Ground-State Theorem for Free Polarons

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A ground-state theorem for the Fröhlich polaron is derived. We show that the zeroth moment of the current-current correlation function is proportional to the kinetic energy of the polaron. While the electron-phonon interaction does not depend on the electron mass, the coupling constant α does; this allows us to relate the kinetic energy with the ground-state energy using the Feynman-Helmann theorem. As an example we compare the polaron ground-state energy on variational grounds with the ground-state energy obtained from the function $\chi(\omega)$ calculated by Feynman, Hellwarth, Iddings, and Platzman. For $\alpha < 5$ both ground-state energies turn out to be identical, as can be concluded from numerical calculations.

INTRODUCTION

It is well known that the nth moment of a response function (for $T=0$) can be written as the average of an operator over the ground state. In some cases the average can be calculated directly and one obtains a sum rule,[1] in other cases the average can be correlated with the ground-state energy. For instance: In the degenerate electron gas, the first moment of the electronic polarizability is proportional to the interaction energy. With the use of the Feynman-Hellman theorem, this energy can be converted into the ground-state energy by considering the electron charge as a parameter.[2] One then obtains a method to compare an approximative calculation of the polarizability with an energy that can be calculated on variational grounds.

We derive here a ground-state theorem valid for the self-field of a particle, relying only on the long-wavelength behavior of the current-current correlation function. Using the scale properties of the polaron system, we were able to relate the ground-state and the kinetic energy by a differential equation with an appropriate initial condition; it was also possible to show that the absolute value of the interaction energy equals four times the kinetic energy and that a simple relation between the number of virtual phonons in the polaron cloud and the ground-state energy could be established.

As an example, we have compared the ground-state energy derived from the function $\chi(\omega)$ calculated by Feynman, Iddings, Hellwarth, and Platzman (henceforth denoted by FHIP)[3,4] and the ground-state energy calculated by Feynman.[5] It turns out that for the range of the coupling constant that we have investigated ($\alpha<5$) there is no deviation between both values for the ground-state energy.

DERIVATION OF A SUM RULE

Let us consider the current-current correlation function for a free-charge carrier in interaction with a phonon field. This function is given in the linear-response theory by the following expression[6]:

$$\chi_{jj}(\omega)=\int_{-\infty}^{\infty} dt\,\tilde{\chi}_{jj}(t)e^{i\omega t} , \tag{1}$$

where $\tilde{\chi}_{jj}(t)$ is an average over the ground state for low temperature:

$$\tilde{\chi}_{jj}(t)=(i/\hbar)\Theta(t)\langle[\bar{j}_x(t),\bar{j}_x(0)]\rangle . \tag{2}$$

$\bar{j}_x(t)$ is the current operator in the Heisenberg picture and is given by the momentum of the charge carrier multiplied by the ratio of the charge and mass of the carrier, at least in the Fröhlich model[7,8] where a parabolic energy-momentum relation is considered for the charge carrier. The mass is the band mass of the carrier. $\Theta(t)$ is the Heaviside step function:

$$\bar{j}_x(t)=e^{(i/\hbar)Ht}(e/m)\bar{p}_x e^{-(i/\hbar)Ht} , \tag{3}$$

where H is the Fröhlich Hamiltonian:

$$H=\frac{p^2}{2m}+\sum_{\vec{k}}\hbar\omega_L a_{\vec{k}}^\dagger a_{\vec{k}}+\sum_{\vec{k}} V_k a_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}+V_k^* a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{r}} . \tag{4}$$

The component V_k of the electron-phonon interaction matrix is given by

$$V_k=-(i/k)[(2\pi\omega_L/V)e^2(1/\epsilon_\infty-1/\epsilon_0)]^{1/2} , \tag{5}$$

where ϵ_∞ and ϵ_0 are, respectively, the dynamic and static dielectric constant. The electron-phonon interaction is independent of the electron mass; this is a consequence of the electrostatic nature of the interaction.

Writing down the spectral representation of the current-current correlation function, one shows that the integral over the positive frequencies of this function is proportional to the kinetic energy. To obtain the spectral representation one introduces the complete set of eigenfunctions of the Fröhlich Hamiltonian and integrates over the time explicitly:

$$\chi_{jj}(\omega)=\sum_n \frac{1}{\hbar}\,|\langle\Phi_0|\,\bar{j}_x\,|\Phi_n\rangle|^2 \times\left(\frac{-1}{\omega+i\epsilon-\omega_{n0}}+\frac{1}{\omega+i\epsilon+\omega_{n0}}\right), \tag{6}$$

where

$$\omega_{n0}=(1/\hbar)(E_n-E_0)\ .$$

An integration over all the positive frequencies of the imaginary part of the current-current correlation function can be done easily considering that

$$\frac{1}{x+i\epsilon}=\mathcal{P}(1/x)-i\pi\,\delta(x)\ , \tag{7}$$

where $\mathcal{P}$ stands for principal value and $\delta(x)$ is the Dirac δ function:

$$\int_0^\infty d\omega\,\mathrm{Im}\chi_{jj}(\omega)=(\pi/\hbar)\sum_n\,|\langle\Phi_0|\,\bar{j}_x\,|\Phi_n\rangle|^2\ . \tag{8}$$

After summation over the complete set one obtains

$$\int_0^\infty d\omega\,\mathrm{Im}\chi_{jj}(\omega)=\frac{2\pi e^2}{\hbar m}\,\langle\Phi_0|\,p_x^2/2m\,|\Phi_0\rangle=\frac{2\pi e^2}{3m\hbar}\,E_{\mathrm{kin}} \tag{9}$$

For symmetry reasons the x component of the kinetic energy is one-third of the total kinetic energy.

GROUND-STATE THEOREM AND SCALE TRANSFORMATION

The ground-state energy of the polaron is given by

$$E^0=\langle\Phi_0|\,H\,|\Phi_0\rangle\ ; \tag{10}$$

if this energy depends on a parameter, than the Feynman-Hellmann theorem states that

$$\frac{dE^0}{d\lambda}=\left\langle\Phi_0\left|\,\frac{dH}{d\lambda}\,\right|\Phi_0\right\rangle\ . \tag{11}$$

If one takes the inverse of the mass $\lambda=1/m$ as a parameter, one obtains

$$\frac{dE^0}{d\lambda}=\langle\Phi_0|\,\tfrac{1}{2}p^2\,|\Phi_0\rangle=\frac{1}{\lambda}\,E_{\mathrm{kin}}\ . \tag{12}$$

Although one now obtains a differential equation that relates the kinetic energy with the ground-state energy, the integral of this equation is difficult to solve due to the lack of an appropriate initial condition. Now, one changes the Hamiltonian to dimensionless units by the following scale transformation[9]: As the unit of energy one uses the energy of the longitudinal-optical phonons

$$E^0\to F^0\hbar\omega_L \tag{13}$$

and as the unit of length one uses

$$\vec{r}\to\vec{u}(2m\omega_L/\hbar)^{-1/2}\ ; \tag{14}$$

the wave vector then becomes

$$\vec{k}\to\vec{v}(2m\omega_L/\hbar)^{1/2}\ . \tag{15}$$

The dimensionless Hamiltonian is then given by

$$F^0|\,\Phi_0\rangle=\Big(-\nabla^2+\sum_{\vec{v}}a_{\vec{v}}^\dagger a_{\vec{v}}+\sum_{\vec{v}}\,(\gamma_v a_{\vec{v}}e^{i\vec{v}\cdot\vec{u}}+\gamma_v^* a_{\vec{v}}^\dagger e^{-i\vec{v}\cdot\vec{u}})\Big)\,|\,\Phi_0\rangle, \tag{16}$$

where

$$\gamma_v=-(i/v)(4\pi\alpha/V)^{1/2} \tag{17}$$

and α is the well-known polaron coupling constant

$$\alpha=\tfrac{1}{2}(e^2/\hbar\omega_L)(1/\epsilon_\infty-1/\epsilon_0)(2m\omega_L/\hbar)^{1/2}\ . \tag{18}$$

This shows that F^0 is a function of α only. It should be stressed that the scale transformation is not a scale symmetry for the Hamiltonian, but only an elegant way to indicate the dependence of the ground-state energy on the coupling constant. Based on this property of the ground-state energy, one obtains some useful relations for this energy. Using the mass dependence of the coupling constant one can express the kinetic energy as a function of the derivative of the ground-state energy with respect to α:

$$E_{\mathrm{kin}}=\lambda\,\frac{dE^0}{d\lambda}=\lambda\,\frac{dE^0}{d\alpha}\,\frac{d\alpha}{d\lambda}=-\tfrac{1}{2}\alpha\,\frac{dE^0}{d\alpha} \tag{19}$$

because

$$\frac{d\alpha}{d\lambda}=-\frac{1}{2}\,\frac{\alpha}{\lambda}\ . \tag{20}$$

In the same way, the interaction energy can be derived from the ground-state energy

$$E_{\mathrm{int}}=2\alpha\,\frac{dE^0}{d\alpha}\ . \tag{21}$$

From Eqs. (19) and (21) it follows that the ratio of the interaction energy to the kinetic energy is a constant for all values of the coupling constant:

$$E_{\mathrm{int}}/E_{\mathrm{kin}}=-4\ . \tag{22}$$

This is a generalization for the whole range of the coupling constant of the 1:4 relation of a theorem derived by Pekar[10] for free polarons in a classical dielectric (strong-coupling limit). Combining Eqs. (19) and (21) one finds the number of virtual phonons in the polaron cloud, i.e., the energy of those phonons divided by the energy of one phonon,

$$N(\alpha)=F^0(\alpha)-\tfrac{3}{2}\alpha\,\frac{dF^0(\alpha)}{d\alpha}\ . \tag{23}$$

Equation (19) allows for solving the differential equations formally with the initial condition that the ground-state energy is equal to $E^0(0)$ for α zero:

$$E^0(\alpha)-E^0(0)=-2\int_0^\alpha\frac{d\alpha'}{\alpha'}\,E_{\mathrm{kin}}(\alpha')\ . \tag{24}$$

Using the sum rule for the kinetic energy, we obtain the ground-state theorem for the current-

current correlation function

$$E^0(\alpha) - E^0(0) = -\frac{3m\hbar}{e^2}\int_0^\alpha \frac{d\alpha'}{\alpha'}\int_0^\infty \frac{d\omega}{\pi}\,\mathrm{Im}\chi_{jj}(\omega,\alpha') \tag{25}$$

DISSIPATION AND GROUND-STATE THEOREM

As an example, one obtains the ground-state energy in the weak-coupling limit (α small) using the expression of Gurevich, Lang, and Firsov[11] for the current-current correlation function

$$-3\int_0^\alpha \frac{d\alpha'}{\alpha'}\int_0^\infty \frac{d\omega}{\pi}\,\mathrm{Im}\chi_{jj}^{\mathrm{GLF}}(\omega,\alpha') = -\alpha\ , \tag{26}$$

where

$$\begin{aligned}\mathrm{Im}\chi_{jj}^{\mathrm{GLF}} &= \tfrac{2}{3}\alpha\pi\omega^{-2}(\omega-1)^{1/2} \quad (\omega>1)\\ &= 0 \quad (\omega<1)\ .\end{aligned} \tag{27}$$

The units are $m=\omega_L=\hbar=e=1$.

In order to obtain an expression for the ground-state energy, which is valid for a wider range of the coupling constant, we have used the function $\chi(\omega)$ as defined in FHIP. Therefore, it is useful to indicate the relation between the current-current correlation function and the function $\chi(\omega)$. The current-current correlation function is defined as the linear coefficient that relates the change of the current in the system with the vector potential applied to the system:

$$\Delta\bar{j}_\omega = \chi_{jj}(\omega)\bar{A}_\omega\ . \tag{28}$$

In FHIP, the impedance function $Z(\omega)$ is defined as the coefficient between the current and the applied electric field:

$$\Delta\bar{j}_\omega = [1/Z(\omega)]\bar{E}_\omega\ . \tag{29}$$

Using the relation between the electric field and the vector potential one obtains

$$\chi_{jj}(\omega) = -i\omega/Z(\omega)\ . \tag{30}$$

Combining relation (30) with the equation for $\chi(\omega)$, which happens to be an auxiliary correlation function in the FHIP approach, we obtain

$$i\omega Z(\omega) = \omega^2 - \chi(\omega)\ . \tag{31}$$

One obtains

$$\mathrm{Im}\chi_{jj}(\omega) = \frac{\omega^2\,\mathrm{Im}\chi(\omega)}{\omega^4 - 2\omega^2\,\mathrm{Re}\chi(\omega) + |\chi(\omega)|^2}\ . \tag{32}$$

An expression equivalent to (32) was first considered in the earlier work of the present authors[4,12]; using the expression for $\mathrm{Re}\chi(\omega)$ obtained in Ref. 4, we were able to perform numerically the two integrations on the IBM 1130 computer of the University of Antwerp. The range for the integration over the frequency is divided in two parts; the first part contains the basic physical information, i.e., one integrates until a frequency, which is greater than the characteristic frequencies of the system which are the one-phonon relaxed-excited-state and the Franck-Condon frequency; the second part handles the asymptotic behavior, the current-current correlation function:

$$\lim_{\omega\to\infty} \mathrm{Im}\chi_{jj}(\omega) = \tfrac{2}{3}\pi(\alpha/\omega^2)(\omega)^{1/2}\ . \tag{33}$$

The first part is treated by an adaptive integration technique[13] and the second by Gaussian quadrature.[14]

After the integrating over the frequency, one obtains the kinetic energy: It is a monotonic increasing function of the coupling constant, and the numerical integration is done using standard methods. As a result, one obtains a ground-state energy which is equal to the Feynman ground-state energy. The two energies are compared in Fig. 1, and in Table I, the ground-state energy resulting from the calculation is given for a set of coupling constants.

DISCUSSION

We have derived this ground-state theorem for free polarons. It can be generalized without any difficulty for a whole class of particle-field interactions, which do not depend on the mass of the particle as long as the energy-momentum relation of the particle is parabolic the last restriction is

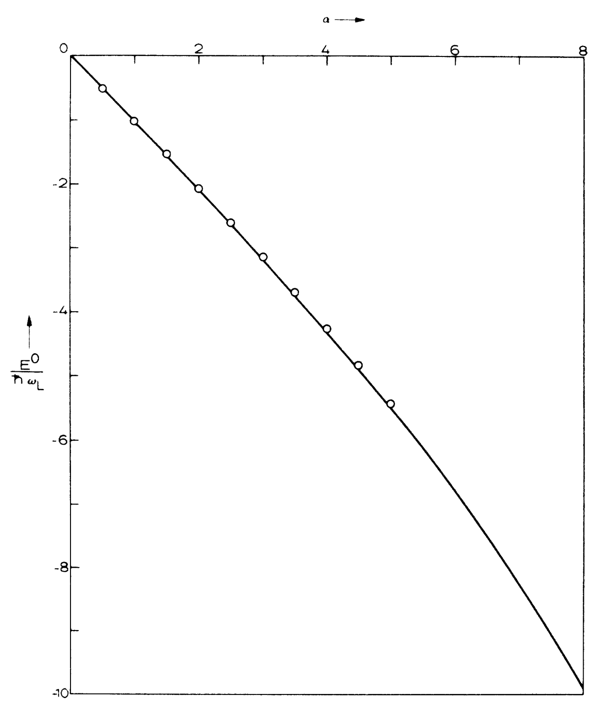

FIG. 1. Feynman ground-state energy is indicated by a solid line, while the dots are the energies calculated using the ground-state theorem.

TABLE I. Ground-state energy.

α	E^0 theorem
0.5	−0.503
1.0	−1.014
1.5	−1.533
2.0	−2.059
2.5	−2.593
3.0	−3.135
3.5	−3.687
4.0	−4.251
4.5	−4.831
5.0	−5.430

necessary, otherwise the expectation value of the square of the velocity is not directly proportional to the kinetic energy, and there is an additional term in the current-current correlation function arising from the nonparabolicity.[15]

The analysis we made, concerning the relations between the ground-state energy and other expectation values over the ground state, can also be generalized for the same class of particle-field interactions.

From the Gurevich-Lang-Firsov expression for the current-current correlation function we obtain the same ground-state energy as the second-perturbation ground-state energy[7] or the Lee-Low-Pines ground-state energy[7]; there is no way to make a distinction between both with the use of the ground-state theorem, because the current-current correlation function happens to be identical for both approximations as far as the weak-coupling limit is concerned.[12]

From the function $\chi(\omega)$ of FHIP we obtained the Feynman ground-state energy. Although both calculations are evaluated in the framework of the path-integral formulation of quantum mechanics, there is a *a priori* reason why they should be equivalently accurate. The accuracy of the Feynman variational approach was tested on a exactly soluble model.[16] Obtaining the same result for the ground state using FHIP $\chi(\omega)$ function, we may claim that this function treats the excited states of the polaron with relatively great accuracy. The asymptotic expansion of the $\chi(\omega)$ function turns out to be the asymptotic expansion obtained from the Gurevich-Lang-Firsov expression of the current-current correlation function. This is not so surprising because the expansion is the tail of the one-phonon contribution to the current-current correlation function. This contribution does not strongly depend on the range of the coupling constant, at least for $\alpha < 5$. Since for this range of the coupling constant all the basic phenomena are incorporated in the spectrum of the current-current correlation function, we felt it not opportune to extend the numerical calculations for greater coupling.

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