Time-retarded interactions in systems with tunneling states and strong electron-phonon coupling

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A path integral approach to the problem of the time-retarded interactions between tunneling states and fermionic excitations in systems with strong electron-phonon coupling is presented. The full partition function is derived up to third order in the coupling constant and the interaction strengths, which weigh both the attractive and the repulsive forces, are renormalized as a function of temperature. The conditions for localization of polarons in double well potentials related to the tunneling states are discussed. The model is applied to evaluate the contribution to the electrical resistivity in systems with structural lattice instabilities.

I. INTRODUCTION

Quantum mechanical systems whose state belong to a two-dimensional Hilbert space have been found in many branches of the solid state physics.[1] In dilute magnetic alloys, a single magnetic impurity of spin $-1/2$ provides a potential with an internal degree of freedom for exchange scattering of conduction electrons.[2] The time retarded interaction between two electrons via the impurity spin causes the anomalous increase in the electrical resistivity observed at low temperatures, the Kondo effect.[3] In amorphous systems, the atoms move back and forth between two equilibrium positions separated by a potential barrier. These low-lying energy excitations determine the low temperature properties (acoustic attenuation, thermal conductivity, specific heat) of amorphous insulators[4] and, in amorphous metals, they are the source of the *nonmagnetic interaction* with conduction electrons leading to the peculiar low-temperature resistivity behavior.[5,6] In A15 compounds, the high-temperature Pauli susceptibility and saturating resistivity have been explained by a model[7] in which double well potentials (i.e., for the vanadium atom in V_3Si) arise as a consequence of strong electron-phonon coupling and violation of Migdal's theorem. Recently, extended x-ray-absorption fine structure measurements in high-T_c superconductors[8] have revealed the existence of two split positions for the apex oxygen atoms and several investigations have pointed out the anharmonic character of the apex oxygen vibrations. The lattice instabilities due to the high polarizability of the oxygen ions have been related[9,10] to the occurrence of the superconducting transition and support polaronic theories for the normal state of the high-T_c superconductors.[11] These motivations have led us to study the general problem of the interaction between a double well potential in its two-state configuration [two level system (TLS)] and the fermionic excitation in a phonon bath (polaron). In this paper we apply a path integral formalism to describe the coupling of the TLS to the polaron. This approach is particularly powerful to deal with the time-retarded interactions for any value of the coupling constant.[12] In Sec. II the full partition function for the interacting system is derived and in Sec. III, the renormalized coupling constants are used to evaluate the electrical resistivity as a function of temperature. The conclusions are drawn in Sec. IV.

II. THE MODEL

We assume to describe the tightly bound electronic states of the system by the independent boson model (IBM) in which one fixed electron interacts with a set of phonons. A fixed particle cannot respond to the changes in the potential field due to the ionic motion and therefore the IBM simplifies the physical situation. However, relaxation effects can be suitably studied by taking into account the fluctuations in the phonon cloud surrounding the electron: this is done through the finite temperature Green's function which can be exactly obtained in the IBM. This is the advantage of the model. Moreover, we notice that the one phonon self-energy in the IBM coincides with the Rayleigh-Schrödinger (RS) perturbative theory if the electron kinetic energies can be taken as a constant.[13] Since the RS theory provides a good description for the ground state polaron problem also for intermediate values of the coupling constant, our model should be reliable in the low-temperatures regime. The IBM Hamiltonian is given by

$$H_{\mathrm{IBM}}=\bar{\epsilon}\tilde{c}^{\dagger}\tilde{c}+\sum_{\mathbf{q}}\ \omega(\mathbf{q})a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}},$$

$$\bar{\epsilon}=\epsilon-\sum_{\mathbf{q}}\ \frac{M_{\mathbf{q}}^{2}}{\omega(\mathbf{q})}, \tag{1}$$

where $\tilde{c}^{\dagger},\tilde{c}$ are the electronic creation and annihilation operators and $\bar{\epsilon}$ is the renormalized energy for the electron interacting with a set of phonons with frequency $\omega(\mathbf{q})$. $M_{\mathbf{q}}$ is the electron-phonon matrix element, ϵ is the free electron energy, and $a_{\mathbf{q}}^{\dagger},a_{\mathbf{q}}$ are the phononic creation and annihilation operators, respectively. The spin variable is not taken into account in the IBM. The one particle Green's function related to H_{IBM} can be derived exactly and the result is

$$G^{(0)}(\tau)=-[1-n_F(\bar{\epsilon})]e^{-\tau\bar{\epsilon}}e^{-\phi(\tau)},$$

$$\phi(\tau)=\sum_{\mathbf{q}}\ \left(\frac{M_{\mathbf{q}}}{\omega(\mathbf{q})}\right)^{2}[N_{\mathbf{q}}(1-e^{\omega(\mathbf{q})\tau})+(N_{\mathbf{q}}+1)$$

$$\times(1-e^{-\omega(\mathbf{q})\tau})]. \tag{2}$$

τ is the time according to the Matsubara Green's function formalism. $N_{\mathbf{q}}$ is the phonon occupation factor and $n_F(\bar{\epsilon})$ is

the Fermi distribution. In the Einstein model, $\bar{\epsilon}$ is given by $\bar{\epsilon}=\epsilon-g\omega_0$ where ϵ is the free electron energy, ω_0 is the frequency common to all phonons in the system, and g is the effective electron-lattice coupling. Then, $G^{(0)}(\tau)$ can be rewritten as follows:

$$G^{(0)}(\tau)=Be^{A\cosh[\omega_0(\tau-\beta/2)]}e^{-\tau\bar{\epsilon}},$$

$$B=-[1-n_F(\bar{\epsilon})]e^{-g(2N_0+1)},$$

$$A=2g[N_0(N_0+1)]^{1/2},$$

$$g=\sum_{\mathbf{q}}\left(\frac{M_{\mathbf{q}}}{\omega(\mathbf{q})}\right)^2. \tag{3}$$

We consider the double well potential in the symmetric ground state configuration which is represented by a two level system (TLS) whose Hamiltonian matrix is

$$(H_{\mathrm{TLS}})=\begin{pmatrix}0 & \Delta\\ \Delta & 0\end{pmatrix}, \tag{4}$$

where Δ is the tunneling energy between the minima of the TLS. The dynamics of the TLS's can be described by a path integral approach that permits one to map the real space quantum oscillations onto the time scale, where the time is the above defined τ. Then, Δ can be suitably expressed by $\Delta=\lambda Q$ where λ is the electron-phonon coupling constant for the vibrational mode giving origin to the TLS and Q is the one-dimensional (1D) atomic displacement which depends linearly[14] on τ.

$$Q(\tau)=-Q_0+\frac{2Q_0}{\tau_0}(\tau-t_i), \tag{5}$$

where τ_0 is the hopping time between the minima of the TLS which are located at $\pm Q_0$ and t_i is the instant at which the ith-hop takes place. One path is characterized by the number $2n$ of hops, by the set of t_i $(0<i\leqslant 2n)$, and by τ_0. This particular form for the tunneling energy is physically plausible and it allows one to introduce the τ dependence of the interaction Hamiltonian $H_{\mathrm{int}}(\tau)$ between the TLS and the polaron described by H_{IBM}:

$$H_{\mathrm{int}}(\tau)=-2\lambda Q(\tau)\tilde{c}^{\dagger}(\tau)\tilde{c}(\tau). \tag{6}$$

We remark that (i) a single lattice site has been considered so that intersite polaron-polaron interaction[15] is not accounted for by the present model. (ii) The tightly bound electrons interact with a potential having an internal degree of freedom provided by the local lattice instability. This interaction is not magnetic in origin since the spin variables have not been considered. (iii) The wave vector dependence of the polaronic operators in H_{int} can be neglected only if elastic s-wave scattering is assumed to be dominant. In general, the directional dependence of the TLS in momentum space should be taken into account: for instance, in high-T_c superconducting systems, it could lead to an anisotropic gap function via anisotropic effective electron-electron interaction.[16] By taking into account Eqs. (5) and (6), the one path contribution to the partition function of the system is given by

$$Z(n,t_i)=Z_0\left\langle T_\tau\exp\left(-\int_0^\beta d\tau\, H_{\mathrm{int}}(\tau)\right)\right\rangle, \tag{7}$$

where Z_0 is the partition function related to the free Hamiltonian $H_0=H_{\mathrm{IBM}}+H_{\mathrm{TLS}}$, T_τ is the ordering operator with respect to τ, β is the inverse temperature, and $\langle\,\rangle$ denotes the thermal average with respect to the free Hamiltonian. The full partition function of the system will be obtained by integrating over the times t_i and summing over all possible even number of hops. Following the method outlined by Hamann,[14] we multiply $\lambda Q(\tau)$ by a fictitious coupling constant s $(0\leqslant s\leqslant 1)$ and, by differentiating with respect to s, one derives the following expression:

$$\ln[Z(n,t_i)/Z_0]=-2\lambda\int_0^1 ds\int_0^\beta d\tau\, Q(\tau)\lim_{\tau'\to\tau^+}G(\tau,\tau')_s, \tag{8}$$

where $G(\tau,\tau')_s$ is the full propagator for polarons satisfying the Dyson's equation,

$$G(\tau,\tau')_s=G^{(0)}(\tau-\tau')+s\int_0^\beta d\tau'' G^{(0)}(\tau-\tau'')\lambda Q(\tau'')G(\tau''-\tau') \tag{9}$$

and $G^{(0)}(\tau-\tau')$ is given in Eq. (3). Then, to second order in s, from Eqs. (8) and (9), we obtain

$$\ln[Z^{(2)}(n,t_i)/Z_0]=-2\lambda\int_0^\beta d\tau\, Q(\tau)G^{(0)}(\tau,\tau^+)-\lambda^2\int_0^\beta d\tau\, Q(\tau)\int_0^\beta d\tau'' G^{(0)}(\tau-\tau'')Q(\tau'')G^{(0)}(\tau''-\tau^+)$$
$$-\frac{2}{3}\lambda^3\int_0^\beta d\tau\, Q(\tau)\int_0^\beta d\tau'' G^{(0)}(\tau-\tau'')Q(\tau'')\int_0^\beta d\tau''' G^{(0)}(\tau''-\tau''')Q(\tau''')G^{(0)}(\tau'''-\tau^+). \tag{10}$$

The time integrations will be carried out by taking into account that, for any function $f(\tau)$,

$$\int_0^\beta d\tau\, Q(\tau) f(\tau) = -Q_0(2n-1)\int_0^{\tau_s} d\tau\, f(\tau) + \frac{2Q_0}{\tau_0}\sum_{i=1}^{2n}\int_{t_i}^{t_i+\tau_0} d\tau(\tau - t_i) f(\tau), \tag{11}$$

where τ_s (the time one atom is sitting in a well) is determined by the closure condition: $(2n-1)\tau_s + 2n\tau_0 = \beta$. The first order term on the right-hand side of Eq. (10) describes TLS-polaron scattering. However, the propagator is essentially time independent so that the polaron cannot see the internal degree of freedom of the TLS and no correlation effect arise in the system by virtue of this nonretarded interaction term. Its explicit expression is derived by using Eqs. (3) and (11):

$$-2\lambda\int_0^\beta d\tau\, Q(\tau) G^{(0)}(\tau,\tau^+) = 2\lambda Q_0 B e^{A\cosh(\omega_0\beta/2)}(\beta - 4n\tau_0). \tag{12}$$

The second and third order terms in Eq. (10) account for both the attractive and repulsive part of the retarded interaction mediated by the lattice deformations. The details of the lengthy calculations are reported on in the Appendix. The final expression for these two terms are respectively

$$-\lambda^2\int_0^\beta d\tau\, Q(\tau)\int_0^\beta d\tau'' G^{(0)}(\tau-\tau'')Q(\tau'')G^{(0)}(\tau''-\tau^+) = -(\lambda Q_0)^2 B^2 e^{2A}\left[\omega_0^2\tau_0^2\sum_{i>j}^{2n}(t_i-t_j)^2 + g(n,\tau_0,\omega_0,\beta)\right] \tag{13}$$

and

$$-\frac{2}{3}\lambda^3\int_0^\beta d\tau\, Q(\tau)\int_0^\beta d\tau'' G^{(0)}(\tau-\tau'')Q(\tau'')\int_0^\beta d\tau''' G^{(0)}(\tau''-\tau''')Q(\tau''')G^{(0)}(\tau'''-\tau^+)$$

$$= -\frac{2}{3}(\lambda Q_0)^3 B^3 e^{3A}\left[3\omega_0^2\tau_0^2(2n\tau_0 - \beta/2)\sum_{i>j}^{2n}(t_i-t_j)^2 + h(n,\tau_0,\omega_0,\beta)\right]. \tag{14}$$

The functions $g(n,\tau_0,\omega_0,\beta)$ and $h(n,\tau_0,\omega_0,\beta)$ are given in Eqs. (A7) and (A16), respectively. Equations (13) and (14) have been derived under the very assumption that short range interactions are dominant on the time scale governed by the hopping time τ_0. This is consistent with the *local* nature of the wave function in polaronic theories and permits one to approximate the time dependent propagators as shown in Eqs. (A2) and (A9). Let us define by $K^{(2)}$ and $K^{(3)}$ the effective couplings for the two physical processes (polaron-polaron attraction and TLS-polaron repulsion) described by Eqs. (13) and (14). The analytical expressions of the interaction strengths are given by the dimensionless constants which multiply the time-retarded terms:

$$K^{(2)} = -(\lambda Q_0)^2 B^2 e^{2A}\omega_0^2\tau_0^4,$$

$$K^{(3)} = -2(\lambda Q_0)^3 B^3 e^{3A}\omega_0^2\tau_0^4(2n\tau_0 - \beta/2). \tag{15}$$

$K^{(2)}$ has a negative sign and it is therefore related to the attractive part of the interaction. An attraction between polarons can take place in the system as a consequence of the self-trapping induced by the double well potential. We point out that the attraction arises to second order in λ and two linear paths are involved but one single atom mediates the interaction which is therefore local in the real space. $K^{(3)}$ depends on the number of hops in the path: if the inequality $2n\tau_0 > \beta/2$ is fulfilled then $K^{(3)}$ is repulsive. Since τ_0 corresponds to the inverse of the tunneling energy between the minima of the TLS, it turns out that the condition $4nK_BT > \tau_0^{-1}$ is satisfied over a large temperature range. For instance, by taking $n=3$ (6 hops in the path) and $\tau_0^{-1} \simeq 10$ meV, one gets $K^{(3)} > 0$ at any $T > T^* \simeq 10$ K whereas $K^{(3)}$ becomes attractive below T^*. Paths with many hops tend to favor repulsive scattering also in the low temperature region. On the other hand, the closure condition for the path poses a lower bound on τ_0^{-1}, $\tau_0^{-1} \geqslant 2nK_BT$, where the equality is satisfied in the limit $\tau_s \to 0$. As a consequence, once τ_0 has been fixed on the base of the physical problem, the subset of relevant paths depends on the temperature range and paths with an increasing number of hops are more effective at de-

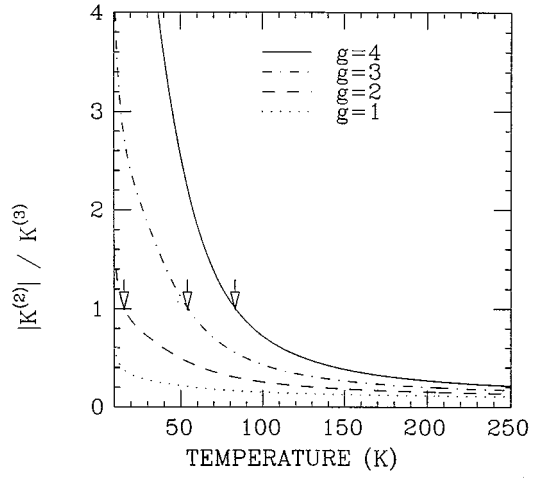

FIG. 1. The ratio between the absolute value of the attractive polaron-polaron coupling and the repulsive coupling constant versus temperature for four values of the overall electron-phonon coupling constant g. The phonon frequency ω_0 is 20 meV. The tunneling energy λQ_0 between the minima of the two level system is 6.5 meV. In the strong coupling cases, the arrows indicate the temperatures at which attractive and repulsive forces are comparable.

creasing temperatures. The temperature dependence of $K^{(2)}$ and $K^{(3)}$ is given by the combination of Bose factors through the parameters A and B in Eq. (3). It turns out that both renormalized couplings are increasing functions of temperature. Then, as we enhance T, the dynamic of the TLS and the motion of the charge carriers become more and more correlated: the atom in the TLS sees only the surrounding fermionic gas which screens the quantum motion between the minima of the double well potential. As a consequence, the atom tends to sit in a well rather than flipping back and forth and the relevant paths are characterized by a low number of hops. Because of the large amount of screening, the interaction between pairs of TLS can be neglected at high temperatures.[17] The full partition function of the system is obtained by integrating over the times t_i and summing over all possible even number of hops,

$$
\begin{aligned}
Z_T &= Z_0 \sum_{n=0}^{\infty} \int_0^{\beta} \frac{dt_{2n}}{\tau_0} \cdots \int_0^{t_2-\tau_0} \frac{dt_1}{\tau_0} Z^{(2)}(n,t_i) \\
&= \sum_{n=0}^{\infty} \exp\Big(2\lambda Q_0 B e^{A\cosh(\omega_0\beta/2)}(\beta - 4n\tau_0) - (\lambda Q_0)^2 B^2 e^{2A} g(n,\tau_0,\omega_0,\beta) \\
&\quad - \frac{2}{3}(\lambda Q_0)^3 B^3 e^{3A} h(n,\tau_0,\omega_0,\beta) \Big) \int_0^{\beta} \frac{dt_{2n}}{\tau_0} \cdots \int_0^{t_2-\tau_0} \frac{dt_1}{\tau_0} \exp\left[(K^{(2)}+K^{(3)}) \sum_{i>j}^{2n} \left(\frac{t_i - t_j}{\tau_0} \right)^2 \right]. \qquad (16)
\end{aligned}
$$

From Eq. (16) we see that the energy $E(n,t_i,\tau_0)$ for a path is given by

$$
\begin{aligned}
E(n,t_i,\tau_0) = \frac{1}{\beta} \Bigg[& 2\lambda Q_0 B e^{A\cosh(\omega_0\beta/2)}(4n\tau_0 - \beta) + (\lambda Q_0)^2 B^2 e^{2A} g(n,\tau_0,\omega_0,\beta) \\
& + \frac{2}{3}(\lambda Q_0)^3 B^3 e^{3A} h(n,\tau_0,\omega_0,\beta) - (K^{(2)}+K^{(3)}) \sum_{i>j}^{2n} \left(\frac{t_i - t_j}{\tau_0} \right)^2 \Bigg] \qquad (17)
\end{aligned}
$$

and, by minimizing $E(\tau_0)$, one can determine τ_0 for the dominant path. This would complete the fully renormalized treatment of the interacting system and would permit one to account for the effects of the polaron-TLS coupling on the dynamics of the TLS.[18] Hereafter we avoid this mathematically lengthy steps and treat τ_0 as a phenomenological parameter. Now we study the competition between attractive and repulsive forces above T^* up to room temperature. The input parameters of our model are Q_0, λ, ω_0, τ_0, and g. We assume that the two equilibrium positions in the TLS are separated by 0.13 Å.[8] λ can be varied in the range 20–200 meV Å^{-1} to ensure a bare tunneling energy λQ_0 between the minima of the TLS of order 1.3–13 meV and the hopping time τ_0 is set equal to $(\lambda Q_0)^{-1}$. In Fig. 1, the ratio $|K^{(2)}|/K^{(3)}$ is reported on versus T for four values of g. The bare tunneling energy λQ_0 is 6.5 meV and $\omega_0 = 20$ meV. Let us define T_p the temperature at which the attraction starts to overcome the repulsion: one sees that very strong electron-lattice interactions ($g = 2,3,4$) provide a temperature range below T_p in which attractive forces are relevant whereas, in the case $g = 1$, the repulsive TLS-polaron scattering dominates throughout the whole temperature region. T_p is an increasing function of g. It should be remarked that these results pose a constraint to the validity of the perturbative expansion in Eq. (10): in fact, whenever the condition $K^{(3)} > |K^{(2)}|$ is fulfilled higher order terms in the λ parameter should be taken into account. Our model is therefore consistent with those values of the input parameters which allow for $|K^{(2)}| > K^{(3)}$ below T_p. In Fig. 2, $|K^{(2)}|/K^{(3)}$ is plotted versus T for the same values of λQ_0 and g as in Fig. 1 but with $\omega_0 = 50$ meV. Larger phonon frequencies imply, for a given g, larger electron-phonon matrix elements and polaron coupling constant. Under these conditions localization of polarons is likely to occur in a wider temperature range. Accordingly, T_p is shifted upwards both for $g = 3$ and $g = 4$ with respect to Fig. 1, whereas for $g = 2$, T_p is locked at $\simeq 16$ K and it does not depend essentially on the phonon frequency. This trend is even more evident in Fig. 3 where we set $\omega_0 = 100$ meV: for $g = 3$ we get $T_p = 250$ K and for $g = 4$ the attractive forces are dominant in the whole temperature

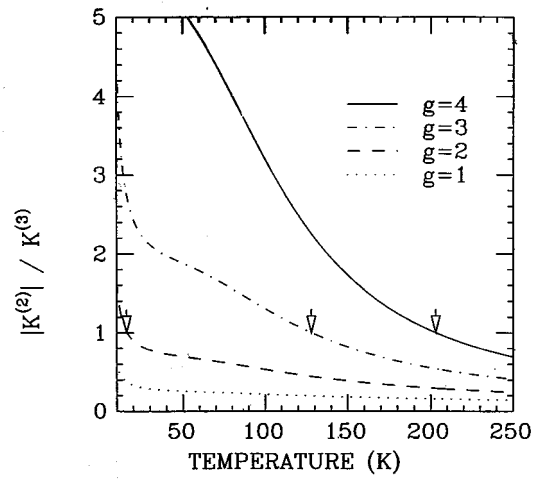

FIG. 2. As in Fig. 1 but with $\omega_0 = 50$ meV.

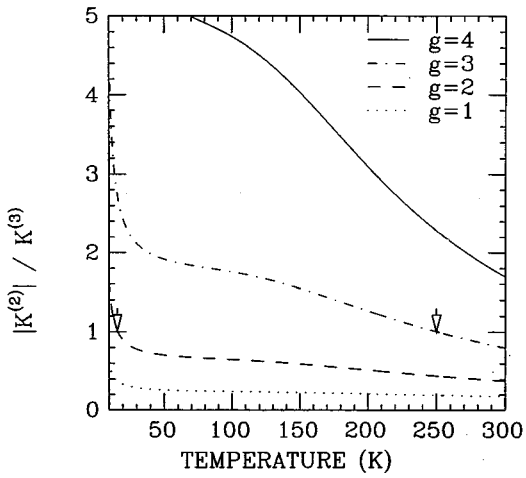

FIG. 3. As in Fig. 1 but with $\omega_0=100$ meV.

range. By decreasing λ, the hopping time gets longer and also paths with a low number of hops give rise to repulsive $K^{(3)}$ at low temperatures: i.e., $\lambda=20$ meV Å^{-1} implies $K^{(3)}>0$ at any $T>2$ K for a 6 hops path. However, the magnitude of both interaction constants grows with increasing τ_0 and no substantial changes in T_p are observed.

III. RESULTS AND DISCUSSION

Hereafter we calculate the contribution to the electrical resistivity ρ arising from the scattering mechanisms which have been studied in the previous section. As noticed above, a full calculation[18] should take into account the effects of a distribution of coupling constants: in fact, the subset of paths which mostly contribute to the scattering properties varies as a function of temperature through the parameters n and τ_0. Here we simplify the procedure and evaluate the resistivity by using the *one path interaction strengths* shown in Figs. 1–3. Assuming s-wave scattering by the impurity potential due to the TLS, one gets[13]

$$\rho=\rho_0 \sin^2 \eta,$$

$$\rho_0=\frac{3n_s}{\pi e^2 v_F^2 (N_0/V)^2 \hbar}, \tag{18}$$

where n_s is the density of two level systems which act as scatterers, v_F is the Fermi velocity, V is the volume, e is the electron charge, and $\hbar$ is the Planck constant. η is the phase shift to the electron s-wave function at the Fermi surface. η is related to the depth of the double well potential and therefore to the interaction strengths $K^{(i)}$ which have been derived in the previous section by the following relation:[19]

$$\eta^2=\frac{\pi^2}{8}(K^{(2)}+K^{(3)}) \tag{19}$$

and, expanding for large phase shift angles, from Eq. (18), one gets

$$\rho=\rho_0(a+b\,\eta+c\,\eta^2),$$

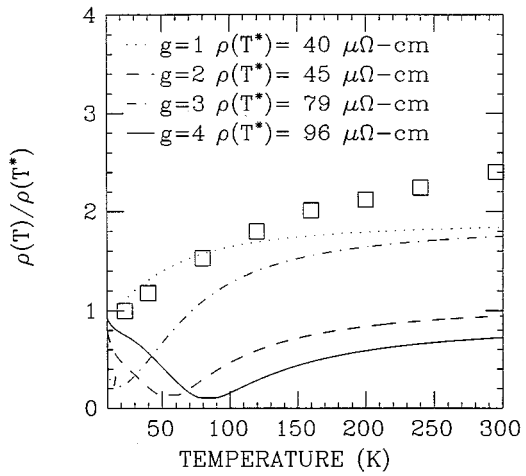

FIG. 4. Electrical resistivity versus temperature for four values of the g parameter by assuming $\omega_0=20$ meV and $\lambda Q_0=6.5$. The experimental data □ are taken from Ref. 20.

$$a=1-\frac{\pi^2}{4}(1-\pi^2/12),$$

$$b=\pi(1-\pi^2/6),$$

$$c=(\pi^2/2-1). \tag{20}$$

ρ_0 is fixed according to the system through the parameters n_s, N_0, and v_F. For instance, in A15 compounds, we should expect ρ_0 in the range $\simeq 100$ $\mu\Omega$ cm,[20] while in fully oxygenated high-T_c superconductors, the experimental out of plane resistivity implies $\rho_0\simeq 10$ mΩ cm.[21] In Fig. 4, the temperature dependent resistivity is reported on for four values of the electron-lattice coupling constant. $\rho(T)$ is normalized to $\rho(T^*)$ with $T^*=20$ K, the order of the highest critical temperature achievable in A15 superconductors. By taking $n_s\simeq 6\times 10^{22}$ cm^{-3}, $N_0\simeq 8\times 10^{22}$ states eV^{-1} cm^{-3}, and $v_F\simeq 6\times 10^7$ cm sec^{-1}, we choose values that are compatible with the system Nb_3Ge and yield a residual resistivity $\rho_0 a\simeq 20$ $\mu\Omega$ cm. The Einstein phonon frequency is set at 20 meV and the tunneling energy between the minima of the TLS is $\lambda Q_0=6.5$ meV. This value yields a hopping time τ_0 of order of 10^{-13} sec which is consistent with previous estimates in A15 compounds.[7] In the case $g=1$, $\rho(T)$ saturates with increasing temperatures, starting from $T\simeq 50$ K. This behavior implies that the relatively strong electron-phonon scattering has reduced the electronic mean free path to the order of the lattice constant. The experimental data published by Testardi *et al.*[20] for the Nb_3Ge film with $T_c\simeq 23$ K are also reported on in Fig. 4. Note that our theory reproduces the anomalous temperature dependence of ρ first pointed out by Woodward and Cody[22] in Nb_3Sn. These authors had found a negative curvature in ρ starting at high temperatures and down to $\simeq 50$ K with an inflection point and positive curvature at lower T. This behavior, general in A15 compounds, is related to the presence of defects which strongly influence the electron-phonon interactions and, moreover, are responsible for the violation of the Matthiessen's rule. The flattening in $\rho(T)$ with increasing T predicted by our model is more pronounced than that shown by experiments. This discrep-

ancy could be due to the fact that, for $g=1$, the TLS-polaron repulsive interaction is dominant and therefore higher order terms in Eq. (10) should be taken into account to make the model consistent. We expect[18] that higher order interaction strengths in λ yield a positive $d\rho/dT$ at high T, via Eqs. (19) and (20). For $g=2$, $\rho(T)$ develops a minimum in the low-temperature region and, by increasing g, the minimum shifts at higher T. Note that above the minimum, $\rho(T)$ shows a linear contribution which is then obscured by logarithmic like[23] saturation effects. In the case $g=2$, the linear $\rho(T)$ is visible between 20 and 80 K and, above 80 K, $d\rho/dT$ decreases but less rapidly than in the previous case. Many theoretical and experimental determinations of the electron-phonon coupling constant in A15 compounds assessed that g should range between 1 and 2 (Ref. 24) with values possibly closer to 2 (Ref. 25) for Nb_3Ge. Our fit of the experimental slope also suggests a coupling g about 2. The $\rho(T^*)$ values grow with g. The low-temperature $\rho(T)$ that we obtain in the very strong coupling cases ($g=3,4$) reminds us of the typical resistivity behavior encountered in amorphous metals.[26] In these systems the well settled presence of TLS acting as scattering centers for the electrons yields a negative $d\rho/dT$ below a characteristic crossover temperature at which a resonant state is built up.[5] The crossover is usually in the region $\simeq 1-10$ K for metallic glasses but in some cases[27] the resistivity minimum occurs at higher $T(\simeq 50-100$ K), that is, in the range predicted by our model. Here we see the analogy between anomalous $\rho(T)$ in amorphous metals and anomalous $\rho(T)$ in A15 compounds: the nature of the defects in A15 superconductors seems connected to structural instabilities which cause the loss of the translational symmetry of the lattice. By increasing the number of defects, the critical temperature is progressively suppressed, the Woodward-Cody anomaly is lost, and the residual resistivity is enhanced.[28] These features point to the formation of an amorphous structure with low lying energy excitations, the TLS. It is interesting that both the normal state resistivity in A15 superconductors and the low temperature ρ in amorphous systems can be understood in the framework of the present model which focuses on the role of the TLS. The g parameter drives the evolution of the resistivity from A15-like behavior ($g=1$) with saturation at high temperatures to the amorphouslike behavior ($g=3,4$) with negative $d\rho/dT$ below a crossover temperature. The reason why, by increasing g, a negative $d\rho/dT$ arises at low T is the following: strong electron-phonon coupling implies that electrons become heavy and their probability amplitude to propagate is reduced; in fact, at low T, $G^{(0)}(\tau)$ decreases exponentially with g [see Eq. (3)]. Then, tightly bound electrons can be easily trapped in the double well potential and they can favor off-diagonal scattering between the minima of the TLS. As a consequence ρ increases with decreasing T. Our theory is consistent with the observation[29] that a negative $d\rho/dT$ is associated to high resistivity values ($\rho \geq 100\ \mu\Omega$ cm).

In Fig. 5, $\rho(T)$ is reported on by assuming $\omega_0=100$ meV. $\rho(T)$ is normalized to $\rho(T^*)$ with $T^*=10$ K, which is an increasing function of g. A higher phonon spectrum broadens the temperature range in which our model is fully consistent (see Fig. 3). We take $n_s=1.2\times10^{22}$ cm^{-3}, $N_0\simeq 1.5\times10^{22}$ states eV^{-1} cm^{-3} and $v_F\simeq 1\times10^7$ cm sec^{-1}, that is values peculiar of the high-T_c superconductor system $YBa_2Cu_3O_{7-\delta}$

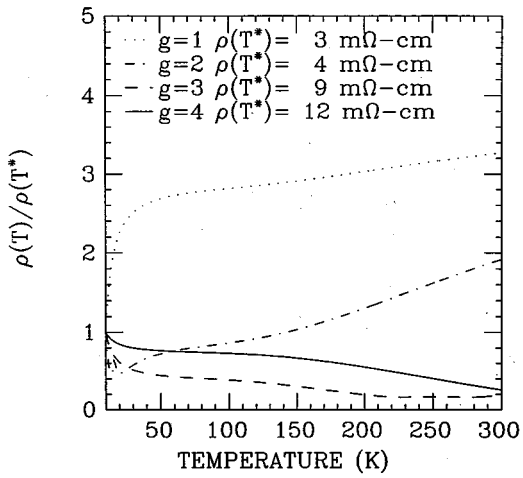

FIG. 5. As in Fig. 4 but with $\omega_0=100$ meV.

which yield $\rho_0\simeq 6$ mΩ cm as expected. We remark that any comparison with the electrical resistivity in high-T_c superconductors can be here only qualitative and limited to $T \geqslant T_c \simeq 100$ K since the occurence of the critical transition is not accounted for by the present model. The most important feature emerging from Fig. 5 is that $d\rho/dT$ changes from positive ($g=1,2$) to negative ($g=3,4$) by increasing the strength of the electron-lattice interaction. Localization of polarons is possible in a very strong coupling regime *and* in the presence of local lattice instabilities (TLS) throughout a wide temperature range. The enhancement of the characteristic phonon frequency (with respect to Fig. 4) smears the minimum in $\rho(T)$ and extends the region of negative $d\rho/dT$, an effect that is actually observed in some high-T_c compounds.[30] In these systems the high frequency vibrations of the apical oxygen atoms (perpendicular to the CuO_2) planes produce anharmonic double well potentials which could influence the out of plane electrical transport.[19] The questions related to the low-temperature semiconductorlike behavior of the c-axis resistivity in high-T_c compounds are currently a matter of intensive investigations.[31] We point out that our model predicts a change from metallic to nonmetallic $\rho_c(T)$ accompanied by an increase of ρ_c above 10 mΩ cm at low temperatures. This value agrees with the estimated[21] Mott-Ioffe-Regel (MIR) limit for metallic conductivity in high-T_c systems. Also superconducting fluctuations tend to increase ρ_c on cooling in the critical region above T_c.[32] This contribution is believed to be relevant in highly anisotropic layered cuprates as Bi-2:2:1:2.[33] However, the $\rho_c(T)$ dependence and the high ρ_c indicate that the c-axis mean free path is of order of the c-axis lattice constant, i.e., the MIR criterion for metallic transport is not fulfilled and this fact cannot be ascribed to critical fluctuations alone. Recently, Zha *et al.*[34] have suggested a phenomenological model to account for the experimental ρ_c in high-T_c systems. According to these authors, the linear ρ_c at high temperatures is determined by in plane electron scattering which makes ρ_c proportional to the in plane resistivity ρ_{ab}. At low T (above T_c) the enhanced c-axis scattering rate arises from the out of plane vibrations of the apical oxygen atoms. This picture seems to be consistent with the here presented calculations. My model neglects spin variables so that I am dealing with dielectric polarons whose properties generally differ from

those of spin polarons.[35] However, Vigren[36] suggested that the diffusion coefficient of spin polarons does not depend on temperature so that, in the presence of lattice instabilities, spin polarons could be trapped. In this case, a nonmetallic contribution to the electrical resistivity is expected[37] and this effect superimposes to that which we calculated in Fig. 5 for the strong g regime. Then, our qualitative conclusions regarding the effect of the lattice instabilities on ρ_c should not be altered by inclusion of spin carriers. On the other hand, spin effects are believed to influence the charge transport in the CuO_2 planes.[38,39] It should be added that also interlayer disorder induced by a low hole concentration in underdoped high-T_c compounds affects ρ_c.[40] In particular, a negative $d\rho_c/dT$ arises from boson assisted interlayer tunneling, where the boson can be both a phonon or a spin excitation.

IV. CONCLUSIONS

In this paper I have studied the general problem of the coupling between an atom in a two state configuration and electronic excitations in a phonon bath (polarons). The quantum tunneling between the minima of the two level system gives rise to a potential with an internal degree of freedom which, in turn, causes time-retarded interactions in the fermionic system. The path integral method allows one to map the real space quantum oscillations onto the time scale so that the time dependence of the interacting Hamiltonian can be easily taken into account. The spinless polaron has been described in the exactly solvable independent boson model which provides an analytical expression for the polaron Green's function at finite temperature. We have written the full partition function of the interacting system up to third order in λ, where λ is the coupling constant between double well potential and polaron. An attractive polaron-polaron interaction arises in the system to second order in λ, as due to the local lattice instability which favors the trapping of the tightly bound electrons. The attractive forces compete with the repulsive two level system-polaron scattering and, in a very strong electron-lattice coupling regime, the attraction overcomes the repulsion at low temperatures. Localization of polarons is more likely to occur throughout a wide temperature range in systems with an high average phonon frequency, $\omega_0 \simeq 50-100$ meV. The model has been applied to calculate the contribution to the electrical resistivity $\rho(T)$ due to electron scattering by an impurity, where the impurity is the two level system modeling the lattice instability. In systems with $\omega_0 \simeq 20-50$ meV a saturating $\rho(T)$ is found at high temperatures, a behavior typical of A15 compounds in which a large electron-phonon coupling reduces the electron mean free path to the order of the lattice constant. By increasing the overall electron-phonon coupling to values larger than one, we see an anomalous $\rho(T)$, with negative $d\rho/dT$, on the low-temperature side below a certain crossover temperature. This phenomenon, which is peculiar of amorphous structures, is related to the electron trapping in the double well potential provided by the local lattice instability. The trapped electrons can, in turn, favor off diagonal scattering between the two wells so that many hops paths for the two level system are expected to be dominant at low temperatures. Finally, we suggest that the present model could contribute to clarify the effects of the structural instabilities on the electrical resistivity of the high-T_c superconductors.

APPENDIX

In this appendix we derive the second and third order contribution to the one path partition function of the interacting system given in Eq. (10). Let us assume that the 1D atomic displacement giving rise to the dynamical TLS depends linearly on time. Then, by using Eq. (11) in the text, the λ^2 term in Eq. (10) can be rewritten as

$$
\begin{aligned}
-\lambda^2 \int_0^\beta d\tau\, Q(\tau) \int_0^\beta d\tau'' G^{(0)}(\tau-\tau'') Q(\tau'') G^{(0)}(\tau''-\tau^+) = &-(2n-1)^2(\lambda Q_0)^2 \int_0^{\tau_s} d\tau \int_0^{\tau_s} d\tau'' G^{(0)}(\tau-\tau'') G^{(0)}(\tau''-\tau^+) \\
&-\left(\frac{2\lambda Q_0}{\tau_0}\right)^2 \sum_{i>j}^{2n} \int_{t_i}^{t_i+\tau_0} d\tau(\tau-t_i) \int_{t_j}^{t_j+\tau_0} d\tau''(\tau''-t_j) \\
&\times G^{(0)}(\tau-\tau'') G^{(0)}(\tau''-\tau^+) + \frac{(2\lambda Q_0)^2}{\tau_0}(2n-1) \\
&\times \int_0^{\tau_s} d\tau \sum_{i=1}^{2n} \int_{t_i}^{t_i+\tau_0} d\tau''(\tau''-t_i) G^{(0)}(\tau-\tau'') G^{(0)}(\tau''-\tau^+).
\end{aligned}
\tag{A1}
$$

$G^{(0)}(\tau-\tau'')$ is the probability amplitude for the polaron to propagate from τ'' to τ and, if the hopping time τ_0 is sufficiently small, we can take $\tau'' \simeq t_j$ and $\tau \simeq t_i$, where t_j and t_i are the instants at which two hops take place. Note that the distance between two successive hops cannot be shorter that τ_0. Then, if short range interactions are dominant, it seems plausible to assume that $\tau-\tau''$ is of order $\beta/2$, where the inverse temperature β measures the length of the path. Under these conditions, the product of two free propagators in the independent boson model can be approximated as follows:

$$
\begin{aligned}
G^{(0)}(\tau-\tau'') G^{(0)}(\tau''-\tau) &= B^2 \exp\{A[\cosh(\omega_0(\tau-\tau''-\beta/2)) + \cosh(\omega_0(\tau''-\tau-\beta/2))]\} \\
&\simeq B^2 e^{2A}[1 + (\omega_0\beta/2)^2 + \omega_0^2(\tau-\tau'')^2].
\end{aligned}
\tag{A2}
$$

By inserting Eq. (A2) in Eq. (A1), the three addenda can be analytically calculated. The first addendum in the right-hand side of Eq. (A1) yields

$$-(2n-1)^2(\lambda Q_0)^2\int_0^{\tau_s}d\tau\int_0^{\tau_s}d\tau''G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau^+)=-(\beta-2n\tau_0)^2(\lambda Q_0)^2B^2e^{2A}\left[1+\left(\frac{\omega_0\beta}{2}\right)^2+\frac{\omega_0^2}{6}\left(\frac{\beta-2n\tau_0}{2n-1}\right)^2\right]; \tag{A3}$$

the second addendum yields

$$-\left(\frac{2\lambda Q_0}{\tau_0}\right)^2\sum_{i>j}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau''(\tau''-t_j)G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau^+)$$
$$=-(\lambda Q_0\tau_0)^2B^2e^{2A}\left[(2n)^2\left(1+\left(\frac{\omega_0\beta}{2}\right)^2+\frac{\omega_0^2\tau_0^2}{9}\right)+\omega_0^2\sum_{i>j}^{2n}(t_i-t_j)^2\right], \tag{A4}$$

where the following result has been used:

$$\sum_{i>j}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau''(\tau''-t_j)(\tau-\tau'')^2=\frac{\tau_0^4}{4}\sum_{i>j}^{2n}(t_i-t_j)^2+(2n)^2\frac{\tau_0^6}{36}; \tag{A5}$$

and the third addendum in Eq. (A1) yields

$$\frac{(2\lambda Q_0)^2}{\tau_0}(2n-1)\int_0^{\tau_s}d\tau\sum_{i=1}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau''(\tau''-t_i)G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau^+)$$
$$=\frac{(2\lambda Q_0)^2}{\tau_0}(\beta-2n\tau_0)B^2e^{2A}\left[2n\left(\frac{\tau_0^2}{2}[1+(\omega_0\beta/2)^2]+\frac{(\omega_0\tau_0\tau_s)^2}{6}-\frac{\omega_0^2\tau_s\tau_0^3}{3}+\frac{\omega_0^2\tau_0^4}{4}\right.\right.$$
$$\left.\left.+(2n-1)\tau_0^2\frac{(\tau_0+\tau_s)}{2}\left(\frac{2\tau_0}{3}-\frac{\tau_s}{2}\right)\right)+\frac{\tau_0^2}{2}(\tau_0+\tau_s)^2\sum_{j=1}^{2n-1}j^2\right]. \tag{A6}$$

Summing up the contributions given in Eqs. (A3), (A4), and (A6), we get

$$-\lambda^2\int_0^{\beta}d\tau\,Q(\tau)\int_0^{\beta}d\tau''G^{(0)}(\tau-\tau'')Q(\tau'')G^{(0)}(\tau''-\tau^+)=-(\lambda Q_0)^2B^2e^{2A}\left[\omega_0^2\tau_0^2\sum_{i>j}^{2n}(t_i-t_j)^2+g(n,\tau_0,\omega_0,\beta)\right],$$

$$g(n,\tau_0,\omega_0,\beta)=(2n\tau_0)^2\left(1+\frac{1}{4}(\omega_0\beta)^2+\frac{\omega_0^2\tau_0^2}{9}\right)+(\beta-2n\tau_0)^2\left(1+\frac{1}{4}(\omega_0\beta)^2+\frac{\omega_0^2}{6}\left(\frac{\beta-2n\tau_0}{2n-1}\right)^2\right)-2\tau_0(\beta-2n\tau_0)\left[2n\left(1\right.\right.$$
$$\left.\left.+\frac{1}{4}(\omega_0\beta)^2-\frac{2}{3}\omega_0^2\tau_0\tau_s+\frac{\omega_0^2\tau_0^2}{2}+\frac{\omega_0^2\tau_s^2}{3}+(2n-1)\left(\frac{4}{3}\tau_0-\tau_s\right)\left(\frac{\tau_0+\tau_s}{2}\right)\right)+(\tau_0+\tau_s)^2\sum_{j=1}^{2n-1}j^2\right]. \tag{A7}$$

By taking into account Eq. (11) in the text, the λ^3 term in Eq. (10) can be rewritten as

$$-\frac{2}{3}\lambda^3\int_0^{\beta}d\tau\,Q(\tau)\int_0^{\beta}d\tau''G^{(0)}(\tau-\tau'')Q(\tau'')\int_0^{\beta}d\tau'''G^{(0)}(\tau''-\tau''')Q(\tau''')G^{(0)}(\tau'''-\tau^+)$$
$$=\left[\frac{2}{3}(2n-1)^3(\lambda Q_0)^3\int_0^{\tau_s}d\tau\int_0^{\tau_s}d\tau''\int_0^{\tau_s}d\tau'''-\frac{16}{3}\left(\frac{\lambda Q_0}{\tau_0}\right)^3\sum_{i>j>k}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau''(\tau''-t_j)\right.$$
$$\times\int_{t_k}^{t_k+\tau_0}d\tau'''(\tau'''-t_k)-4\frac{(\lambda Q_0)^3}{\tau_0}(2n-1)^2\int_0^{\tau_s}d\tau''\int_0^{\tau_s}d\tau'''\sum_{i=1}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)$$
$$\left.+8\frac{(\lambda Q_0)^3}{\tau_0^2}(2n-1)\int_0^{\tau_s}d\tau''\sum_{i>j}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau'''(\tau'''-t_j)\right]G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau). \tag{A8}$$

Following the same arguments which lead to Eq. (A2) we notice that the product of three propagators can be approximated as

$$G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau)\simeq B^3e^{3A}\left[1+\frac{3}{8}(\omega_0\beta)^2+\frac{\omega_0^2}{2}[(\tau-\tau'')^2+(\tau''-\tau''')^2+(\tau'''-\tau)^2]\right] \tag{A9}$$

and, by means of Eq. (A9), we evaluate the four addenda in the right-hand side of Eq. (A8). The first addendum yields

$$\frac{2}{3}(2n-1)^3(\lambda Q_0)^3\int_0^{\tau_s}d\tau\int_0^{\tau_s}d\tau''\int_0^{\tau_s}d\tau'''G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau)$$

$$=\frac{2}{3}(\beta-2n\tau_0)^3(\lambda Q_0)^3B^3e^{3A}\left[1+\frac{3}{8}(\omega_0\beta)^2+\frac{\omega_0^2\tau_s^2}{4}\right]. \tag{A10}$$

The second addendum yields

$$-\frac{16}{3}\left(\frac{\lambda Q_0}{\tau_0}\right)^3\sum_{i>j>k}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau''(\tau''-t_j)\int_{t_k}^{t_k+\tau_0}d\tau'''(\tau'''-t_k)G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau)$$

$$=-\frac{2}{3}(\lambda Q_0\tau_0)^3B^3e^{3A}\left[(2n)^3\left(1+\frac{3}{8}(\omega_0\beta)^2+\frac{\omega_0^2\tau_0^2}{6}\right)+2n\,\frac{3\omega_0^2}{2}\sum_{i>j}^{2n}(t_i-t_j)^2\right], \tag{A11}$$

where Eq. (A5) has been used. The third addendum yields

$$-4\frac{(\lambda Q_0)^3}{\tau_0}(2n-1)^2\int_0^{\tau_s}d\tau''\int_0^{\tau_s}d\tau'''\sum_{i=1}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau)$$

$$=-\frac{4}{3}(\lambda Q_0)^3\tau_0(\beta-2n\tau_0)^2B^3e^{3A}\left[2n\left[\left(\frac{1}{2}+\frac{3}{16}(\omega_0\beta)^2\right)+\frac{5}{24}\omega_0^2\tau_s^2-\frac{1}{3}\omega_0^2\tau_s\tau_0+\frac{1}{4}\omega_0^2\tau_0^2\right.\right.$$

$$\left.\left.-(2n-1)\frac{(\tau_0+\tau_s)}{4}\omega_0^2\left(\tau_s-\frac{4}{3}\tau_0\right)\right]+\omega_0^2\frac{(\tau_0+\tau_s)^2}{2}\sum_{j=1}^{2n-1}j^2\right], \tag{A12}$$

where the following integral has been used:

$$\sum_{i=1}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_0^{\tau_s}d\tau''(\tau-\tau'')^2=2n\tau_0\tau_s\left[\frac{\tau_s^2\tau_0}{6}-\frac{\tau_s\tau_0^2}{3}+\frac{\tau_0^3}{4}+\left(\frac{2\tau_0^2}{3}-\frac{\tau_s\tau_0}{2}\right)\sum_{i=1}^{2n}t_i+\frac{\tau_0}{2}\sum_{i=1}^{2n}t_i^2\right] \tag{A13}$$

and

$$\sum_{i=1}^{2n}t_i=2n(2n-1)\frac{\tau_0+\tau_s}{2},\quad \sum_{i=1}^{2n}t_i^2=(\tau_0+\tau_s)^2\sum_{j=i}^{2n-1}j^2. \tag{A14}$$

The fourth addendum yields

$$8\frac{(\lambda Q_0)^3}{\tau_0^2}(2n-1)\int_0^{\tau_s}d\tau''\sum_{i>j}^{2n}\int_{t_i}^{t_i+\tau_0}d\tau(\tau-t_i)\int_{t_j}^{t_j+\tau_0}d\tau'''(\tau'''-t_j)G^{(0)}(\tau-\tau'')G^{(0)}(\tau''-\tau''')G^{(0)}(\tau'''-\tau)$$

$$=8(\lambda Q_0)^3\tau_0^2(\beta-2n\tau_0)B^3e^{3A}\left[\frac{\omega_0^2}{8}\sum_{i>j}^{2n}(t_i-t_j)^2+(2n)^2\left[\frac{1}{4}\left(1+\frac{3}{8}(\omega_0\beta)^2\right)+\frac{5\tau_0^2\omega_0^2}{36}+\frac{\omega_0^2\tau_s^2}{12}\right.\right.$$

$$\left.\left.-\frac{\omega_0^2\tau_s\tau_0}{6}+(2n-1)\frac{\omega_0^2}{4}(\tau_0+\tau_s)\left(\frac{2}{3}\tau_0-\frac{1}{2}\tau_s\right)\right]+2n\frac{\omega_0^2}{4}(\tau_0+\tau_s)^2\sum_{j=1}^{2n-1}j^2\right], \tag{A15}$$

where Eqs. (A5), (A13), and (A14) have been used. Summing the contributions in Eqs. (A10)–(A15), one gets the λ^3 term:

$$-\frac{2}{3}\lambda^3\int_0^{\beta}d\tau\,Q(\tau)\int_0^{\beta}d\tau''G^{(0)}(\tau-\tau'')Q(\tau'')\int_0^{\beta}d\tau'''G^{(0)}(\tau''-\tau''')Q(\tau''')G^{(0)}(\tau'''-\tau^+)$$

$$=-\frac{2}{3}(\lambda Q_0)^3B^3e^{3A}\left[3\omega_0^2\tau_0^2(2n\tau_0-\beta/2)\sum_{i>j}^{2n}(t_i-t_j)^2+h(n,\tau_0,\omega_0,\beta)\right],$$

$$h(n,\tau_0,\omega_0,\beta)=[(2n\tau_0)^3-(\beta-2n\tau_0)^3]\left(1+\frac{3}{8}(\omega_0\beta)^2\right)+\frac{\omega_0^2}{2}\left[(2n)^3\frac{\tau_0^5}{3}-\frac{(\beta-2n\tau_0)^5}{2(2n-1)^2}\right]$$
$$+3(\beta-2n\tau_0)(\beta-4n\tau_0)\tau_0\left[\omega_0^2\left(\frac{\beta-\tau_0}{2n-1}\right)^2\sum_{j=1}^{2n-1}j^2+2n\left(1+\left(1+\frac{3}{8}(\omega_0\beta)^2\right)\right.\right.$$
$$\left.\left.-\frac{2}{3}\omega_0^2\tau_0\frac{\beta-2n\tau_0}{2n-1}+2(\beta-\tau_0)\omega_0^2\left(\frac{\tau_0}{3}-\frac{\beta-2n\tau_0}{4(2n-1)}\right)\right)\right]+6(\beta-2n\tau_0)2n\tau_0\left[\frac{\omega_0^2\tau_0^2}{4}\left(\beta-\frac{38}{9}n\tau_0\right)\right.$$
$$\left.+\frac{5}{24}\omega_0^2\left(\frac{\beta-2n\tau_0}{2n-1}\right)^2\left(\beta-\frac{18}{5}n\tau_0\right)\right]. \tag{A16}$$

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