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Vibrational excitations of a one-dimensional electron-phonon system in strong coupling

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We consider an electron interacting with optical phonons through the deformation potential in one dimension. We calculate the energy spectrum of such a system to one order in $1/\alpha^2$ beyond the strong-coupling limit. We calculate the self-energy, effective mass and modified phonon spectrum to this order. The modified phonon spectrum is determined by the solution of a homogeneous linear integral equation. We are able to solve this integral equation in closed form for the odd-parity phonon modes. The result is a frequency spectrum $\Omega_n = \omega_0[1 - 4/n(n+3)]^{1/2}$, where $n = 1,3,5,...$ and ω_0 is the unperturbed optical-phonon frequency. For $n = 1$, $\Omega_1 = 0$ and this mode is a translation. For even-parity modes, the phonon frequency spectrum is determined numerically.

I. INTRODUCTION

Since its formulation in terms of particle-field interaction by Fröhlich,[1] the dynamics of an electron in a crystal lattice has attracted interest in two main directions. On the one hand, the importance of the electron-phonon interaction in solids is now well established and culminates, in this regard, in the explanation of superconductivity. On the other hand, the polaron, first studied quantum mechanically by Pekar,[2] serves generally as a model of particle-field interaction. Since particle-field interaction is of interest not only in solid-state physics, but also in such areas as quantum liquids and elementary-particle physics, it is important to study simple model systems for the purpose of extracting the content of specific features of more involved models. This approach is particularly useful in strongly interacting systems for which the usual methods of weak-coupling perturbation theory are invalid.

The Pekar theory is a variational treatment that is valid in the strong-coupling limit. This result suggests that a perturbation-theory analysis in inverse powers of the coupling constant should be useful in obtaining systematic corrections to the Pekar theory. However, an apparent difficulty in such a perturbation analysis arises in the attempt to incorporate fully the effects of the inherent translational invariance of the electron-phonon system. Bogoliubov and Tyablikov[3] developed a theory which maintains this translational invariance by introducing coordinates for the center of the polarization packet as additional dynamical variables together with subsidiary conditions. They showed that the Pekar theory was rigorous in the limit of infinite coupling. Although in principle the theory can yield corrections beyond the Pekar result, in practice it is difficult to extract these corrections in a systematic manner. A more recent theory has been developed by Gross[4] in which the translational invariance is made manifest by the introduction of the coordinates of the polarization packet as dynamical variables through a change of variables. The novel manner in which this is done leads to a theory which allows the energy spectrum to be computed as a power series in reciprocal powers of the coupling constant. Although the Gross theory is quite general in that it can be used to describe various types of polarons, it too is a rather involved theory.

In the present work we solve the more modest problem of a straightforward diagonalization of the Hamiltonian through the next order beyond the Pekar result. The model that we investigate is that of an electron interacting with optical phonons through the deformation potential in one dimension. For such a model both the phonon frequencies and the interaction form factor are independent of wave vector. As a consequence, the model is soluble in the sense that certain key features, upon which subsequent analysis depends, can be determined analytically. To the order of approximation in this work, we find that the spectrum is that of a set of lattice vibrations with frequencies that have been lowered from their optical-phonon value by the electron-phonon interaction. These localized vibrational modes were first discussed by Melnikov and Rashba[5] and later by Gross.[4] We have been able to determine the frequencies and mode description *analytically* for the odd-parity modes. The lowest such frequency turns out to be identically zero and the resulting mode is a translation rather than a vibration. This translational degree of freedom is characterized by a quadratic polaron energy-momentum relation with an effective mass that is identical to that found by Gross.[4] We stress that the translational mode appears naturally in the analysis and does not need to be introduced separately. The vibrational spectrum found here is

analogous to that recently obtained numerically by Miyaki[6] for the three-dimensional polaron with polarization interaction and optical phonons. In that work the zero-frequency mode is justified on general theoretical grounds. In addition to the free-polaron kinetic energy and the modified-phonon spectrum, we also obtain the Pekar self-energy and the lowest-order localization and fluctuation energy.

We also indicate to some degree how to go beyond the order of approximation considered here. In particular, we show how to construct an effective Hamiltonian that operates only in the space of the phonon variables and which gives the exact spectrum of the electron-phonon system. A similar effective Hamiltonian method was also used by Gross.[4] In the present theory, the exact effective Hamiltonian takes a particularly simple form and is determined by an equation of the Dyson type. In a separate publication we will discuss a more general analysis of this effective Hamiltonian.

In Sec. II of the paper we develop the general approach to the problem and in Sec. III we determine the phonon spectrum by the solution of a linear integral equation. The details of the solution are discussed in the Appendix. In Sec. IV we return to the question of translational invariance, and determine the polaron-effective mass together with the localization and fluctuation energies.

II. GENERAL FORMALISM

We start with the Fröhlich Hamiltonian in dimensionless form,

$$H = -\frac{\partial^2}{\partial x^2} + \sum_k a_k^\dagger a_k + \left(\frac{4\pi\alpha}{l}\right)^{1/2} \sum_k (a_{-k}^\dagger + a_k) e^{ikx} . \tag{1}$$

We have used $(\hbar/2m\omega_0)^{1/2}$ for a unit of length and $\hbar\omega_0$ for the unit of energy. The electron band mass is m, ω_0 is the unperturbed phonon frequency, and l is the length of the crystal lattice. Equation (1) is appropriate for an electron interacting with optical modes via a deformation potential interaction. However, it is often introduced as the simplest form of a polaron Hamiltonian [i.e., both the phonon frequency ω_0 and the interaction form factor $(4\pi\alpha/l)^{1/2}$ are independent of wave vector]. We have omitted the zero point energy in Eq. (1). The electron position is x and the phonon creation and destruction operators satisfy the usual commutation relations

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} . \tag{2}$$

Since we are interested in the strong-coupling theory where we expand in a series in $1/\alpha$, it is convenient to introduce an additional change of units, scaling energies with a factor $(2\pi\alpha)^2$ and lengths by a factor $(2\pi\alpha)^{-1}$, i.e.,

$$2\pi\alpha x \to x , \quad 2\pi\alpha l \to l \tag{3}$$

and

$$H/(2\pi\alpha)^2 \to H . \tag{4}$$

In terms of the new variables we have

$$H = -\frac{\partial^2}{\partial x^2} + \frac{1}{8\pi^2\alpha^2} \sum_k (p_k p_{-k} + q_k q_{-k} - 1) + \frac{1}{\pi\alpha l^{1/2}} \sum_k q_k e^{ikx} , \tag{5}$$

where the dimensionless lattice displacement coordinates q_k and their conjugate momenta p_k can be written in terms of phonon creation and annihilation operators

$$\begin{aligned} q_k &= (1/\sqrt{2})(a_k + a_{-k}^\dagger) , \\ p_k &= (1/i\sqrt{2})(a_{-k} - a_k^\dagger) , \end{aligned} \tag{6}$$

with

$$[q_k, p_{k'}] = i\delta_{kk'} . \tag{7}$$

Since the basic feature of strong coupling is that the electron creates a static lattice deformation and then becomes self-trapped in the potential well that is established by this deformation, we redefine the lattice-displacement field coordinates and conjugate momenta through the canonical displaced-oscillator transformation

$$\begin{aligned} q_k &\to q_k + d_k , \\ p_k &\to p_k , \end{aligned} \tag{8}$$

where the displacements d_k are taken as real and even functions of k,

$$d_k = d_k^* , \quad d_k = d_{-k} . \tag{9}$$

Under the change of variables of Eq. (8), the q_k and p_k now refer to fluctuations on the displaced field, and in terms of these new variables the Hamiltonian is given by

$$H = -\frac{\partial^2}{\partial x^2} + \frac{1}{8\pi^2\alpha^2} \sum_k (p_k p_{-k} + q_k q_{-k} - 1) + \frac{1}{8\pi^2\alpha^2} \sum_k d_k^2 + \frac{1}{4\pi^2\alpha^2} \sum_k d_k q_k + \frac{1}{\pi\alpha l^{1/2}} \sum_k d_k e^{ikx} + \frac{1}{\pi\alpha l^{1/2}} \sum_k q_k e^{ikx} . \tag{10}$$

We emphasize here that the property of translational invariance holds regardless of whether we express the Hamiltonian in terms of the original field variables or the new field variables. In terms of the original variables, the Hamiltonian of Eq. (5) commutes with the momentum operator

$$P = -i\frac{\partial}{\partial x} + \sum_k a_k^\dagger a_k k , \tag{11}$$

which generates translations of both the electron coordinate and the lattice distortion. In terms of the new variables, the Hamiltonian of Eq. (10) commutes with the momentum operator

$$P = -i\frac{\partial}{\partial x} + \sum_k a_k^\dagger a_k k - i\sum_k k d_k p_k , \tag{12}$$

which is obtained from Eq. (11) by the change of variables given in Eq. (8). In obtaining Eq. (12) we have also used the fact that d_k is an even function of k.

To this point, the displacements d_k have not been determined. We now choose the d_k by making a variational estimate of the ground-state energy of H with a trial eigenfunction of the form

$$|\psi_{tr}(x)\rangle = u(x)|0\rangle , \tag{13}$$

where $|0\rangle$ is the vacuum for phonons which are excitations relative to the displaced field. The expectation value of H in the trial state is given by

$$\begin{aligned} W(u;\{d_k\}) = &-\int_{-\infty}^{\infty} dx\, u^*(x)\frac{\partial^2}{\partial x^2}u(x) \\ &+ \frac{1}{\pi\alpha l^{1/2}}\sum_k d_k \int_{-\infty}^{\infty} dx\, u^*(x)u(x)e^{ikx} \\ &+ \frac{1}{8\pi^2\alpha^2}\sum_k d_k^2 \int_{-\infty}^{\infty} dx\, u^*(x)u(x) , \end{aligned} \tag{14}$$

where we have anticipated the limit $l \to \infty$ by extending the electronic coordinate integration over all space. We choose the "best" displacements and electronic wave function by minimizing W with respect to the set $\{d_k\}$ and with respect to the functional form of $u(x)$. Since we wish to maintain the normalization of $u(x)$ to unity in this procedure, we introduce a Lagrange multiplier λ, and then minimize

$$\tilde{W} = W - \lambda\int_{-\infty}^{\infty} dx\, u^*(x)u(x) . \tag{15}$$

The condition

$$\frac{\partial\tilde{W}}{\partial d_k} = 0$$

then gives

$$d_k = -(4\pi\alpha/l^{1/2})\rho_k \tag{16}$$

where

$$\rho_k = \int_{-\infty}^{\infty} dx\, u^*(x)u(x)e^{ikx} = \rho_{-k} , \tag{17}$$

with $u(x) = u(-x)$, while the condition

$$\delta\tilde{W}/\delta u^*(x) = 0 \tag{18}$$

then gives

$$-\frac{d^2}{dx^2}u(x) + \frac{1}{\pi\alpha l^{1/2}}\sum_k d_k e^{ikx}u(x) = \epsilon u(x) , \tag{19}$$

where

$$\epsilon = \lambda - \frac{1}{8\pi^2\alpha^2}\sum_k d_k^2 . \tag{20}$$

Substitution of Eq. (16) into Eq. (19) then gives a nonlinear Schrödinger-like equation (which is often referred to in the literature as the nonlinear Schrödinger equation)[7]

$$-\frac{d^2}{dx^2}u(x) - 4u^3(x) = \epsilon u(x) , \tag{21}$$

where we have taken $u(x)$ as real. This equation has been discussed previously in a related context[8,9] and possesses only one bound state, for which

$$\begin{aligned} &u(x) = (1/\sqrt{2})\,\mathrm{sech}\,x , \\ &\epsilon = -1 . \end{aligned} \tag{22}$$

For future purposes we also note that the potential well set up by the electron in the state given by Eq. (22) has a set of continuum eigenfunctions which obey the Schrödinger equation

$$-\frac{d^2}{dx^2}u_p(x) - 2\,\mathrm{sech}^2 x u_p(x) = \epsilon_p u_p(x) , \tag{23}$$

with solutions

$$\begin{aligned} &u_p(x) = l^{-1/2}e^{ipx}(p + i\tanh x)/(i+p) , \\ &\epsilon_p = p^2 . \end{aligned} \tag{24}$$

We emphasize that these states are not excited states of the nonlinear equation, Eq. (21), but they do constitute a convenient basis. In the limit of large but finite l these continuum states satisfy the orthonormality relations

$$\int_{-l/2}^{l/2} dx\, u_p^*(x)u_{p'}(x) = \delta_{pp'} . \tag{25}$$

We next calculate ρ_k from Eq. (17) with the result

$$\rho_k = \tfrac{1}{2}k\pi\,\mathrm{csch}\tfrac{1}{2}k\pi \tag{26}$$

and then determine from Eq. (16) that

$$\frac{1}{8\pi^2\alpha^2}\sum_k d_k^2 = \tfrac{2}{3} . \tag{27}$$

The variational estimate of the ground state energy of H is then

$$W_{\min} = -1 + \tfrac{2}{3} = -\tfrac{1}{3} . \tag{28}$$

With the displacements d_k determined above we now go back and write the Hamiltonian in the form $H = H_0 + H_1 + H_2$, where

$$H_0 = -\frac{\partial^2}{\partial x^2} - 2\,\mathrm{sech}^2 x + \tfrac{2}{3},$$

$$H_1 = \frac{1}{\pi\alpha l^{1/2}} \sum_k q_k (e^{ikx} - \rho_k), \tag{29}$$

$$H_2 = \frac{1}{8\pi^2\alpha^2} \sum_k (p_k p_{-k} + q_k q_{-k} - 1),$$

with ρ_k now given by Eq. (26). These various terms making up the Hamiltonian are of order 1, $1/\alpha$, and $1/\alpha^2$, respectively. The factor $l^{-1/2}$ in H_1 makes the factors e^{ikx} and ρ_k of the same scale as q_k.

As a next step in determining the energy eigenvalue spectrum, we expand any energy eigenfunction of the system as

$$|\psi(x)\rangle = u(x)\,|\phi\rangle + \sum_p u_p(x)\,|\phi_p\rangle, \tag{30}$$

where

$$H\,|\psi(x)\rangle = E\,|\psi(x)\rangle. \tag{31}$$

Because of the completeness of the $u(x)$ and $u_p(x)$, Eq. (30) is entirely general. The states $|\phi\rangle$ and $|\phi_p\rangle$ are the phonon parts of the state vector and are determined below. The normalization of $|\psi(x)\rangle$ and the orthonormalization of the electronic wave functions $u(x)$ and $u_p(x)$ then imply that

$$\langle\phi\,|\,\phi\rangle + \sum_p \langle\phi_p\,|\,\phi_p\rangle = 1. \tag{32}$$

By substitution of Eq. (30) into Eq. (31) we form the *partial* inner products with respect to the electronic wave functions $u(x)$ and $u_p(x)$ and obtain reduced coupled Schrödinger equations for the phonon parts of the energy eigenfunction

$$\int_{-\infty}^{\infty} dx\, u(x) H u(x)\,|\phi\rangle + \sum_p \int_{-\infty}^{\infty} dx\, u(x) H u_p(x)\,|\phi_p\rangle = E\,|\phi\rangle$$

and

$$\int_{-\infty}^{\infty} dx\, u_p^*(x) H u(x)\,|\phi\rangle + \sum_{p'} \int_{-\infty}^{\infty} dx\, u_p^*(x) H u_{p'}(x)\,|\phi_{p'}\rangle = E\,|\phi_p\rangle. \tag{33}$$

By explicit calculation using Eq. (29) we then find that

$$(-\tfrac{1}{3} + H_2)\,|\phi\rangle + \sum_p H_{1p}^{\dagger}\,|\phi_p\rangle = E\,|\phi\rangle \tag{34}$$

and

$$H_{1p}\,|\phi\rangle + \sum_{p'} H_{1pp'}\,|\phi_{p'}\rangle + (p^2 + \tfrac{2}{3} + H_2)\,|\phi_p\rangle = E\,|\phi_p\rangle, \tag{35}$$

where

$$H_{1p} = \int_{-\infty}^{\infty} dx\, u_p^*(x) H_1 u(x) \tag{36}$$

and

$$H_{1pp'} = \int_{-l/2}^{l/2} dx\, u_p^*(x) H_1 u_{p'}(x). \tag{37}$$

We note that all operators in Eqs. (34) and (35) are operators in the phonon space; the electronic coordinate has been removed from the problem. Equation (35) may now be solved for $|\phi_p\rangle$ in terms of $|\phi\rangle$. This may be done formally by writing

$$|\phi_p\rangle = D_p(E) H_{1p}\,|\phi\rangle + D_p(E) \sum_{p'} H_{1pp'}\,|\phi_{p'}\rangle, \tag{38}$$

where

$$D_p(E) = (E - p^2 - \tfrac{2}{3} - H_2)^{-1}. \tag{39}$$

By iteration we then find

$$|\phi_p\rangle = \Delta_p(E) H_{1p}\,|\phi\rangle, \tag{40}$$

where $\Delta_p(E)$ satisfies a type of Dyson equation

$$\Delta_p(E) = D_p(E) + D_p(E) \sum_{p'} H_{1pp'} \Delta_{p'}(E). \tag{41}$$

Upon substitution of Eq. (40) back into Eq. (34) we obtain

$$H_{\mathrm{ph}}\,|\phi\rangle = E\,|\phi\rangle, \tag{42}$$

where H_{ph} is an effective phonon Hamiltonian given by

$$H_{\mathrm{ph}} = -\tfrac{1}{3} + H_2 + \sum_p H_{1p}^{\dagger} \Delta_p(E) H_{1p}. \tag{43}$$

This effective Hamiltonian operates only in the phonon space but, in principle, gives the spectrum of the full Hamiltonian H. From Eq. (43) it is evident that H_{ph} is generally energy dependent in that it depends on E through $\Delta_p(E)$. In the present paper we will not attempt a general analysis of Eqs. (42) and (43), and we restrict the computation of H_{ph} to second order in $1/\alpha$. To this end we note that because H_{1p} is of order $1/\alpha$ we need $\Delta_p(E)$ only in the infinite α limit. From Eqs. (41) and (39) we then obtain

$$\lim_{\alpha\to\infty} \Delta_p(E) = (-\tfrac{1}{3} - p^2 - \tfrac{2}{3})^{-1} = -(1 + p^2)^{-1}, \tag{44}$$

where we have used the fact that $E \to -\frac{1}{3}$ in the in-

finite α limit. Hence through order $1/\alpha^2$ we obtain

$$H_{\rm ph} = -\tfrac{1}{3} + H_2 - \sum_p \frac{H_{1p}^\dagger H_{1p}}{p^2+1}. \tag{45}$$

From Eqs. (36), (22), (24), and (29) we calculate the operator

$$H_{1p} = \frac{1}{\sqrt{2}\alpha l}\sum_k q_k \frac{k}{p-i}\,\mathrm{sech}\frac{\pi}{2}(p-k), \tag{46}$$

in terms of which $H_{\rm ph}$ may be cast into a final form,

$$H_{\rm ph} = -\frac{1}{3} + \frac{1}{8\pi^2\alpha^2}\sum_k \left(p_k p_{-k} + q_k q_{-k} - 1 - \sum_{k'} V_{kk'} q_k q_{-k'} \right), \tag{47}$$

where

$$V_{kk'} = \frac{(2\pi)^2}{l^2} kk' \sum_p \frac{\mathrm{sech}\frac{1}{2}\pi(k-p)\,\mathrm{sech}\frac{1}{2}\pi(k'-p)}{(p^2+1)^2}. \tag{48}$$

Equations (47), (48), and (42) form the basis for most of the remaining work in this paper. From these equations the energy spectrum of the Hamiltonian H can be calculated, and from the form of Eq. (47) it is clear that the energy eigenvalue problem is reduced to finding new normal modes of the lattice vibrations. To this end we construct a set of linear combinations of the coordinates and conjugate momenta

$$\eta_n = \sum_k f_{nk} q_k, \quad \xi_n = \sum_k f_{nk}^* p_k, \tag{49}$$

where the coefficients f_{nk} comprise a unitary square matrix of dimension ν (equal to the number of optical degrees of freedom in the finite lattice) so that

$$q_k = \sum_{n=0}^{\nu-1} f_{nk}^* \eta_n, \quad p_k = \sum_{n=0}^{\nu-1} f_{nk} \xi_n. \tag{50}$$

If we choose the f_{nk} to obey the eigenvalue equation

$$\sum_{k'} V_{kk'} f_{nk'} = \lambda_n f_{nk}, \tag{51}$$

then the unitarity of f_{nk} is ensured by the Hermitian nature of the $V_{kk'}$. It is evident from Eq. (48) that $V_{kk'} = V_{-k,-k'}$, and it is therefore possible to choose the coefficients f_{nk} to have the property

$$f_{nk}^* = f_{n,-k}. \tag{52}$$

This ensures that the new coordinates η_n and conjugate momenta ξ_n are Hermitian. With the use of Eqs. (50) and (51), the phonon Hamiltonian $H_{\rm ph}$ may be written in terms of the new phonon coordinates η_n and conjugate momenta ξ_n as

$$H_{\rm ph} = -\frac{1}{3} + \frac{1}{8\pi^2\alpha^2}\sum_{n=0}^{\nu-1} (\xi_n^2 + \Omega_n^2 \eta_n^2 - 1), \tag{53}$$

with

$$\Omega_n^2 = 1 - \lambda_n. \tag{54}$$

In dimensionless units the unperturbed phonon frequencies are all unity. The effect of the electron-phonon interaction has been to shift these frequencies to the value $(1-\lambda_n)^{1/2}$. In fact, the eigenvalues λ_n all lie between zero and unity, and hence the modified frequencies are all real and *lower* than the unperturbed frequency. This lowering of the phonon frequencies can be understood by noting that the lattice vibrations under consideration are localized vibrations imposed on top of the static deformation created by the self-trapped electron. The static deformation constitutes the new equilibrium for the lattice, so that if the lattice were to vibrate around this position with the electron-charge density held fixed, it would vibrate with the original frequency $\omega_0 = 1$. It is then easy to see that if the electron-charge density is permitted to follow the lattice vibrations adiabatically, the restoring force, and hence the the frequency, will be reduced. Finally, before undertaking the calculation of the modified-phonon spectrum, we comment here that these frequencies are determined from the eigenvalues of the matrix $V_{kk'}$. From Eq. (48) it is clear that since $V_{kk'}$ is *independent* of the coupling constant α, then the phonon spectrum is — in the strong-coupling limit — independent of α.

III. INTEGRAL EQUATION FOR THE PHONON SPECTRUM

In order to facilitate the computation of the phonon spectrum, we take the limit of Eq. (51) as $l \to \infty$. In that limit the phonon wave number k and the unperturbed electron energy eigenvalue p^2 become continuous, and Eq. (51) then becomes an integral equation for the function $f_n(k)$. This equation will have nontrivial solutions only for certain eigenvalues λ_n. The integral equation obtained in the above limit is

$$\lambda_n f_n(k) = \int_{-\infty}^{\infty} dk' K(k,k') f_n(k'), \tag{55}$$

with

$$f_n(k) = (l/2\pi)^{1/2} f_{nk}, \tag{56}$$

where the kernel $K(k,k')$ is given by

$$K(k,k') = kk' \int_{-\infty}^{\infty} dp\, \frac{\mathrm{sech}\frac{1}{2}\pi(k-p)\,\mathrm{sech}\frac{1}{2}\pi(k'-p)}{(p^2+1)^2}. \tag{57}$$

We note that this kernel is both real and sym-

metric, and is positive in the sense that

$$\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\, \psi^*(k) K(k,k') \psi(k') \geq 0 \tag{58}$$

for any $\psi(k)$ for which the integral exists. From the theory of integral equations,[10] the eigenvalues λ_n are positive and the eigenfunctions are orthogonal to one another and can be normalized so that

$$\int_{-\infty}^{\infty} dk\, f_n^*(k) f_m(k) = \delta_{nm}. \tag{59}$$

In addition to the above properties of the kernel, we also note that it is an even function of its arguments in the sense that

$$K(-k,-k') = K(k,k'). \tag{60}$$

From this property it then follows that the eigenfunctions of the kernel are either even or odd. The index n can be chosen to reflect the parity of the eigenfunctions with

$$f_n(-k) = (-1)^n f_n(k) \tag{61}$$

and

$$\lambda_n f_n(k) = \int_0^{\infty} dk'\, K_+(k,k') f_n(k'), \quad n = 0, 2, 4, \ldots,$$
$$\lambda_n f_n(k) = \int_0^{\infty} dk'\, K_-(k,k') f_n(k'), \quad n = 1, 3, 5, \ldots, \tag{62}$$

where

$$K_\pm(k,k') = K(k,k') \pm K(k,-k'). \tag{63}$$

Furthermore, the property expressed in Eq. (52) can be attained by making $f_n(k)$ real for n even and pure imaginary for n odd. From the theory of integral equations,[10] the fact that the kernels $K_\pm(k,k')$ are positive and continuous enables us to write

$$K_\pm(k,k') = \sum_n{}' \lambda_n f_n^*(k) f_n(k'), \tag{64}$$

where the prime on the summation means that the sum is over either even or odd integers. In this way we may obtain two sum rules,

$$\sum_n{}' \lambda_n = \int_0^{\infty} dk\, K_\pm(k,k). \tag{65}$$

From Eqs. (63) and (57) we then find

$$\sum_n{}' \lambda_n = 4\,\frac{\ln 2 + \frac{1}{2}}{3} \quad (n \text{ even}),$$
$$\sum_n{}' \lambda_n = 4\,\frac{\frac{3}{2} - \ln 2}{3} \quad (n \text{ odd}). \tag{66}$$

It is interesting to note that for the odd-parity case, the integral equation can be solved exactly. The details of this fact are described in the Appendix, in which we show that for n odd

TABLE I. The polynomials $p_n(u)$ which are orthonormal in the sense of Eq. (68). Only those polynomials for odd n are related to the eigenfunctions of $K(k,k')$.

n	$p_n(u)$
0	$\frac{\sqrt{3}}{\pi}$
1	$\frac{\sqrt{15}}{\pi}\left(\frac{u}{\pi}\right)$
2	$\frac{1}{\pi}\left(\frac{7}{6}\right)^{1/2}\left[5\left(\frac{u}{\pi}\right)^2 - 1\right]$
3	$\frac{1}{\pi}\left(\frac{5}{8}\right)^{1/2}\left[7\left(\frac{u}{\pi}\right)^3 - 5\left(\frac{u}{\pi}\right)\right]$
4	$\frac{1}{\pi}\left(\frac{11}{240}\right)^{1/2}\left[21\left(\frac{u}{\pi}\right)^4 - 35\left(\frac{u}{\pi}\right)^2 + 4\right]$
5	$\frac{1}{\pi}\left(\frac{91}{1200}\right)^{1/2}\left[11\left(\frac{u}{\pi}\right)^5 - 35\left(\frac{u}{\pi}\right)^3 + 14\left(\frac{u}{\pi}\right)\right]$
6	$\frac{1}{\pi}\left(\frac{1}{6720}\right)^{1/2}\left[143\left(\frac{u}{\pi}\right)^6 - 770\left(\frac{u}{\pi}\right)^4 + 707\left(\frac{u}{\pi}\right)^2 - 60\right]$

$$f_n(k) = i\left(\frac{\pi}{2}\right)^{1/2} \frac{(\frac{1}{2}k\pi)\, p_n(\frac{1}{2}k\pi)}{\sinh(\frac{1}{2}k\pi)}, \tag{67}$$

where $p_n(u)$ is a polynomial of degree n. According to Eq. (59) these polynomials are thus orthonormal in the sense that

$$\int_{-\infty}^{\infty} du\, \frac{u^2}{\sinh^2 u}\, p_n(u) p_m(u) = \delta_{nm}. \tag{68}$$

Thus the polynomials can be generated by orthogonalization.[11] A few of the polynomials are given in Table I. For even n, we were not able to obtain a closed form solution.

Furthermore, as we show in the Appendix, the eigenvalues λ_n can be determined for the case of odd n by the simple formula

$$\lambda_n = 4/n(n+3), \quad n \text{ odd} \tag{69}$$

for which it follows that

$$\Omega_n = [1 - 4/n(n+3)]^{1/2}, \quad n \text{ odd}. \tag{70}$$

Again no such simple formula was found for the even-parity eigenvalues. We also point out that for $n = 1$, Eq. (70) gives $\Omega_1 = 0$, which means that this particular mode is not a vibration at all but is, in fact, a translation. The presence of this zero-frequency mode is then a manifestation of the fact that the strong-coupling perturbation theory developed here is inherently translationally invariant. We discuss this more thoroughly in Sec. IV.

While the even-parity eigenfunctions and eigenvalues are not found in closed form, we can determine them numerically. The eigenvalues λ_n were

TABLE II. Modified phonon frequencies Ω_n/ω_0.

Even-parity modes		Odd-parity modes		
n	Numerical	n	Exact	Numerical
0	0.647 50	1	0.	0.000 00
2	0.912 21	3	0.881 92	0.881 92
4	0.958 12	5	0.948 68	0.948 68
6	0.975 28	7	0.971 00	0.971 01
8	0.983 60	9	0.981 31	0.981 30
10	0.988 28	11	0.986 93	0.986 91
12	0.991 13	13	0.990 34	0.990 27
14	0.992 93	15	0.992 57	0.992 38
16	0.994 07	17	0.994 10	0.993 72
18	0.994 75	19	0.995 20	0.994 54

actually determined by first transforming the integral equation into one in which the kernel is given in closed form. To this end we note that the kernel $K(k,k')$ is of the form

$$K(k,k')=\int_{-\infty}^{\infty} dp\, G(k,p)G(k'p)\,, \tag{71}$$

where

$$G(k,p)=\frac{k\,\mathrm{sech}\frac{1}{2}\pi(k-p)}{p^2+1}. \tag{72}$$

Thus, upon multiplication of Eq. (55) by $G(k,p)$ and integration over k, we obtain

$$\lambda_n g_n(p)=\int_{-\infty}^{\infty} dp' J(p,p')g_n(p')\,, \tag{73}$$

where

$$J(p,p')=\int_{-\infty}^{\infty} dk\, G(k,p)G(k,p') \tag{74}$$

and

$$g_n(p)=\int_{-\infty}^{\infty} dk\, G(k,p)f_n(k)\,. \tag{75}$$

The new kernel is also symmetric and its eigenfunctions $g_n(p)$ have parity $(-1)^{n+1}$ [which is *opposite* that of the $f_n(k)$]. The eigenvalues λ_n are, of course, the same as before. The advantage of the new integral equation is that the internal integration of Eq. (74) can be done by contour integration to give the kernel in closed form,

$$J(p,p')=\frac{2}{3}\frac{p^2+p'^2+pp'+1}{(p^2+1)(p'^2+1)}\frac{p-p'}{\sinh\frac{1}{2}\pi(p-p')}\,. \tag{76}$$

The integral equation Eq. (73) can then be approximated by a matrix eigenvalue equation in a large but finite-dimensional space using Gaussian quadrature methods. The results of the eigenvalue determination using this numerical method are given in Table II for both even and odd values of n together with the exact eigenvalues for odd values of n.

IV. TRANSLATIONAL INVARIANCE

The translational invariance of the Hamiltonian H is expressed through the relation

$$[P,H]=0\,, \tag{77}$$

where H is given by Eq. (10) and P is given by Eq. (12). These operators can be decomposed as $H=H_0+H_1+H_2$ and $P=P_0+P_{-1}$, where the subscripts indicate the order, in $1/\alpha$, of the relevant terms. In particular H_0, H_1, and H_2 are given in Eq. (29), while

$$P_0=-i\frac{\partial}{\partial x}+\sum_k a_k^\dagger a_k k\,, \tag{78}$$

and

$$\Pi\equiv P_{-1}=-i\sum_k k d_k p_k\,. \tag{79}$$

Equation (77) may be separated into groups of terms of the same order in $1/\alpha$, and each group will then vanish separately with the result

$$[\Pi,H_0]=0\,, \tag{80a}$$

$$[P_0,H_0]+[\Pi,H_1]=0\,, \tag{80b}$$

$$[P_0,H_1]+[\Pi,H_2]=0\,, \tag{80c}$$

$$[P_0,H_2]=0\,. \tag{80d}$$

We now use these equations to see how translational invariance is manifest in $H_{\rm ph}$. Equations (80a) and (80d) can be easily verified by inspection and will not be needed. From Eqs. (80b) and (80c) we calculate the commutator of $H_{\rm ph}$ with the operator Π and show that it vanishes. To see this we multiply Eq. (80b) from the left by $u_p^*(x)$ and from the right by $u(x)$, and then integrate over x to obtain

$$[\Pi,H_{1p}]=\int_{-\infty}^{\infty} dx\, u_p^*(x)P_0u(x)(p^2+1)\,, \tag{81}$$

from which it also follows that

$$[\Pi,H_{1p}^\dagger]=-\int_{-\infty}^{\infty} dx\, u(x)P_0u_p(x)(p^2+1)\,. \tag{82}$$

In Eqs. (81) and (82) H_{1p} is the phonon operator defined in Eq. (36), and we have used the fact that Π is independent of electron variables. From Eqs. (81) and (82) we may now compute the commutator

$$[\Pi,H_{\rm ph}]=[\Pi,H_2]-\sum_p\frac{[\Pi,H_{1p}^\dagger]H_{1p}}{p^2+1}-\sum_p\frac{H_{1p}^\dagger[\Pi,H_{1p}]}{p^2+1}$$

$$=[\Pi,H_2]+\sum_p\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\,u(x)P_0u_p(x)u_p^*(y)H_1u(y)-\sum_p\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\,u(y)H_1u_p(y)u_p^*(x)P_0u(x)\,. \tag{83}$$

In Eq. (83) the electronic part of P_0 is a function of x and H_1 is a function of y. Since H_1 has zero expectation value in the state $u(y)$, we may include the bound state in the sum over intermediate states in Eq. (83) and then invoke closure to obtain

$$[\Pi, H_{\rm ph}] = [\Pi, H_2] + \int_{-\infty}^{\infty} dx\, u(x)[P_0, H_1]u(x)$$

$$= \int_{-\infty}^{\infty} dx\, u(x)([\Pi, H_2] + [P_0, H_1])u(x), \quad (84)$$

where in the last integral we use the fact that neither Π nor H_2 involves the electronic variables. Since the integrand in the last line of Eq. (84) vanishes by Eq. (80c), we conclude that the translational invariance of the system is expressed in terms of the effective-phonon Hamiltonian by

$$[\Pi, H_{\rm ph}] = 0. \quad (85)$$

By using Eq. (47) for $H_{\rm ph}$, we may write Eq. (85) as

$$\sum_k q_k \left(k d_k - \sum_{k'} V_{kk'} k' d_{k'} \right) = 0 \quad (86)$$

from which it follows that

$$k d_k = \sum_{k'} V_{kk'} k' d_{k'}. \quad (87)$$

This result is simply the statement that $k d_k$ is an eigenfunction of $V_{kk'}$ with eigenvalue equal to 1. From Eq. (54) this leads to a zero-frequency mode which is a translation of the system. From Eqs. (16) and (26) we also note that $d_k \sim \frac{1}{2}k\pi/\sinh\frac{1}{2}k\pi$ and hence the eigenfunction of $V_{kk'}$ associated with the translation is proportional to $\frac{1}{2}(k\pi)^2/\sinh\frac{1}{2}k\pi$, which is of the form given in Eq. (67) with $n = 1$. By normalizing this eigenfunction and giving it the phase needed to make the new coordinate and conjugate momentum Hermitian we obtain

$$f_{1k} = i k d_k \Big/ \left(\sum_k k^2 d_k^2 \right)^{1/2}. \quad (88)$$

Thus the relation between the new coordinate η_1 and the old coordinates q_k is given by Eq. (49)

$$\eta_1 = \sum_k f_{1k} q_{1k} = \chi \left(\sum_k k^2 d_k^2 \right)^{1/2}, \quad (89)$$

where

$$\chi = \chi^\dagger \equiv i \sum_k k d_k q_k \Big/ \left(\sum_k k^2 d_k^2 \right). \quad (90)$$

In addition, the new conjugate momentum ξ_1 is given by

$$\xi_1 = \sum_k f_{1k}^* p_k = \Pi \Big/ \left(\sum_k k^2 d_k^2 \right)^{1/2}, \quad (91)$$

where Π is defined in Eq. (79). It follows then from the canonical commutation rule

$$[\eta_1, \xi_1] = i \quad (92)$$

that

$$[\chi, \Pi] = i. \quad (93)$$

Hence χ is a coordinate which is conjugate to the operator Π which in turn generates translations to the order of approximation considered in this paper, and we may think of these variables as *polaron* position and momentum operators to that order. When higher-order terms are taken into account in $H_{\rm ph}$, the expressions for the polaron variables will change accordingly, and will be discussed in a separate publication. To justify this interpretation of χ and Π as polaron variables we express the phonon Hamiltonian in terms of Π, the generator of translations, rather than ξ_1. The effective Hamiltonian of Eq. (53) then becomes

$$H_{\rm ph} = -\frac{1}{3} + \frac{\Pi^2}{m^*} + \frac{1}{4\pi^2\alpha^2} \sum_{n\neq 1}^{\infty} A_n^\dagger A_n \Omega_n$$

$$+ \frac{1}{8\pi^2\alpha^2} \sum_{n=0}^{\infty} (\Omega_n - 1), \quad (94)$$

where

$$A_n = [1/(2\Omega_n)^{1/2}](\Omega_n \eta_n + i\xi_n), \quad n \neq 1 \quad (95)$$

is the localized phonon annihilation operator, and m^* is given (in units of the electron mass) by

$$m^* = 8\pi^2\alpha^2 \sum_k k^2 d_k^2 = \tfrac{2}{15}(4\pi\alpha)^4 \quad (96)$$

and is identical with the polaron effective mass obtained by Gross[4] when $4\pi\alpha$ of our work is replaced by $g^2/\sqrt{2}$ of his work.[12] We also note that in the units of our paper Π^2/m^* is the appropriate kinetic energy rather than $\Pi^2/2m^*$. To order $1/\alpha^2$ the Hamiltonian of Eq. (94) describes a free polaron of self-energy $-\frac{1}{3}$ and effective mass m^*, and free phonons of frequency Ω_n ($n \neq 1$).

Finally, the last term in Eq. (94) remains to be calculated. We write this term as

$$\frac{1}{8\pi^2\alpha^2} \sum_{n=0}^{\infty} (\Omega_n - 1) = \frac{1}{4\pi^2\alpha^2} \left(-\frac{1}{2} + \frac{1}{2} \sum_{n\neq 1} (\Omega_n - 1) \right). \quad (97)$$

The overall factor of $(4\pi^2\alpha^2)^{-1}$ is just the scale of energy. The term $-\frac{1}{2}$ is usually referred to as the localization energy, and is a lowering of the sys-

tem energy due to the fact that the translational degree of freedom should have no zero point energy associated with it. The term $\frac{1}{2}\sum_{n\neq 1}(\Omega_n - 1)$ is usually referred to as the fluctuation energy, and is a lowering of the system energy due to the fact that the electron responds to the zero-point motion of the lattice. This response shows up as a lowering of the phonon frequencies as discussed at the end of Sec. II. Each term in the sum $\sum_{n\neq 1}(1-\Omega_n)$ is positive, less than one, and rapidly approaches zero as n increases since $\Omega_n \to 1$ as $n \to \infty$. To make the convergence more rapid we use the identity

$$1-\Omega_n = \tfrac{1}{2}[(1-\Omega_n)^2 + \lambda_n], \tag{98}$$

where $\lambda_n = 1-\Omega_n^2$ is the eigenvalue of $V_{kk'}$. We now sum Eq. (98) over all n to obtain

$$\sum_{n=0}^{\infty}(1-\Omega_n) = \frac{1}{2}\sum_{n=0}^{\infty}(1-\Omega_n)^2 + \frac{1}{2}\sum_{n=0}^{\infty}\lambda_n . \tag{99}$$

The first sum on the right-hand side of Eq. (99) now converges more rapidly than does the left-hand side and the second sum on the right-hand side can be evaluated in the infinite-lattice limit by use of the sum rules of Eq. (66),

$$\frac{1}{2}\sum_{n=0}^{\infty}\lambda_n = \frac{4}{3}. \tag{100}$$

By numerical evaluation we find

$$\frac{1}{2}\sum_{n=0}^{\infty}(1-\Omega_n)^2 = 0.5764 . \tag{101}$$

Thus the combined localization energy and fluctuation energy is given by

$$\frac{1}{8\pi^2\alpha^2}\sum_{n=0}(\Omega_n - 1) = -\frac{0.9549}{4\pi^2\alpha^2} . \tag{102}$$

A numerical evaluation of the analogous term for the three-dimensional polaron with polarization interaction and optical phonons has been made by Miyaki.[6]

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APPENDIX

In this appendix we study integral transforms of the form

$$b_\mu(k) = \int_{-\infty}^{\infty} dk' K(k,k') a_\mu(k') , \tag{A1}$$

where

$$K(k,k') = kk' \int_{-\infty}^{\infty} dp \frac{\operatorname{sech}\frac{1}{2}\pi(k-p)\operatorname{sech}\frac{1}{2}\pi(k'-p)}{(p^2+1)^2} \tag{57}$$

and

$$a_\mu(k) = k^{\mu+1}/\sinh(\tfrac{1}{2}\pi k) . \tag{A2}$$

We will show below that *if* μ is an odd integer, then $b_\mu(k)$ is of the form

$$b_\mu(k) = \sum_{\sigma=1}^{\mu}{}' \gamma_{\sigma\mu} a_\sigma(k) , \tag{A3}$$

where the prime on the summation indicates that the sum is over odd integers only. We note that the integral transform contains only terms with $\sigma \leq \mu$. Invoking Eq. (A3) as an ansatz, we next construct the linear combination

$$\sum_{\mu=1}^{n}{}' C_\mu^{(n)} b_\mu(k) = \sum_{\mu=1}^{n}{}' \sum_{\sigma=1}^{\mu}{}' C_\mu^{(n)} \gamma_{\sigma\mu} a_\sigma(k) , \tag{A4}$$

where n is an odd integer. We then choose the coefficients $C_\mu^{(n)}$ to satisfy the eigenvector equation

$$\sum_{\mu=1}^{n}{}' \Gamma_{\sigma\mu}^{(n)} C_\mu^{(n)} = \lambda_n C_\sigma^{(n)} , \tag{A5}$$

where λ_n is an eigenvalue of the matrix

$$\Gamma_{\sigma\mu}^{(n)} = \begin{cases} \gamma_{\sigma\mu}, & 1 \leq \sigma \leq \mu \\ 0, & \mu < \sigma \leq n . \end{cases} \tag{A6}$$

The index n on the matrix $\Gamma_{\sigma\mu}^{(n)}$ has been introduced simply to make explicit the dimensionality of the vector space. Equation (A5) then implies that

$$\sum_{\mu=1}^{n}{}' \sum_{\sigma=1}^{\mu}{}' C_\mu^{(n)} \gamma_{\sigma\mu} a_\sigma(k) = \lambda_n \sum_{\sigma=1}^{n}{}' C_\sigma^{(n)} a_\sigma(k) , \tag{A7}$$

and from Eq. (A4) it then follows that

$$f_n(k) \equiv \sum_{\mu=1}^{n}{}' C_\mu^{(n)} a_\mu(k) \tag{A8}$$

is an eigenfunction of the kernel $K(k,k')$ for which the eigenvalue λ_n is an eigenvalue of the matrix $\Gamma_{\sigma\mu}^{(n)}$. More explicitly, we note that because $\Gamma_{\sigma\mu}^{(n)}$ is a triangular matrix, as stated in Eq. (A6), the secular equation for Eq. (A5) reduces to

$$\prod_{\mu=1}^{n}{}' (\gamma_{\mu\mu} - \lambda_n) = 0 . \tag{A9}$$

For $n=1$ we obtain $\lambda_1 = \gamma_{11}$. For $n=3$ both $\lambda_3 = \gamma_{11}$

and $\lambda_3=\gamma_{33}$ are solutions of Eq. (A9). However, the solution $\lambda_3=\gamma_{11}$ is extraneous since it would be degenerate with $\lambda_1=\gamma_{11}$, and this degeneracy is not present in the kernel. By increasing n in steps of two and ruling out degeneracy, we find that the eigenvalues of the kernel $K(k,k')$ are given by

$$\lambda_n=\gamma_{nn}, \quad n \text{ odd}. \tag{A10}$$

Although the eigenfunctions $f_n(k)$ can be found from Eq. (A8), it is much simpler to determine them by the Schmidt orthogonalization procedure or by a recursion relation as mentioned in Ref. 11.

We now go back and prove the validity of Eq. (A3) and obtain an expression for γ_{nn}. The integral transform in Eq. (A1) involves an integration over the phonon wave vector k' and, in the definition Eq. (57) of the kernel, an integration over the electron momentum p. The k' integration involves the integral

$$I_\mu(p)=\int_{-\infty}^{\infty} dk' \frac{k'^{\mu+2}}{\sinh\frac{1}{2}\pi k' \cosh\frac{1}{2}\pi(k'-p)}, \tag{A11}$$

which can be written as

$$I_\mu(p)=\left(\frac{\partial^{\mu+2}}{\partial t^{\mu+2}}\int_{C_1} dk' \frac{e^{tk'}}{\sinh\frac{1}{2}\pi k' \cosh\frac{1}{2}\pi(k'-p)}\right)_{t=0}, \tag{A12}$$

where the contour C_1 in the complex k' plane consists of the real axis with an infinitesimal semicircular displacement into the upper-half plane around the origin. The integral in Eq. (A12) can be evaluated from the residue theorem by considering the integral over the contour C_1 together with a similar integral over a contour displaced upward from C_1 in the complex k' plane by an amount $4i$. By this means we obtain

$$I_\mu(p)=N_\mu(p)/\cosh\tfrac{1}{2}\pi p, \tag{A13}$$

where

$$N_\mu(p)=2\left[\frac{\partial^{\mu+2}}{\partial t^{\mu+2}}\left(\frac{\cosh pt-\cos t}{\sin t}\right)\right]_{t=0}. \tag{A14}$$

By analytic continuation from real values of p, we note from Eq. (A11) that

$$I_\mu(\pm i)=\int_{-\infty}^{\infty} dk' \frac{k'^{\mu+2}}{\sinh\frac{1}{2}\pi k' \cosh\frac{1}{2}\pi(k'\mp i)} = \mp i\int_{-\infty}^{\infty} dk' \frac{k'^{\mu+2}}{\sinh^2\frac{1}{2}\pi k'}. \tag{A15}$$

Since μ is an odd integer, we conclude that $I_\mu(\pm i)=0$. However, from Eqs. (A13) and (A14) we note that $N_\mu(p)$ is a polynomial in p^2, and that because $\cosh(\pi i/2)=0$ and $I_\mu(\pm i)=0$, it follows that $N_\mu(p)$ must be of the form

$$N_\mu(p)=(p^2+1)^2 R_\mu(p), \tag{A16}$$

where $R_\mu(p)$ is a residual polynomial in p of even parity. To determine the degree of $R_\mu(p)$, we apply the Cauchy integral formula to Eq. (A14) and obtain

$$N_\mu(p)=\frac{(\mu+2)!}{\pi i}\oint_{C_2} dt \frac{\cosh pt-\cos t}{t^{\mu+3}\sin t}, \tag{A17}$$

where the contour C_2 encircles the origin in the complex t plane with $|t|<\pi$. The leading power of p is then determined by expanding $(\sin t)^{-1}=t^{-1}+t/6+\cdots$ and obtaining

$$N_\mu(p)=\frac{(\mu+2)!}{\pi i}\oint_{C_2} dt \frac{\cosh pt}{t^{\mu+4}}+\cdots = \frac{2}{\mu+3}p^{\mu+3}+\cdots. \tag{A18}$$

Thus $R_\mu(p)$ is a polynomial of degree $\mu-1$ and even parity.

We next do the integration over the electron momentum p which is implicit in the transform kernel. From Eqs. (A1), (57), and (A11) we have

$$b_\mu(k)=k\int_{-\infty}^{\infty} dp \frac{I_\mu(p)}{(p^2+1)^2\cosh\frac{1}{2}\pi(p-k)} \tag{A19}$$

which reduces through Eqs. (A13) and (A16) to

$$b_\mu(k)=k\int_{-\infty}^{\infty} dp \frac{R_\mu(p)}{\cosh\frac{1}{2}\pi p\cosh\frac{1}{2}\pi(p-k)}. \tag{A20}$$

It is important to note that the factors of p^2+1 have cancelled in Eq. (A20). If μ were an *even* integer, Eq. (A16) would not be true and there would remains a factor of p^2+1 in the denominator of Eq. (A20) which would invalidate the following analysis.

We next retain only the leading power of p in R_μ and calculate the integral

$$b_\mu(k)=\frac{2k}{\mu+3}\int_{-\infty}^{\infty} dp \frac{p^{\mu-1}}{\cosh\frac{1}{2}\pi p\cosh\frac{1}{2}\pi(p-k)}+\cdots=\frac{2k}{\mu+3}\left(\frac{\partial^{\mu-1}}{\partial t^{\mu-1}}\int_{-\infty}^{\infty} dp \frac{e^{tp}}{\cosh\frac{1}{2}\pi p\cosh\frac{1}{2}\pi(p-k)}\right)_{t=0}+\cdots, \tag{A21}$$

which, by a contour integration similar to that used in evaluating Eq. (A12), gives

$$b_\mu(k)=\frac{4k}{\mu+3}\frac{1}{\sin\frac{1}{2}\pi k}\left(\frac{\partial^{\mu-1}}{\partial t^{\mu-1}}\frac{e^{tk}-1}{\sin t}\right)_{t=0}+\cdots, \quad \text{(A22)}$$

where the expression in parentheses is a polynomial in k. Another application of the Cauchy integral formula then shows that $b_\mu(k)$ is of the form Eq. (A3) with the leading term given by

$$b_\mu(k)=\frac{4k}{\mu+3}\frac{(\mu-1)!}{\sinh\frac{1}{2}\pi k}\oint_{C_2}\frac{dt}{2\pi i}\frac{e^{tk}}{t^{\mu+1}}+\cdots$$

$$=\frac{4}{\mu(\mu+3)}\frac{k^{\mu+1}}{\sinh\frac{1}{2}\pi k}+\cdots. \quad \text{(A23)}$$

Since the lower even powers of p in $R_\mu(p)$ will produce only lower even powers of k in $b_\mu(k)$ through Eq. (A20), we have proven the ansatz equation (A3) and have determined that

$$\lambda_n=\gamma_{nn}=4/n(n+3). \quad \text{(A24)}$$

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