q\delta)/2$ yielding

$$\sum_q\left\{zJ\left(1-\Delta\right)\sqrt{1-\left[\left(1-\Delta\right)\frac{\cos(q\delta)}{2}\right]^2}\right\}\left(\beta^{\dagger}_q\beta_q+\frac{1}{2}\right)-2NzJ\left(1-\Delta\right). \tag{212}$$

The renormalized frequency

$$\hbar\Omega_q=zJ\left(1-\Delta\right)\sqrt{1-\left[\left(1-\Delta\right)\frac{\cos(q\delta)}{2}\right]^2} \tag{213}$$

is the product of the bare frequency $zJ\left(1-\Delta\right)$ and the softening factor $\sqrt{1-\left[\left(1-\Delta\right)\cos(q\delta)/2\right]^2}$ in close analogy with the discussion following Eq. (75) for the squeezed phonon case.

Finally we can rewrite $H^{\rm SP}$ in terms of the diagonalized AF spin wave operators $\beta_q^\dagger, \beta_q$ as follows:

$$H^{\rm SP} = -zJ\,(1-2\Delta)\sum_k h_k^\dagger h_k - \sqrt{\frac{2}{N}}\,(2zt)\sum_{kq}\left[h_{k-q}^\dagger h_k\left(\beta_q^\dagger \mathcal{B}_{k,q} + \beta_{-q}\mathcal{C}_{k,q}\right)\right] + \sum_q \hbar\Omega_q\left(\beta_q^\dagger\beta_q + \frac{1}{2}\right) - \frac{N}{2}zJ\,(1-\Delta) - \left(\frac{NzJ}{4}\right)\left[1-2\Delta^2\right]\ , \quad (214)$$

where we define:

$$\begin{aligned}\mathcal{B}_{k,q} &= \cos\left[(k-q)\delta\right]\cosh\left(\vartheta_q\right) + \cos(k\delta)\sinh\left(\vartheta_q\right)\ ,\\ \mathcal{C}_{k,q} &= \cos\left[(k-q)\delta\right]\sinh\left(\vartheta_q\right) + \cos(k\delta)\cosh\left(\vartheta_q\right)\ .\end{aligned} \quad (215)$$

The effective Hamiltonian we have obtained is roughly similar to the one for interacting electrons and phonons, leading to the phonon polarons. Indeed, $H^{\rm SP}$ features a sort of "Holstein term" coupling linearly spin waves and hole density, in addition to the "polaronic shift" already mentioned. However, there is one important difference, that is the absence of a hole hopping term. The coefficient of the first term in Eq. (214), which should do the job, has no dispersion, so that it does not describe the hopping of the holes. To see that the holes dressed by spin waves can nevertheless hop around as coherent quasi-particles, one has , for instance, to evaluate the Green's function. This has been done by several people, and we refer the reader to the bibliography [17] for details. Let us, however, mention that a general result [18] is that the the spin polaron exists over a wide range of parameters as a coherent itinerant particle, whose bandwidth W_{SP} goes as $W_{SP} \approx (t/J)\exp\left[-\left(\kappa t/J\right)^2\right]$ where κ is a known constant. The bandwidth vanishes both for $t/J \to 0$ and for $t/J \to \infty$. The first case has an obvious meaning. In the opposite limit, realised by a "soft" magnetic structure, the polaron uses all its energy to excite spin waves, and gets trapped in a kind of "magnetic quicksand".

We leave as an exercise for the patient reader to verify if it is possible to transform Eq. (214) into an effective fermion-only Hamiltonian, as we did for the phonon polaron problem.

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Appendix A

To prove Eq. (76) we follow [20]. Let us rewrite it, by dropping the state label q, as:

$$\exp\left[-2\alpha u\frac{d}{du}\right]F(u) = F(\mathrm{e}^{-2\alpha}u)\,. \tag{A.1}$$

By expanding both, the exponential

$$\exp\left[-2\alpha u\frac{d}{du}\right] = \sum_m \frac{(-2\alpha)^m}{m!}\left(u\frac{d}{du}\right)^m\,, \tag{A.2}$$

and $F(u) = \sum_n \frac{u^n}{n!}F^{(n)}(0)$ with $F^{(n)}(0) = |d^nF(u)/du^n|_0$, yields:

$$\exp\left[-2\alpha u\frac{d}{du}\right]F(u) = \sum_{m,n}\frac{(-2\alpha)^m}{m!}\left(\frac{1}{n!}\right)\left(u\frac{d}{du}\right)^m\left[u^nF^{(n)}(0)\right]\,. \tag{A.3}$$

Now, for any m one has $\left(u\frac{d}{du}\right)^m\left[u^nF^{(n)}(0)\right] = n^mu^nF^{(n)}(0)$ so that:

$$\begin{aligned}\exp\left[-2\alpha u\frac{d}{du}\right]F(u) &= \sum_{m,n}\frac{(-2\alpha)^m}{m!n!}n^mu^nF^{(n)}(0)\\ &= \sum_n\frac{1}{n!}\left[\sum_m\frac{(-2\alpha n)^m}{m!}\right]u^nF^{(n)}(0) = \sum_n\frac{1}{n!}\left[\mathrm{e}^{-2\alpha n}\right]u^nF^{(n)}(0)\\ &= \sum_n\frac{(u\mathrm{e}^{-2\alpha})^n}{n!}F^{(n)}(0) = F\left(u\mathrm{e}^{-2\alpha}\right)\,.\end{aligned} \tag{A.4}$$

which proves Eq. (A.1).

Note added in proofs. After the conclusion of the School, a very interesting paper [19] has been published, in which an analytical solution of the problem of the spin polaron in the $t-J$ model, obtained through displacement transformations, is proposed.

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