Two Aspects of Electron-Phonon Interaction

Bayo Lau

I. INTRODUCTION

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The interaction between electron and lattice vibration is an interesting and on-going research topic in condensed matter physics. To the lowest-order in the lattice displacement (see Appendix), the general Hamiltonian is

$$H_{ep} = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{kq} M_q c_k^\dagger c_{k-q}(b_{-q}^\dagger + b_q) \tag{1}$$

This report discusses two aspects of the study of electron-phonon interaction. First, a general diagrammatic expansion is discussed, followed by a brief discussion of the solution in metallic system. Second, the single polaron problem is discussed analytically and numerically.

II. THE DIAGRAMS OF ELECTRON-PHONON COUPLING

A general form of Dyson's equation is derived for electron-phonon interaction[1]. In general, equation (1) is capable of modeling a N-electron system. The derivation can be done with and external phonon source $J_{-q}\phi_q$ to equation (1) [2].

$$\phi_q = b_{-q}^\dagger + b_q \tag{2}$$

$$H_{ep} = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q b_q^\dagger b_q + \sum_{kq} M_q c_k^\dagger c_{k-q}\phi_q + \sum_q J_{-q}\phi_q \tag{3}$$

$$G(k,t;k',t') = -i\langle T\{c_k(t)c_{k'}^\dagger(t')\}\rangle \tag{4}$$

$$D(q,t;q',t') = \frac{\delta\langle\phi_q(t)\rangle}{\delta J_{q'}(t')} = -i\left(\langle T\{\phi_q(t)\phi_{q'}^\dagger(t')\}\rangle - \langle\phi_q(t)\rangle\langle\phi_{q'}^\dagger(t')\rangle\right) \tag{5}$$

A differential equation for $G(k,t;k',t')$ can be obtained from the equation of motion of the electron annihilation operator.

$$\left[i\frac{\partial}{\partial t} - \epsilon_k\right]G(k,t;k',t') + i\sum_q M(q)\langle T\phi_q(t)c_{k-q}(t)c_{k'}^\dagger(t')\rangle = \delta_{kk'}\delta(t-t') \tag{6}$$

Due to the presence of the external source J, the expectation value of the time-ordered triple product can be rewritten as

$$\begin{aligned}
-i\langle T\phi_q(t)c_{k-q}(t)c_{k'}^\dagger(t')\rangle &= \frac{\delta\langle Tc_{k-q}(t)c_{k'}^\dagger(t'))\rangle}{\delta J_{-q}(t'')} - i\langle\phi_q(t'')\rangle\langle Tc_{k-q}(t)c_{k'}^\dagger(t'))\rangle \\
&= \frac{\delta G(k,t;k',t')}{\delta J_{-q}(t'')} - i\langle\phi_q(t'')\rangle G(k,t;k',t')
\end{aligned} \tag{7}$$

Using the functional analogs of quotient rule and chain rule as well as equation (5), the first term of the right-hand-side can be expressed as, $\frac{\delta G^{-1}()}{\delta\langle\phi\rangle}D()$. The differential equation can then be written as

$$\begin{aligned}
&\left[i\frac{\partial}{\partial t} - \epsilon_k\right]G(k,t;k',t') - \sum_q M(q)\langle\phi_q(t)\rangle G(k-q,t;k',t') \\
&+i\sum_q M(q)G(k-q,t;k_1,t_1)\frac{\delta G^{-1}(k_1,t_1;k_2,t_2)}{\delta\langle\phi(q_3,t_3)\rangle}G(k_2,t_2;k',t')D(q_3,t_3,-q,t)
\end{aligned} = \delta_{k,k'}\delta(t-t') \tag{8}$$

Next, a "free" electron Green's function is defined implicitly along with the self-energy, which includes the vertex function Γ.

$$G_0^{-1}(k,t;k_2,t_2) = \left[\left[i\frac{\partial}{\partial t} - \epsilon_k\right]\delta_{k_2,k} - M(k-k_2)\langle\phi_{k-k_2}(t)\rangle\right]\delta(t_2-t) \tag{9}$$

$$\Sigma(k,t,k2,t2) = i\int dt_1 dt_3 \sum_{q,k_1,q_3} M(q)M(q_3)G(k-q,t,k_1,t_1)\Gamma(k_1,t_1,k_2,t_2,q_3,t_3)D(q_3,t_3;-q,t) \tag{10}$$

$$\Gamma(k_1,t_1,k_2,t_2,q_3,t_3) = -\frac{1}{M(q_3)}\frac{\delta G^{-1}(k_1,t_1;k_2,t_2)}{\delta\langle\phi(q_3,t_3)\rangle} \tag{11}$$

The result is a Dyson's equation for the electron Green's function. The same procedure can be applied to the phonon's green's function. After fourier transform and taking care of momentum conservation, the result is

$$G(k) = G_0(k) + G_0(k)\Sigma(k)G(k) \tag{12}$$
$$D(q) = D_0(q) + D_0(q)\Pi(q)D(q) \tag{13}$$

The self-energies can be expressed in terms of the vertex function Γ, resulting in the following diagrams.

$$\Sigma(k) = i\int \frac{dq^4}{(2\pi)^3}|M(q)|^2 G(k+q)\Gamma(k,q)D(q) \tag{14}$$

$$\Pi(q) = -i2|M(q)|^2\int \frac{dk^4}{(2\pi)^3}G(k+q)G(k)\Gamma(k,q) \tag{15}$$

$$\tag{16}$$

The term $M(0)\langle\phi_0(t)\rangle$ in the implicit definition of G_0 leads to a subtle difference between G_0 and the bare electron propagator. $\langle\phi_0(t)\rangle$ can be calculated in the interactive picture.

$$\langle\phi_0(t)\rangle = -i\frac{\sum_{n=0}^{\infty}\frac{1}{n!}(-\frac{i}{\hbar})^n\int dt_1\ldots\int dt_n\langle\phi_0|T\{\hat{V}_I(t_1)\ldots\hat{V}_I(t_n)\phi_{0I}(t)\}|\phi_0\rangle}{\sum_{n=0}^{\infty}\frac{1}{n!}(-\frac{i}{\hbar})^n\int dt_1\ldots\int dt_n\langle\phi_0|T\{\hat{V}_I(t_1)\ldots\hat{V}_I(t_n)\}|\phi_0\rangle} \tag{17}$$

$$\hat{V}_I(t) = \sum_{kq} M_q c_k^\dagger c_{k-q}\phi_q \tag{18}$$

The evaluation of the series is the same as the evaluation of Green's function. The non-zero terms in the sum are those with even number of ϕ_0, which means only the odd terms contribute. $\langle\phi_0(\omega=0)\rangle$ can be expressed as a diagrammatic series. For each odd order n, there are $\frac{n+1}{2}$ phonon lines and n bare electron lines

$$\tag{19}$$

From equation(9), the "free" greens function satisfies the Dyson's Equation

$$\tag{20}$$

which reduces to the bare electron Green's function when $M(0) = 0$.

Despite the apparent simplicity of the self-energy equations, the vertex function is implicitly defined by the electron Green's function (equation (11)), which is an infinite series of diagrams itself. The vertex function is an infinite series diagrams. Under the ladder approximation, which essentially neglects the variation of the phonon field with respect to the external source, the vertex can be expressed as a recursion

$$\Gamma(k,q) = 1 + i \int \frac{d^4 p}{(2\pi)^4} |M(k-p)|^2 G(p+q)\Gamma(p,q)G(p)D(k-p) \tag{21}$$

The ladder approximation is not the focus of the report, the reader is referred to papers such as [1] for the details. Noting that the G and D are merely the sum of different diagrams, so to the lowest order in G_0 and D_0, $\Gamma(k,q)$ can be written as

$$\tag{22}$$

Note that the outer lines are just "connection points", not actual propagators; therefore either dressed or undressed propagators can be connected to the simplified vertex.

A. Migdal's Treatment of the Metals

The Migdal's theorem greatly simplifies the diagrammatic evaluation of Green's function in a special class of system [3]. A metallic metal with a large number of electrons coupled to acoustic phonons (see Chapter 26 in [4]).

$$H_{metal} = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{q<q_D} \omega_D q b_q^\dagger b_q + \sum_{k,q<q_D} g_q c_{k+q}^\dagger c_q (b_{-q}^\dagger + b_q) \tag{23}$$

where q_D and $\omega_D(q)$ is the Debye wave vector and (linear) dispersion, respectively, and

$$g_q^2 = \lambda \frac{\omega_D(q)}{k_f} \tag{24}$$

with λ a scaling constant and k_f the fermi wave vector of the electrons. Atomic unit is used here. Migdal argued that the vertex diagrams for metals (equation (23)) can be approximated to a good degree by unity.

The second diagram in equation (22) can be written as

$$\begin{aligned}
\Gamma_1(k,q) &= i \int \frac{d^3 p}{(2\pi)^3} \int \frac{de}{2\pi} g_{k-p}^2 D_0(k-p, E-e) G_0(p+\tfrac{q}{2}, e+\tfrac{\omega}{2}) G_0(p-\tfrac{q}{2}, e-\tfrac{\omega}{2}) \\
&= i \frac{2\lambda}{k_f} \int \frac{d^3 p}{(2\pi)^3} \int \frac{de}{2\pi} \frac{\omega_D^2(k-p)}{(E-e)^2 - \omega_D^2(k-p)} G_0(p+\tfrac{q}{2}, e+\tfrac{\omega}{2}) G_0(p-\tfrac{q}{2}, e-\tfrac{\omega}{2})
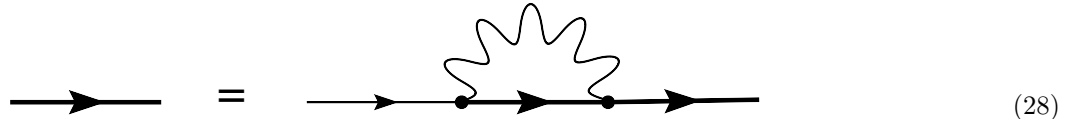\end{aligned} \tag{25}$$

Migdal argued that the fraction in the integrand can be treated as a "hat" function. Please refer to the left vertex of the second term in equation (22) in the following discussion. In normal metal, the important electronic behavior happens near the Fermi surface. The dominant scattering process is the ones with the in-coming electron has $E \sim E_f$ and $|E_f - e|$ small, in the scale of the Debye frequency. One way to understand Migdal's argument is to consider a system that has very steep electron energy dispersion $\epsilon(k)$ and a very flat phonon dispersion $\omega_D(k-p)$. By conservation of momentum and energy, a change in the integration variable e would require a small change of electron momentum because of energy dispersion. That very same change of momentum would also change $\omega_D(k-p)$, but not as drastically because of the difference in dispersion. In a normal metal, the Debye frequency is orders of magnitude smaller than the Fermi energy, and it becomes obvious that $(E_f - e)^2$ crosses over $\omega_D(k-p)$ extremely fast as one changes e due to the steep electronic dispersion at E_f. Because the fraction drops off as the inverse of the fast changing $(E_f - e)^2$, Migdal treated the fraction as -1 and introduced a characteristic frequency, ω_0 as the bound of integration over e.

$$\Gamma_1(k,q) \sim -i \frac{2\lambda}{k_f} \int \frac{d^3 p}{(2\pi)^3} \int_{E-\frac{\omega_0}{2}}^{E+\frac{\omega_0}{2}} \frac{de}{2\pi} G_0(p+\frac{q}{2}, e+\frac{\omega}{2}) G_0(p-\frac{q}{2}, e-\frac{\omega}{2}) \tag{26}$$

The e integral would yield a factor of ω_0 because $E \sim E_f \gg \omega_0$. Migdal set out to get an upper bound of the remaining 3D convolution integral, and the result turns out to be

$$\max(|\Gamma_1(k,q)|) \sim \frac{\lambda}{\sqrt{M}} \tag{27}$$

Because of the recursive nature of the vertex, the higher order terms are even smaller. That is, when the system has steep electronic dispersion, flat phonon dispersion, and large fermi wave-vector, the phonon propagator can be treated as a "hat" function, and the vertex can also be treated as unity with an error of order $\frac{1}{\sqrt{M}}$ for the usual coupling constant $\lambda \sim 1$. From this result, Migdal treated $\Gamma \sim 1$ and performed direct integration on equation 13 and showed that the phonon Green's function D(q) can be roughly treated as $D_0(q)$ when the Debye frequency is close to the true phonon frequency. The combined result is the electron's green's function can be treated accurately by the self-consistent born approximation

$$\tag{28}$$

III. SINGLE POLARON

Let's look at electron-phonon interaction in a system that contrasts the aforementioned metallic system. Instead of having a N free electron coupling to acoustic phonon in a 3D metal, we now discuss the property of a single electron coupling to a branch of optical phonon, negligible Umklapp process, and localized (tight-binding) electronic behavior in 1D[5].

$$H_t = -t \sum_{<ij>} c_i^\dagger c_j + c_j^\dagger c_i + \sum_q \omega_q b_q^\dagger b_q + \sum_{jq} e^{iq \cdot R_j} M_q c_j^\dagger c_j (b_{-q}^\dagger + b_q) \tag{29}$$

Holstein [6] extended the tight-binding method and proposed an investigation of molecular-crystal. It was argued that the ions do not have long-range effect on the localized electronic orbits such that V_{ea} can be approximated by a linear function. The result is that the gradient in equation (62), and hence M_q becomes just a constant. Lastly, if we consider a system in which electrons are coupled most strongly to optical phonons, the phonon frequency can be taken as a constant. The above arguments lead to the Holstein Hamiltonian in real and reciprocal space. M_q and ω_q becomes $\frac{-g}{\sqrt{N}}$ and ω_0 in equation (29), respectively.

$$H_h = -t \sum_{<ij>} c_i^\dagger c_j + c_j^\dagger c_i + \omega_0 \sum_i b_i^\dagger b_i - g \sum_i c_i^\dagger c_i (b_i^\dagger + b_i) \tag{30}$$

$$H_h = -t \sum_{\mathbf{k}} E(\mathbf{k}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \omega_0 \sum_q b_q^\dagger b_q - \frac{g}{\sqrt{N}} \sum_{\mathbf{k},q} c_{\mathbf{k}+q}^\dagger c_{\mathbf{k}} (b_{-q}^\dagger + b_q) \tag{31}$$

The Hamiltonian commutes with the total momentum operator $K = k + \sum q$, and its eigenstates can be characterized by this quantum number.

The polaron problem has not yet been solved exactly, but insights can be gained from different solution methods in different parts of the parameter space. It is obvious that when the coupling constant is small, the solution will resemble the usual tight-binding wave function with a cosine-energy dispersion. As the constant increases, the negative sign of the Hamiltonian would lead to phonon-dressing of the electron wave function. The phonon-dressing is best described by perturbing the strong-coupling solution. When the hopping term in equation (29) is small, it can be treated as perturbation (V) to the last two terms (H_0), which are merely harmonic oscillators with shifted equilibrium points ($x \sim b^\dagger + b$). The most elegant way to proceed is the transformation

$$\begin{aligned} \overline{H}_t &= e^S H_t e^{-S} \\ &= H_t + [S, H_t] + \frac{1}{2!}[S, [S, H_t]] + ... \\ &= \overline{H}_{t0} + \overline{V}_t \end{aligned} \tag{32}$$

Such transformation has the properties

$$\overline{\prod \hat{O}_i} = \prod \overline{\hat{O}_i} \tag{33}$$

$$S^\dagger = -S \tag{34}$$

The transformation

$$
\begin{aligned}
S &= \sum_{jq} \frac{e^{iq \cdot R_j} M_q}{\omega_q} c_j^\dagger c_j (b_{-q}^\dagger - b_q) \\
\overline{b}_q &= b_q - \sum_j e^{-iq \cdot R_j} \frac{M_{-q}}{\omega_{-q}} c_j^\dagger c_j \\
\overline{c}_i &= c_i X_i
\end{aligned}
\tag{35}
$$

gives

$$X_j = \exp[-\sum_q \frac{e^{iq \cdot R_j} M_q}{\omega_q}(b_{-q}^\dagger - b_q)] = (X_j^\dagger)^{-1} \tag{36}$$

$$\overline{H}_{t0} = \sum_q \omega_q b_q^\dagger b_q - \sum_{ijq} e^{iq \cdot (R_i - R_j)} \frac{M_q^2}{\omega_q} c_i^\dagger c_i c_j^\dagger c_j \tag{37}$$

$$\overline{V} = -t \sum_{<ij>} c_i^\dagger c_j X_i^\dagger X_j + c_j^\dagger c_i X_j^\dagger X_i \tag{38}$$

A. The Holstein Model in the Strong Coupling Limit

In the Holstein model, the above three operators are greatly simplified because $\frac{M_q}{\omega_q} = \frac{-g}{\omega_0 \sqrt{N}}$ allows simplification by Fourier summation.

$$S = -\frac{g}{\omega_0} \sum_i c_i^\dagger c_i (b_i^\dagger - b_i) \tag{39}$$

$$X_i = \exp[\frac{g}{\omega_0}(b_i^\dagger - b_i)] \tag{40}$$

$$\overline{H}_{h0} = \omega_0 \sum_i b_i^\dagger b_i - \frac{g^2}{\omega_0} \sum_i c_i^\dagger c_i \tag{41}$$

$$\overline{V} = -t \sum_{<ij>} c_i^\dagger c_j X_i^\dagger X_j + c_j^\dagger c_i X_j^\dagger X_i \tag{42}$$

$\overline{H}_{h0}$ is obviously diagonal, and there are N degenerate unperturbed single-electron ground states

$$\overline{|GS, i\rangle}_0 = c_i^\dagger |0\rangle \quad ; \quad i\epsilon\{1...N\} \tag{43}$$

These ground states can be projected into the original basis by considering the inverse transform

$$H_{h0} = e^{-S} \overline{H}_{h0} e^S \tag{44}$$

That is, the ground state in the original basis satisfy the equation

$$c_i^\dagger |0\rangle = e^S |GS, i\rangle_0 \tag{45}$$

The solution can be obtained by using fermionic algebra and the Baker-Hausdorft identity.

$$
\begin{aligned}
|GS, i\rangle_0 &= e^{-S} c_i^\dagger |0\rangle \\
&= e^{\frac{g}{\omega_0}(b_i^\dagger - b_i)} c_i^\dagger |0\rangle \\
&= e^{\frac{g}{\omega_0} b_i^\dagger} e^{-\frac{g}{\omega_0} b_i} e^{-\frac{1}{2}\frac{g^2}{\omega_0^2}} c_i^\dagger |0\rangle \\
&= e^{-\frac{1}{2}\frac{g^2}{\omega_0^2}} e^{\frac{g}{\omega_0} b_i^\dagger} c_i^\dagger |0\rangle
\end{aligned}
\tag{46}
$$

The N unperturbed ground states each have one electron and a phonon coherent state located at site i. A coherent state $|z\rangle = e^{-\frac{1}{2}|z|^2} e^{zb_i^\dagger}|0\rangle$ is an eigenstate of the annihilation operator b_i with complex eigenvalue z. The real part of z is proportional to $\langle \mathbf{Q}_i \rangle$, and the imaginary part is proportional to $\langle \mathbf{P}_i \rangle$. A coherent state has the property of $\triangle Q_i \triangle P_i = \frac{\hbar}{2}$. Therefore, the ground state has $z = \frac{g}{\omega_0}$ unperturbed ground state in the real space can be interpreted as an electron dressed by a phonon cloud with zero average momentum. The phonon statistic is found to be a Poisson distribution.

$$N_{p0} = {}_0\langle GS, i|b_i^\dagger b_i|GS, i\rangle_0 = \frac{g^2}{\omega_0^2} \tag{47}$$

$$P_0(n) = |\langle n|c_i|GS, i\rangle_0|^2 = e^{-N_{p0}} \frac{1}{n!}(N_{p0})^n \tag{48}$$

To go one step further, there are N^2 first excited state of two kinds: N of $|1, i, i\rangle_0$ with one electron, and one phonon at the same site and $N(N-1)$ of $|1, i, j\rangle_0$ with one electron and one phonon at different site. The transformation to real space is the same as equation (46). The mechanic is to commute the extra creation operator through e^{-S}, and the operator e^{-b_i} would introduce an extra if the phonon and electron are on the same site. This leads to a simple correction to the ground state.

$$|1, i, i\rangle_0 = (b_i^\dagger - \frac{g}{\omega_0})|GS, i\rangle \tag{49}$$

$$|1, i, j\rangle_0 = b_j^\dagger|GS, i\rangle \tag{50}$$

$|1, i, j\rangle_0$ is $|G, i\rangle_0$ plus a free [9] phonon at site j, and $|1, i, j\rangle_0$ is the superposition of $|GS, i\rangle_0$ and $|GS, i\rangle_0$ plus a free phonon at site i. The phonon statistic is a correction to the ground state. The mean of the Poisson distribution remains as N_{p0} but there is a scaling as a function of the number of phonons, n. For the one-off-site-phonon states, the probability of finding n-1 phonons in the phonon cloud at site i is needed. For the on-site phonon states, the probability for finding n phonons at site i is needed.

$$P_{1ii}(n) = |\langle n_i = n|c_i|1, i, i\rangle_0|^2 = \frac{P_0(n_i)}{N_{p0}}(n - N_{p0})^2 \tag{51}$$

$$P_{1ij}(n) = |\langle n_i = n-1|b_j c_i|1, i, j\rangle_0|^2 = P_0(n-1) \tag{52}$$

This procedure can be generalized to the mth-excited state with n-phonons. The N^m can be categorized into n+1 groups by the number of on-site phonons, $n_{os}\epsilon\{0...m\}$. The result of each n_{os} is

$$|m, i, n_{os}\rangle_0 = \left(\prod_{(m-n_{os})offsite} b_j^\dagger\right) \sum_{l=0}^{n_{os}} \frac{(-1)^l}{l!} \left(\frac{g}{\omega_0}\right)^l \frac{\sqrt{n_{os}!}}{(n_{os}-l)!} b_i^{\dagger(n_{os}-l)}|GS, i\rangle \tag{53}$$

$$P_{m,i,n_{os}}(n) = P_0(n-(m-n_{os}))\frac{n_{os}!}{(N_{p0})^{n_{os}}} \left(\sum_{l=\max\{0,m-n\}}^{n_{os}} \frac{(-N_{p0})^l}{l!} \frac{(n-m+n_{os})!}{(n-m+l)!(n_{os}-l)!}\right)^2 \tag{54}$$

The polynomial in $P_{m,i,n_{os}}(n)$ has a maximum of $m = \max\{n_{os}\}$ zeros in n for all possible $\frac{g}{\omega_0}$.

The perturbation $\overline{V}$ in equation (42) introduces off-diagonal matrix elements between the eigenstates of $\overline{H}_{h0}$ in equation (41). In addition to the usual nearest-site hopping, the operator $X_j^\dagger X_i$ couples states of adjacent site with different number of phonons. To get a better feel of the solution, the influence of $\overline{V}$ can be thought of two types of coupling: one couples the states with the same phonon configuration around the electron, and one couples the states with different phonon configuration. Incidentally, the operation of $c_i X_i$ on a state is basically the same as the transformation to real space in equation (46).

The N degenerate ground states are coupled to one another by the first type of coupling.

$$_0\langle \overline{GS, i}|\overline{V}|\overline{GS, j}\rangle_0 = -te^{-\frac{g^2}{\omega^2}}(\delta_{j=i+1} + \delta_{j=i-1}) \tag{55}$$

Therefore, the N ground state actually forms a tight-binding band with exponentially suppressed bandwidth. The N degenerate on-site first excited state are also coupled by the matrix element

$$_0\langle \overline{GS, i}|\overline{V}|\overline{GS, j}\rangle_0 = -t\left(\frac{g}{\omega}\right)^2 e^{-\frac{g^2}{\omega^2}}(\delta_{j=i+1} + \delta_{j=i-1}) \tag{56}$$

and the bandwidth is a factor of $\left(\frac{g}{\omega}\right)^2$ greater than that of the ground state, but note that it is exponentially suppressed by the same factor. The other N(N-1) excited states forms N-1 bands, distinguished by the phonon's location relative to the electron site, with the same coupling constant as the ground state. These bands are further coupled with each other by the second type of coupling. The overall result is most easily illustrated by the numerical method discussed in the next subsection.

B.   The Holstein Model in the Intermediate Regime

The evolution of the system from the strong coupling regime to the weak coupling regime is commonly called the crossover regime. The transition from the strong coupling basis into the tight-binding electron basis is most easily illustrated by the numerical result of a matrix digitalization method by Bonca, et.al. [7]. Electron-phonon interaction is numerically challenging because of the phonon space is essentially infinite in dimension, and a clever choice of discretization is required to get accurate result using finite computing resource. To deal with the crossover regime, neither the tight-binding electron plus phonons nor the above coherent state-like basis is a good, it has to be some sort of hybrid. Bonca's numerical basis consists of Bloch waves of different phonon configuration in real space.

$$|S, K\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iKj} c_j^\dagger \prod_{m\epsilon\{S\}} \frac{b_{j+m}^{n_m}}{\sqrt{n_m}} |0\rangle \tag{57}$$

where K is the total momentum, which we know is a good quantum number of the system, and the set S denotes a certain combination of (m, n_m), which determine the phonon configuration around the electron. The matrix elements in the $|S, K\rangle$ basis can be computed using the equation (30).

There are only three types of matrix elements. First, there are $-te^{iK}$ elements between the states whose phonon configurations are the same except for a one-unit-cell translation about the electron site. Second, there are $-g\sqrt{n_{os}}$ elements between the states whose number of on-site phonons differ by one (nos results from the creation/annihlation operator). Lastly, the diagonal elements are just the total number of phonons times the constant phonon frequency $\omega_0 \sum_{m\epsilon\{S\}} n_m$. This formulation divides the problem into one matrix per crystal momentum K leading to the eigenvalue problem of

$$\begin{aligned} H_h|\psi\rangle &= E_{S,K}|\psi\rangle \\ H_h \sum_S \alpha_{S,K}|S, K\rangle &= E_{S,K} \sum_S \alpha_{S,K}|S, K\rangle \\ \hat{H}_h\overline{\alpha}_{S,K} &= E_{S,K}\overline{\alpha}_{S,K} \end{aligned} \tag{58}$$

The matrices are sparse because there are only 2 types of off-diagonal matrix elements coupling each $|S, K\rangle$ to three other states. Arnoldi-type iterative numerical methods can be employed to calculate the low energy eigen-pairs of sparse matrices [8]. To take advantage of the Arnoldi method and our $|S, K\rangle$ formulation, A variational space is constructed starting from $|S_0, K\rangle$, a state with no phonons. Equation (30) is used to couple $|S_0, K\rangle$ to $|S_1, K\rangle$, a state with one on-site phonon with a matrix element $-g$. $|S_1, K\rangle$ would in turn couples with three states by the matrix elements $-g\sqrt{2}$, $-te^{iK}$, and $-te^{-iK}$. The process is repeated until a cut-off has been reach. Bonca suggested that the best way of cut-off in the cross-over region is to define a parameter N_f. According to his rule, a state $|S_i, K\rangle$ is included only if the sum of its number of phonons $(\sum_{m\epsilon S_i} n_m)$ and its maximum difference in m's are smaller or equal to N_f. Calculation is then performed for increasing N_f until the desired quantity, such as eigenvalue or eigenvector, has converged.

The numerical result for K=0 in the 1D model is presented here. The computation parameters are $(t, \omega_0, g) = (2, 1, g)$. It is common practice to define a dimensionless parameter $\alpha = \frac{g^2}{\omega_0}\frac{1}{t}$, which is the ratio of phonon-dressing energy (equation (41)) to the hopping energy of the electron.

Figure 1 shows the energy difference between the first excited state and ground state, minus the phonon energy. When α is small, the first excited state energy is above the ground state energy plus a phonon energy. This shows that the first excited state contain least one free phonon. When α is large, The first excited state falls below that threshold, meaning that the excitation contains some phonons, but not a free one.

The nature of the states is revealed when one calculates the phonon statistics and compare with those calculated in the last subsection. Figure 2 shows the probability of finding certain number of phonon in the ground state, as a function of α. The statistic in the figure is the same as equation (48). This suggests that at K=0, the ground state of the system remains the same over all values of α. Figure 3 shows the same type of phonon statistic for the first excited state. The trench structure in the large α limit obeys the form in equation (51), and the single-peak structure in the small α limit obeys equation (52). The locality of the states in the numerical result have also been verified to be consistent with that of the two equations. At $\alpha_c \sim 1.6$, the first-excited state has a cross-over behavior. α_c also
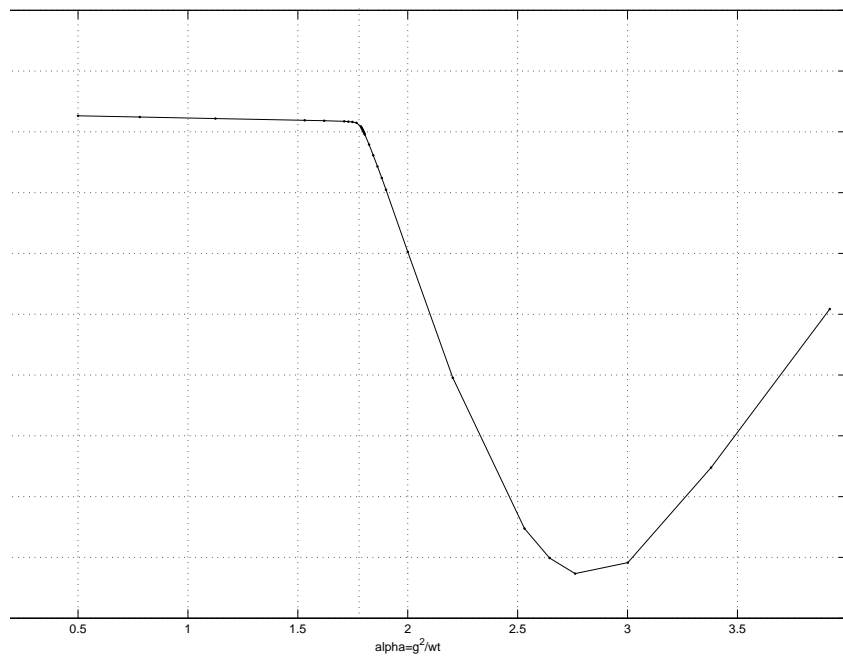
FIG. 1: The energy difference between the first excited state and the ground state, minus the phonon energy ω_0.
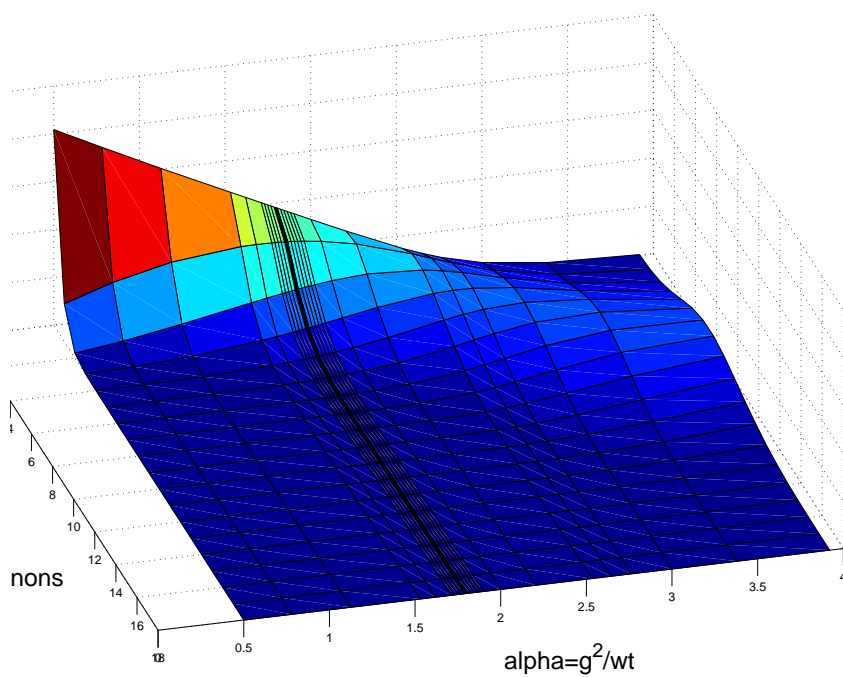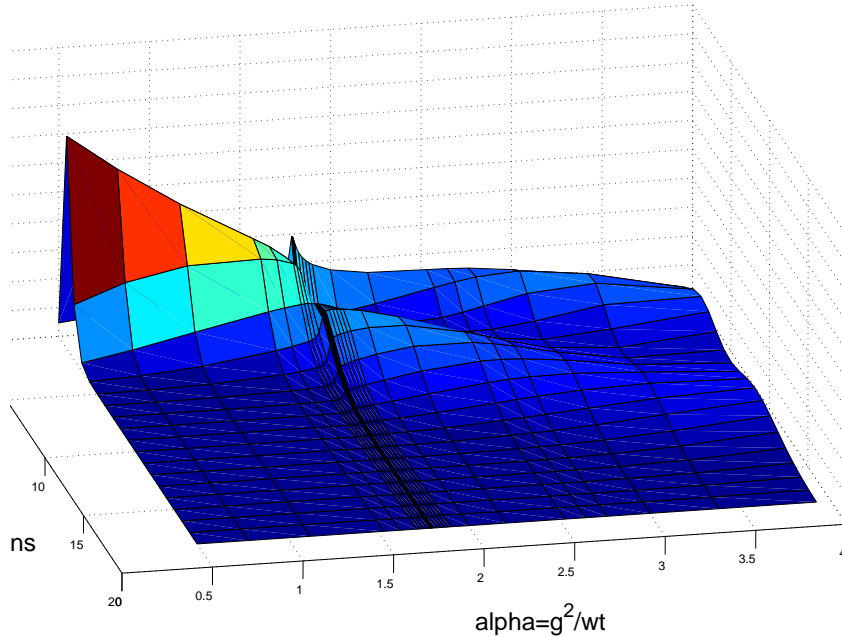

FIG. 2: The phonon statistic of the ground state.

FIG. 3: The phonon statistic of the ground state.

correspond to the energy cross over point in figure 1. For $\alpha < \alpha_c$, the first excited state is the ground state plus a free-phonon described by equation (50). For $\alpha > \alpha_c$, the first excited state is a super position of that and the ground state (equation (49)).

IV. CONCLUSION

Two aspects of the study of electron-phonon has been discussed. A general form of diagrammatic have been derived for electron-phonon interaction. For an idealized metallic system, the self-consistent Born approximation can be used to solve for the Green's function. The single Holstein polaron problem has also been discussed in 1D. It has been shown by a combination of strong-coupling perturbation and numerical solution that the ground state are dressed by a coherent state of phonons, and that the first excited state has a cross-over behavior involving two states as the coupling constant is increased.

Appendix

The usual starting point of the study of electron-phonon coupling is the Hamiltonian

$$
\begin{aligned}
H &= H_e + H_a + H_{ep} \\
H_e &= \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j} \frac{1}{r_{ij}} \\
H_a &= \sum_j \frac{\mathbf{P}_j^2}{2M} + \sum_j V_a(R_j) \\
H_{ea} &= \sum_{ij} V_{ea}(\mathbf{r}_i - R_j)
\end{aligned}
\tag{59}
$$

H_e and H_a model the electron-only and lattice-only part of the energetic, and H_{ea} is the sum of the potential contributed by all electron-atom pairs. Following the Born-Oppenheimer approximation, electrons are treated as fast moving objects and the atoms are assumed to vibrate slightly around their equilibrium positions. The Hamiltonian can be expanded in terms of small oscillations

$$
\mathbf{Q}_j = R_j - R_j^0
\tag{60}
$$

$$V_a(R_j) = V_a(R_j^0) + \frac{K}{2}\mathbf{Q}_j^2 + O(\mathbf{Q}_j^4) \tag{61}$$

$$V_{ea}(\mathbf{r}_i - R_j) = V_{ea}(\mathbf{r}_i - R_j^0) - \mathbf{Q}_j \cdot \nabla V_{ea}(\mathbf{r}_i - R_j^0) + O(\mathbf{Q}_j^2) \tag{62}$$

$V_a(R_j^0)$ is just a constant, and $V_{ea}(\mathbf{r}_i - R_j^0)$ contributes a periodic potential to each electron under a periodic lattice. By defining the operator

$$
\begin{aligned}
a_j &= \sqrt{\tfrac{m\omega}{2\hbar}}(\mathbf{Q}_j + \tfrac{i}{m\omega}\mathbf{P}_j) \\
\omega^2 &= \tfrac{K}{m}
\end{aligned}
\tag{63}
$$

as well as neglecting the indicated high-order terms and an overall constant, the Hamiltonian can be simplified to

$$
\begin{aligned}
H &= H_e + H_p + H_{ep} \\
H_e &= \sum_i \frac{\mathbf{p}_i^2}{2m} + V_{periodic}(\mathbf{r}_i) + \frac{e^2}{2}\sum_{i\neq j}\frac{1}{r_{ij}} \\
H_p &= \sum_{q\lambda}\omega_{q\lambda}(b_{q\lambda}^\dagger b_{q\lambda} + \tfrac{1}{2}) \\
H_{ep} &= \frac{1}{\sqrt{V}}\sum_{q\mathbf{G}\lambda}M_{q+\mathbf{G},\lambda}\rho(q+\mathbf{G})(b_{q\lambda} + b_{-q,\lambda}^\dagger)
\end{aligned}
\tag{64}
$$

Here, the $\mathbf{G}$'s are the reciprocal lattice vectors, the q's are the momenta in the first Brillouin zone, and the λ's are the phonon branch indices. ρ is the electron density in reciprocal space and

$$M_{q+\mathbf{G},\lambda} = (q+\mathbf{G})\cdot\xi_{q\lambda}\sqrt{\frac{\hbar}{2MN\omega_{q\lambda}}}V_{ea}(q+\mathbf{G}) \tag{65}$$

is proportional to the fourier component of V_{ea} as well as the dot-product between the momentum and the phonon branch eigenvector.

The Hamiltonian is still formidable to solve because of the electron-electron interaction as well as the frequency dependence of $M_{q+\mathbf{G},\lambda}$. Study of electron-phonon interaction usually starts with the exclusion of electron-electron interaction as well as a simplified version of $M_{q+\mathbf{G},\lambda}$.

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