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POLARONS BY TRANSLATIONALLY INVARIANT DIAGRAMMATIC PERTURBATION THEORY

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Dedicated to the memory of Professor Vladimir Šips

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The structure of the translationally-invariant diagrammatic perturbation theory for one polaron is examined on the 1D discrete lattice described by the Holstein Hamiltonian. The latter is characterized by the electron hopping t, the phonon frequency ω_0 and the electron-phonon coupling g. It is shown that the polaron localization (and translation) properties are contained in the electron propagator of one electron, intermittently added to the lattice, and/or in the phonon correlation function with one electron permanently present in the lattice. The order by order analysis in g/ω_0 shows that the expansion of the irreducible electron self-energy corresponds to the expansion of the phonon correlation function, rather than of the irreducible phonon self-energy. The range of polaronic correlations is determined in this way. For small t/ω_0 and already to the second order g/ω_0 small, the electron-lattice correlation becomes very short ranged, i.e. the polaron is already localized to one site, although the overall translational symmetry remains unbroken. For large t/ω_0, the second order result is meaningful up to large $g/\omega_0 \approx (t/\omega_0)^{\frac{1}{4}}$, where it becomes degenerate with the results for the large adiabatic Holstein polaron. This suggests that the translationally invariant perturbation theory crosses then over smoothly, without symmetry breaking, into the adiabatic, continuous quantum limit, as rigorously demonstrated in the companion paper. Thus the quantum theory of the large adiabatic Holstein polaron provides a simple, instructive example of the quantum crossover which replaces the behavior in the quantum critical point.

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1. Introduction

Ever since Landau proposed [1] that an electron set into the deformable lattice can form a self-localized ground state called a polaron [2], the question of whether this state can be reached by the translationally invariant perturbation theory, when the latter is summed up to the infinite order in the electron-phonon coupling, has been pending [3−6]. Actually, it is sometimes stated that this is not possible, especially on the discrete lattice [3,4], because the self-localized state breaks the translational symmetry of the unperturbed ground state. The question is of quite general importance, in particular because there are many analogous problems in which one particle is interacting with a large number of bosons and/or fermions [7−12] on the lattice.

There are several versions of the perturbation theory: Schrödinger, Wigner, diagrammatic, among which the last [13] is usually considered as the most effective in calculating the physically relevant correlation functions. It is usually believed that the most convenient one is to be chosen according to the particularity of the polaron problem, and the diagrammatic approach was seldom used [14, 15] in this context. However, it has been realized that the electron self-energy describing one electron intermittently added to the system (the referent number of electrons $N = 0$) contains some properties of the polaron, its translational properties in particular. Here it will be emphasized that it contains also the polaron localization length. The identification of this length is carried out by considering the $N = 1$ phonon correlation function, which is the appropriate counterpart of the $N = 0$ electron propagator.

However, the evaluation of the $N = 0$ electron propagator requires only the knowledge of the $N = 0$ (i.e. of the bare) phonon correlation function. In other words, the development of the local polaronic correlation in the electron propagator, as well as the translation of the polaronic composite, are both associated with the bare phonon correlations, rather then with correlation related to the phonon softening. As will be discussed in detail here, this makes the $N = 0$ electron self-energy the quantity which is most convenient in considering the symmetry-breaking issue by the translationally-invariant diagrammatic perturbation theory.

In addition to this discussion, the lowest-order translationally invariant diagrammatic theory is shown, under appropriate conditions, to lead to the very short-range polaronic, electron-lattice correlations, which are known in one dimension (1D) to evolve smoothly into the Lang–Firsov theory [16] of the small nonadiabatic polaron. This is consistent with the idea that there is no symmetry breaking “phase” transition as a function of the coupling strength. The Landau self-localizing, symmetry breaking argument [1] refers however to the adiabatic regime, which is beyond the reach of the translationally invariant low-order perturbation theory. The discussion of the adiabatic polaron, either large or small, critical for the symmetry-breaking issue, requires thus the analysis of perturbation summation to all orders in the coupling strength.

This discussion will be carried out in the companion paper [17] for the large adiabatic polaron on the 1D lattice. It will be shown there that under appropriate conditions the weak coupling nonadiabatic regime crosses over smoothly, on increasing the coupling strength, into the adiabatic limit of the large polaron. As indicated here and proven in the companion paper, the absence of the symmetry-breaking phase transition at zero temperature is due to quantum fluctuations of the lattice (adiabatically followed by the electron), disregarded in the Landau self-localizing argument, which treats the lattice classically. Actually, the system crosses over between two regimes, reachable either by the translationally invariant perturbation theory from the high symmetry side, or by the Goldstone symmetry-restoring approach [18] from the broken symmetry side. Since there is no symmetry breaking involved in the crossover from the large to the small 1D adiabatic polaron, the results of the companion paper amount in fact to the proof that the translationally invariant perturbation theory on the 1D lattice can describe the polaronic correlations for an arbitrary value of the coupling constant.

2. *General*

The Hamiltonian chosen here to illustrate the points announced in Introduction is the Holstein Hamiltonian on the discrete 1D lattice of L sites (for simplicity L is taken even and $\hbar = 1$) [19]

$$\hat{H} = \sum_{r=-L/2}^{L/2-1} \left[-t\, c_r^\dagger\, (c_{r+1} + c_{r-1}) + \omega_0\, b_r^\dagger b_r - g\, c_r^\dagger c_r\, (b_r^\dagger + b_r) \right], \tag{1}$$

where the fermion and boson operators c_r and b_r are defined in the usual way. Equation (1) describes N electrons subject to hopping t along the chain and to the interaction g with local displacements of the lattice $u_r = x_0(b_r^\dagger + b_r)$. In the absence of interaction, the latter behave as the harmonic oscillators with frequency ω_0 and zero-point displacement x_0. This changes when g is turned on, except for the homogeneous displacement $u = x_0 \sum_r (b_r^\dagger + b_r)$, which continues to behave [20] as a free ω_0 oscillation, but around the equilibrium value

$$u_0 = x_0 \sum_r (b_r^\dagger + b_r) = 2\frac{gN}{\omega_0} x_0\,, \tag{2}$$

N being 0 and 1 in the present paper.

The translationally invariant diagrammatic theory starts from the electron propagators

$$G_0^{(0)}(k,\omega) = \frac{1}{\omega - \xi_k + \mathrm{i}\eta}\,, \tag{3}$$

or

$$G_0^{(1)}(k,\omega) = \frac{\delta_{k,0}}{\omega + \xi_k - \mathrm{i}\eta} + \frac{1-\delta_{k,0}}{\omega - \xi_k + \mathrm{i}\eta}\,, \tag{4}$$

at $N = 0, 1$, respectively. Equation (3) describes an extended electron of energy ξ_k added into the $N = 0$ system during a given lapse of time. On the other hand, the two terms in Eq. (4) correspond respectively to the intermittent suppression of the $N = 1$ electron in the $k = 0$ state and to the intermittent creation of an electron in the k state, in addition to the $N = 1$ electron of the same spin occupying the $k = 0$ state. Only the second term in Eq. (4) is thus the expression of the Pauli principle. To simplify the presentation, the zero of the electron energy ξ_k in Eqs. (3) and (4) is, unlike in Eq. (1), taken to be at $k = 0$, i.e.

$$\xi_k = 2t\,(1 - \cos k)\,, \qquad k = \frac{2\pi}{L} m\,, \tag{5}$$

assuming Born-von Kármán boundary conditions for k.

The free harmonic oscillators are described by the usual displacement-displacement correlation function

$$D_0(q,\omega) = \frac{1}{2}\left[\frac{1}{\omega - \omega_0 + \mathrm{i}\eta} - \frac{1}{\omega + \omega_0 - \mathrm{i}\eta}\right], \tag{6}$$

which describes the propagation in time of one boson added into the free lattice subject to the zero point x_0 oscillations. The Holstein assumption of the locality of g and D_0 is not of essential importance for what follows below, as long as the forces are of sufficiently short range [21].

3. Electron propagation at $N = 0$

The second- and fourth-order diagrams for G are shown in Fig. 1, in the usual diagrammatic presentation. The arrows on the electron propagator are taken to represent the $\pm \mathrm{i}\eta$ parts of the G_0 propagator, and, in accordance with Eq. (3), at $N = 0$ they are always pointing to the right: the electron is advancing in time from its creation to its annihilation, never accompanied by the electron-hole pair because no hole can appear at $N = 0$. It should be noted that when $N = 0$, the Cooper particle-particle pairings in higher orders of Fig. 1 are also eliminated.

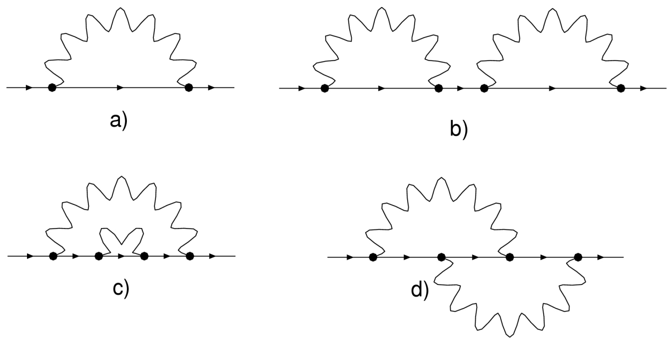

Fig. 1. The second and fourth order diagrams for $G^{(0)}$. The full and wavy lines stand for the electron propagator $G_0^{(0)}$ and the phonon correlation function D_0, as described in the text. The dot denotes the interaction g.

In the next step, the diagrams which, according to the Lehmann representation of $G^{(0)}$ [13], give the leading contributions to the ground-state energy of the system, are selected. These are the (a) and (b) diagrams in Fig. 1, and, before the quartic diagrams (c) and (d), the "reducible" diagrams of the type (b) to all orders in g. In terms of the Dyson equation, this means that the expansion of the irreducible self-energy $\Sigma^{(0)}$ in $G^{-1} = G_0^{-1} - \Sigma$ in terms of g corresponds to the analogous expansion of the ground and excited state energy.

It may seem that the Dyson reduction to the irreducible electron self-energy $\Sigma^{(0)}$ is a self-evident step. That this is not so is shown in Sec. 4, where just the opposite is true for $D^{(1)}$: at $N = 1$, it is $D^{(1)}$, rather than the irreducible phonon self-energy $\Pi^{(1)}$, which has to be expanded in g in order to be consistent with the expansion of the irreducible $\Sigma^{(0)}$. The properties of $\Sigma^{(0)}$ are thus relevant when the order-by-order analysis in g is carried out, in the present paper to the second order in g, and to infinite order in the companion paper. By arguing that in 1D $\Sigma^{(0)}$, which corresponds to the ground state energy, is a regular function of g for any finite g it will be shown [17] that there is no symmetry-breaking phase transition in the 1D polaron problem.

The electron self-energy $\Sigma^{(0)}$ can be easily calculated to the second order in g using the usual diagrammatic rules [13], slightly adapted to the Holstein Hamiltonian on the discrete lattice,

$$\Sigma_2^{(0)}(\varepsilon) = -\frac{g^2}{4\pi t} I(\varepsilon)\,,$$

with

$$I(\varepsilon) = \frac{2\pi}{L} \sum_{m=-L/2}^{L/2-1} \frac{1}{\varepsilon + 2\sin^2(\frac{\pi m}{L})}\,, \tag{7}$$

where $\varepsilon = (\omega_0 - \omega + \mathrm{i}\eta)/2t$ and the number of lattice sites L is kept finite. Separating out the $m = -L/2, 0$ ($q = -\pi, 0$) terms in Eq. (7), $I(\varepsilon)$ can be found in the closed form

$$I(\varepsilon) = \frac{2\pi}{L}\left[\frac{1}{\varepsilon} + \frac{1}{\varepsilon+2} + \frac{2}{\operatorname{sh} x}\,\left(\frac{L}{2}\operatorname{cth}(Lx/2) - \operatorname{cth}(x)\right)\right], \tag{8}$$

where $\varepsilon = \operatorname{sh}(x)\operatorname{th}(x/2)$. $I(\varepsilon)$ of Eq. (8) (i.e. $\Sigma_2^{(0)}$) has three interesting asymptotic regimes. Two occur for $L^2\varepsilon \gg 1$, when $Lx \gg 1$. Equation (8) then gives

$$I(\varepsilon) \approx \frac{2\pi}{\sqrt{\varepsilon(\varepsilon+2)}}. \tag{9}$$

This equation has two qualitatively different limits,

$$1 < \varepsilon: \qquad I(\varepsilon) \approx \frac{2\pi}{\varepsilon}, \tag{10}$$

$$\frac{1}{L^2} < \varepsilon < 1: \qquad I(\varepsilon) \approx \pi\sqrt{\frac{2}{\varepsilon}}. \tag{11}$$

The third important limit corresponds to $\varepsilon \ll 1$, such that not only $x \ll 1$ but also $Lx \approx L\sqrt{\varepsilon} < 1$. Equation (8) then gives

$$\varepsilon < \frac{1}{L^2}: \qquad I(\varepsilon) \approx \frac{2\pi}{L\varepsilon}, \tag{12}$$

i.e. the value (10) divided by L.

It is worthwhile to note that the result (9) can also be obtained from Eq. (7) directly by turning the sum over m for large L into the integral over q, while keeping the full ξ_q electron dispersion (5) in the integral. This amounts to retaining the discreteness of the lattice, and in particular the Umklapp contribution to $\Sigma_2^{(0)}$ of Eq. (7), in the case that the lattice becomes infinitely long. However, the discreteness in Eq. (9) is important in the limit (10), but not in (11). Indeed, this latter result can be obtained from Eq. (7) not only but turning the sum at large L into the integral, but also by taking the continuous approximation in the electron dispersion (5), $\xi_q \sim q^2$. Finally, the result (12) is manifestly a finite-size effect.

The physical meaning of Eqs. (10)–(12) is best understood upon considering the position of poles in G. In the general case, $\Sigma = \Sigma(k,\omega)$, this position is given by

$$\omega = \xi_k + \Sigma_R(k,\omega)\,, \tag{13}$$

where Σ_R is the real part of the irreducible electron self-energy Σ. The lowest $k = 0$ pole is sitting at $-\Delta = \Sigma_R(0, -\Delta)$. According to the Lehmann representation of $G^{(0)}$, Δ is equal to the shift of the ground state energy of the $N = 1$ system, produced by switching g on,

$$\Delta = E_0(0) - E_0(g)\,, \tag{14}$$

remembering that the $E_0(0)$'s at $N = 0$ and $N = 1$ are chosen (by $\xi_{k=0} = 0$) to coincide.

In the lowest-order perturbation theory $\Delta \ll \omega_0$. ε_Δ in $\Sigma_2^{(0)}$ of Eqs. (7) and (8) can thus be set equal to the adiabatic parameter $\alpha = \omega_0/2t$, $\varepsilon_\Delta \approx \alpha$, i.e. the behavior of Δ is governed by $I(\alpha)$. The limits (10), (11) and (12) correspond then, respectively, to

$$1 < \alpha: \qquad \Delta \approx \frac{g^2}{\omega_0}\,, \tag{15}$$

$$\frac{1}{L^2} < \alpha < 1: \qquad \Delta \approx \frac{g^2}{\omega_0}\alpha^{\frac{1}{2}}\,, \tag{16}$$

$$\alpha < \frac{1}{L^2}: \qquad \Delta \approx \frac{g^2}{\omega_0 L}\,. \tag{17}$$

It is very important to realize now that, although the theory started from the translationally invariant states and is only of the second order in g, the condensation energy (14) is equal in Eq. (15) to ε_p, the electron localization energy to one site. In Eq. (16), it can be interpreted as the localization energy to the large number of sites, $\alpha^{-\frac{1}{2}}$, but which can not be larger than L in Eq. (17). This can be made explicit through the identification

$$\Delta = \frac{g^2}{\omega_0 L_d} , \tag{18}$$

where L_d is the number of sites involved. However, rather than being associated with symmetry breaking, those results correspond to the establishment of the local correlations in the system over L_d sites. The question of local correlations will be taken up again in the next section and for this purpose it is convenient to express L_d as

$$L_d = 2\pi\alpha^{-1} I^{-1}(\alpha) , \tag{19}$$

using Eqs. (7), (13) and (18), with the limits (10), (11) and (12) for $I(\alpha)$.

Turning now to the time scales, it should first be noted that the extreme limits (15) and (17) for Δ and L_d correspond to the adiabatic values of Δ, i.e., such Δ are independent of the lattice mass M involved in ω_0. However, for all intermediate values of α in Eq. (19), the low-order ground state energy (14) contains essentially nonadiabatic time/space electron-lattice correlations. This is particularly true for small values of the adiabatic parameter $1 \gg \alpha \gg 1/L^2$. $\alpha \ll 1$ is thus a necessary but not a sufficient condition for adiabaticity. For g/ω_0 sufficiently small, when $\Sigma^{(0)} \approx \Sigma_2^{(0)}$, it ensures however, the applicability of the continuous approximation.

A similar reasoning can be applied to the excited, finite k states. Expanding $\Sigma_2^{(0)}(\omega)$ of Eq. (7) linearly in ω, and solving Eq. (13) with the g^2/ω_0^2 accuracy, leads to

$$\tilde{\xi}_k = -\Delta + (1 - \frac{\Delta}{\omega_0})\xi_k , \tag{20}$$

for the polaron spectrum $\tilde{\xi}_k$.

For $\alpha > 1$, this procedure is valid for any k because the bandwidth in Eq. (20) is smaller than ω_0. In the extreme limit $\alpha \gg 1$, when $L_d = 1$ and $\Delta = \varepsilon_p$, Eq. (20) reduces to the well known Lang–Firsov result [16,20,22,23], expanded in g^2/ω_0^2 small. It is noteworthy that the energy shift $\Delta = \varepsilon_p$ of the $k = 0$ state is then exact to all orders in g/ω_0. This result is in contrast to Eq. (20), which corresponds [20] to the leading term of the Lang–Firsov exponential law [22].

For $\alpha < 1$ it is essential to take into account the full dependence of $\Sigma_2^{(0)}(\omega)$ on ω in the vicinity of k_c given by $\xi_{k_c} = \omega_0$. This leads to the electron-phonon anticrossing at $k = k_c$ and to the polaron dispersion $\tilde{\xi}_k$ which approaches ω_0 from below.

Such result is apparently equivalent to the result of the conventional Wigner perturbation theory, in contrast to the results (18) and (19), for the $k = 0$ ground state, which, by using $\Sigma_2^{(0)}(\omega)$ at $\omega = 0$, amount [14] to the corresponding Schödinger perturbation theory. The expansion of $\Sigma_2^{(0)}$ linearly in ω is applicable only for $k \ll k_c$. It defines the effective mass for the motion of the polaronic correlations

$$M_p^{-1} \approx 2t(1 - \frac{\Delta}{\omega_0}) ,$$

with Δ given by Eq. (16). This result differs [20] from the Migdal adiabatic result, meaning only that the low-order perturbation theory is nonadiabatic for g/ω_0 and α small, rather than that it fails as believed in Ref. [20]. The expectation [20] that the theory has to become adiabatic at α small is shown here to be fulfilled either by assuming α extremely small at g/ω_0 small, making the finite size effects important, Eq. (17), or, as will be argued below, by taking g/ω_0 sufficiently large at α small.

Three questions can be further raised in connection with the discussion in this section. The first concerns when the Schödinger perturbation theory, which in its lowest order involves one phonon corresponding to the single-loop approximation for the irreducible electron self-energy at $\omega = 0$, $\Sigma_2^{(0)}(\omega = 0)$, can be expected to give accurate results. The second question is related to how well justified the identification of the L_d with the range of correlations is. This is because Eq.(18) defines L_d only indirectly, through the energy scale Δ. Consideration of the above effects leads us to the examination of the phonon correlation function $D^{(1)}$, and to the third question. The latter considers the nature of the weak coupling expansion for $D^{(1)}$ which is consistent with the expansion for $E_0(g)$. In the next section, these three questions will be answered in the appropriate order.

4. *Phonon Green function at $N = 1$*

In considering the phonon Green function, the $N = 1$ situation with one reference electron present is of relevance because the processes involved in the build up of $D^{(1)}$ conserve the number of electrons N (in contrast to the case of the electron $N \pm 1$ propagator $G^{(0,1)}$). Therefore, the physics contained in $G^{(0)}$ corresponds to that in $D^{(1)}$. While the determination of $E_0(g)$ to the leading order in g requires the summation of the Dyson series for $G^{(0)}$, and the use of the irreducible electron self-energy $\Sigma^{(0)}$ to the leading order in g, the determination of the average number $\bar{n}_{ph}$ of phonons requires through

$$\bar{n}_{ph} = \sum_q \bar{n}_q \, , \tag{21}$$

and (valid to the leading order in g)

$$2\,\bar{n}_q + \frac{1}{2} \approx \frac{1}{2\pi} \int \mathrm{Im}\{D_q^{(1)}(\omega)\} \mathrm{d}\omega \, , \tag{22}$$

the expansion of $D^{(1)}$ in Eq. (22) to the leading order in g,

$$D_q^{(1)}(\omega) = D_0 + \delta D^{(1)} \approx D_0(q,\omega) + D_0^2(q,\omega)\Pi_2^{(1)}(q,\omega)\,. \tag{23}$$

In contrast to that, the Dyson summation with $\Pi_2^{(1)}$ leads, as is easily seen, to the finite size correction to $D_q^{(1)}$ at small q and ω, which contributes to the integral in Eq. (22) not only the term retained in Eq. (23), but also the terms beyond the leading order in g.

$\Pi_2^{(1)}$ in Eq. (23) consists of two terms shown in Fig. 2. The arrows in Fig. 2 stand for the $\pm \mathrm{i}\eta$ parts of the $N = 1$ electron propagator $G_0^{(1)}$, given by Eq. (4). The disconnected diagram Fig. 2(a) [13] contributes to $\Pi_2^{(1)}$ only the imaginary $\omega = 0$, $q = 0$ term $\Pi_2^{(1a)} = -2\,\mathrm{i}\,\pi g^2 \delta(\omega)\delta_{q,0}/L$, where the energy and momentum conservation rules in the interaction vertices are exhibited explicitly, in order to make Eq. (23) consistent with Eqs. (21) and (22). As discussed below, this term is related to the squared static, homogeneous average displacement u_0^2.

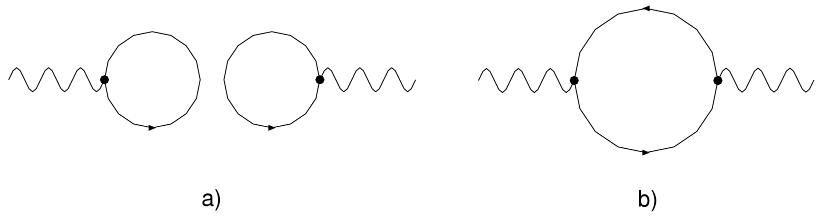

Fig. 2. The second order diagrams for D. Notation as in Fig. 1.

The bubble diagram of Fig. 2(b) can be easily calculated as

$$\Pi_2^{(1b)}(q,\omega) = \frac{g^2}{L}\left(\frac{1}{\omega - \xi_q + 2\mathrm{i}\eta} - \frac{1}{\omega + \xi_q - 2\mathrm{i}\eta}\right) \tag{24}$$

at $q \neq 0$, because the creation of the electron-hole pair requires a finite q. Inserted in Eq. (23), such $\Pi_2^{(1b)}$ leads to $D_q^{(1)}$ with two branches, at $\omega = \omega_0$ and at $\omega = \xi_q$. The spectral weight $\mathrm{Im}\{D_q^{(1)}\}$ of the low-frequency branch $\omega = \xi_q$ is proportional to g^2. This spectral weight contributes in particular to $\bar{n}_q$ of Eq. (21). D_0 of Eq. (23) gives no contribution. The contribution to $\bar{n}_q$ that comes from the product $D_0^2\Pi_2^{(1b)}$ arises when the one and two poles, respectively, are on the opposite sides of the real ω axis. This leads to $\bar{n}_q$ being proportional to

$$(\omega_0 + \xi_q)^{-2} + \omega_0^{-1}(\omega_0 + \xi_q)^{-1}.$$

$\bar{n}_{ph}$ of Eq. (21) can thus be determined in terms of $I(\alpha)$ and $dI(\alpha)/d\alpha$, defined by Eqs. (7) and (8), i.e. in terms of L_d of Eq. (18). This applies also to $D(r-s)$, the Fourier transform of $\bar{n}_q$.

Taking this transform on, including the contribution $\Pi_2^{(1a)}$ of Fig. 2(a) at $q = 0$ and using the notations of Eq. (23), it follows that

$$-\mathrm{i}L\delta D^{(1)}(r-s) = \bar{n}_{ph}\, \mathrm{e}^{-|r-s|/d}\left[1 + |r-s|\,\mathrm{th}\,(1/d)\right], \qquad d \ll L\,. \tag{25}$$

It turns out that the correlation distance d in Eq. (25) is related to L_d of Eqs. (18) and (19) by

$$\frac{1}{2d} = \mathrm{Ar\,cth}\, L_d\,. \tag{26}$$

(Actually, it is technically much easier to derive Eqs. (25) and (26) from the conventional Schrödinger theory [24].) Equation (26) justifies the interpretation of L_d in the ground state energy in terms of the length scale, and gives the precise form of this relation. For $d = 0$ $L_d = 1$ ($\alpha \gg 1$) and for large d ($\alpha \ll 1$, continuous approximation) L_d is, as expected, linear in d.

The existence and the simplicity of Eq. (26) are not surprising when one remembers that $\Sigma^{(0)}$ itself is an electron-lattice correlation function [13]. The remarkable feature of Eqs. (25) and (26) is that they do not exhibit α or g/ω_0 explicitly. As pointed out earlier [24], this is the consequence of the fact that the conventional Schrödinger perturbation theory (to which the approximation $\Sigma_2^{(0)}(\omega) \approx \Sigma_2^{(0)}(0)$ is equivalent) conserves the average displacement $\bar{u}$ equal to u_0 of Eq. (2), order by order in g. To see how this works in the diagrammatic formulation, it is appropriate to take a closer look into Eq. (23) at $q \approx 0$. For a small but finite q, Eq. (24) gives $\Pi_2^{(1b)} \approx -2\mathrm{i}\pi g^2\delta(\omega)/L$, which merges smoothly with the $q = 0$, $\omega = 0$ long-range, long-time order term $\Pi_2^{(1a)}$ of Fig. 2a. At $q = 0$, Eq. (23) amounts [24] to the decomposition

$$\langle u^2\rangle = \langle (u-u_0)^2\rangle + 2\langle (u-u_0)u_0\rangle + u_0^2\,.$$

Here the first term corresponds to the harmonic ω_0 vibration of the homogeneous displacement u around u_0. The second term has to vanish by $\langle u\rangle = u_0$ of Eq. (2) and the third is the signature of the long-range, long-time order [25]. $\langle u\rangle = u_0$ is satisfied on omitting the contribution of $\Pi_2^{(1b)}$ at $q = 0$, which at the same time renders $\bar{n}_q$ continuous around $q = 0$, i.e., the constant depending on g/ω_0, and α is removed from the asymptotic behavior of $D(|r-s|)$ in Eq. (25). In this way d depends on L_d only. (Obviously, such arguments can be generalized beyond the second order perturbation theory.)

This brings up finally the question of the validity of the present weak-coupling approach. The single-loop approximation for the irreducible electron self-energy $\Sigma_2^{(0)}$, corresponding to the conventional second-order one-phonon Schrödinger perturbation theory for $E_0^{(2)}(g)$, is obviously valid when the average number of phonons $\bar{n}_{ph}$ given by Eq. (21) is less than unity. $\bar{n}_{ph}$, appearing also as the normalization factor in Eq. (25), is easily shown to be

$$\bar{n}_{ph} = \frac{g^2}{\omega_0^2}\frac{1+L_d^2}{2L_d^3}\,.$$

at large L. The structure in α of $\bar{n}_{ph}$ is thus given by Eq. (19), and Eq. (9) for $\alpha > 1/L^2$. For $\alpha \gg 1$, the requirement $\bar{n}_{ph} < 1$ becomes thereby $g/\omega_0 < 1$. For $1/L^2 < \alpha < 1$ the requirement turns into

$$\frac{g}{\omega_0} \lesssim \alpha^{-\frac{1}{4}}, \tag{27}$$

or, according to Eq. (16), to $\Delta \lesssim \omega_0$. In other words, the perturbation theory holds in the continuous limit of Eq. (11) up to g/ω_0 much larger than unity. Noteworthy, however, is the fact that, for $g/\omega_0 \approx \alpha^{-\frac{1}{4}}$, the adiabatic coupling constant $\lambda = g^2/2\omega_0 t$ is small ($\lambda \ll 1$). This suggests that the adiabatic weak-coupling limit starts to hold for such (large) values of g/ω_0.

Pursuing this idea further, it is noted that on the line $g/\omega_0 \approx \alpha^{-\frac{1}{4}}$, Eqs. (11), (19) and (26) give $d \approx 1/\lambda$, while Eq. (18) yields $\Delta \approx \lambda^2 t$. Both these results are known to hold for the large, adiabatic, Holstein polaron [19,26]. The ground-state energies of the weak-coupling nonadiabatic polaron and of the large adiabatic Holstein polaron are thus comparable on the line $g/\omega_0 \approx \alpha^{-\frac{1}{4}}$, and it is reasonable to associate this line with the crossover between the two regimes. This becomes even more convincing on noting that the condition (27) was previously derived from the adiabatic side: the nonadiabatic corrections to the local adiabatic dynamics of the Holstein polaron were shown [18,27,28] to become important for $g/\omega_0 \approx \alpha^{-\frac{1}{4}}$.

The standard approach to the adiabatic Holstein polaron starts, however, from the symmetry-broken side, with the translational symmetry restored by the Goldstone mode which corresponds to the polaron translation [18,29]. The rigorous proof that $g/\omega_0 \approx \alpha^{-\frac{1}{4}}$ line is the crossover rather that the phase transition line (line of quantum critical points) thus requires the summation of the series for $E_0(g)$ to all orders in g and the demonstration that $E_0(g)$ (i.e. the corresponding Σ) has no singularity for any finite value of g. This is the program which will be carried out in the companion paper [17], on considering the scaling properties of Σ, as they follow from the translationally-invariant perturbation theory to the infinite order in g.

5. *Final remarks*

One may wonder why the ground-state energy Δ is determined in Sec. 3 from the irreducible $N = 0$ electron self-energy $\Sigma^{(0)}$ rather than from the straightforward [13] diagrammatic $N = 1$ expansion for the energy. In order to answer this question, the latter is shown in Fig. 3 to the second order in g. The electron Green functions in Fig. 3 have to be taken at $N = 1$ and are given by $G_0^{(1)}$ of Eq. (4). The phonon

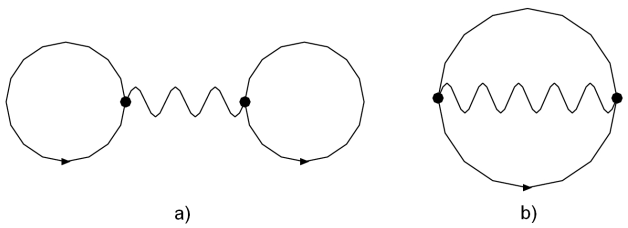

Fig. 3. The second order expansion for the energy. Notations as in Fig. 1.

Green function is obviously corresponding to D_0 of Eq. (6). The first diagram is the "Hartree" diagram related to the time-conserved homogeneous displacement u_0 and the second diagram is usually called the "exchange" diagram.

The intermediate step in evaluating the contribution of Figs. 3(a) and 3(b) is the calculation of the $N = 1$ electron-self energy $\Sigma_2^{(1a)} + \Sigma_2^{(1b)}$, obtained by cutting one-electron line in Figs. 3. The resulting $\Sigma_2^{(1b)}$ is given by Eq. (7) on replacing $I(\varepsilon)$ by

$$I(\varepsilon) - \frac{2\pi}{L}\left(\frac{1}{\varepsilon} + \frac{2t}{\omega + \omega_0}\right).$$

The first term, additional to $I(\varepsilon)$, takes into account the fact that an electron intermittently added into the system cannot occupy the $k = 0$ state that is already occupied by the electron of the same spin. Indeed, this contribution cancels out the first term in Eq. (8) for $I(\varepsilon)$ singular at $\omega = \omega_0$. The second term, singular at $\omega = -\omega_0$, describes the fact that the electron in the $k = 0$ state ($\xi_0 = 0$) can be intermittently turned into the hole at the energy $-\omega_0$ by emitting a phonon of the energy ω_0. This latter process leads to the formation of the resonant band [25] in the Dyson $G^{(1)}$ close above $-\omega_0$, and, concomitantly, to the cancellation around $\omega \approx 0$ of the $N = 1$ Hartree self-energy contribution $\Sigma_2^{(1a)}$ proportional to $2\pi/L\alpha$. However, due to the cancellation of the singularity in $I(\varepsilon)$ at $\omega \approx \omega_0$, there is no additional pole in $G^{(1)}$ close below $+\omega_0$ to the lowest order in g.

Returning to the energy of Fig. 3, it can be seen that the aforementioned additional effects at $\omega \approx -\omega_0, 0$, cancel out between the contributions of Figs. 3(a) and 3(b) to $E_0(g)$, and the result is Δ of Eqs. (18) and (19). Indeed, the latter has nothing to do with Hartree and exchange contributions to the $N = 1$ electron self-energy. However, this result has been obtained herein after cancellations which are already painful in the lowest-order perturbation theory. Such an approach becomes even more so in higher orders. It is therefore more convenient to consider the polaron properties from the $N = 0$ electron self-energy $\Sigma^{(0)}$ given by Fig. 1 than from the $N = 1$ expansion of Fig. 3. This is the course of action that is undertaken in the companion paper [17], which treats the polaron properties to the infinite order in g.

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TRANSLACIJSKI INVARIJANTNA DIJAGRAMSKA TEORIJA SMETNJE ZA POLARONE

Istraživali smo strukturu translacijski invarijantne dijagramske perturbacijske teorije jednog polarona na 1D diskretnoj rešetki opisanoj Holsteinovim hamiltonijanom. Taj je hamiltonijan karakteriziran elektronskim preskokom t, fononskom frekvencijom ω_0, i elektron-fononskim vezanjem g. Pokazali smo da su lokalizacijska (i translacijska) svojstva polarona sadržana u propagatoru jednog elektrona, privremeno dodanog rešetki, i/ili u fononskoj korelacijskoj funkciji s jednim elektronom stalno prisutnim u rešetki. Analiza po potencijama od g/ω_0 pokazuje da razvoj elektronske ireducibilne vlastite energije odgovara razvoju fononske korelacijske funkcije, a ne razvoju fononske ireducibilne vlastite energije. Na taj je način odred ¯en doseg polaronskih korelacija. Za mali t/ω_0, već u drugom redu po g/ω_0 elektron-reetka korelacija postaje vrlo kratkodosena, odnosno polaron je lokaliziran na jedno čvorište rešetke, iako opća translacijska simetrija ostaje sačuvana. Za veliki t/ω_0 rezultat računa u drugom redu ostaje primjenjiv do velikih $g/\omega_0 \approx (t/\omega_0)^{1/4}$, gdje postaje degeneriran s rezultatom za veliki, adijabatski Holsteinov polaron. To naznačuje da translacijski invarijantna perturbacijska teorija tada prelazi glatko, bez loma simetrije, u adijabatsku kontinuiranu kvantnu granicu, što e biti rigorozno dokazano u članku-pratitelju. Kvantna teorija velikog adijabatskog Holsteinovog polarona, dakle, predstavlja jednostavan i poučan primjer kvantnog križanja koje zamjenjuje ponašanje u kvantnoj kritičnoj točki.