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Polaron in N dimensions

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The self-energy of a polaron in general n dimensions is calculated with the use of a dispersion-theory approach. Our result agrees with the result of Peeters *et al.* up to order α, the Fröhlich coupling constant. We also obtain the general expression for the effective mass in n dimensions. As expected, the polaronic effects become negligible as the dimensions of the space increase.

I. INTRODUCTION

For the last 40 years there has been considerable interest[1-3] in theoretical and experimental studies of polaronic properties. It was the first problem in solid-state physics to be treated using field-theoretic methods. The basic concept of the polaron as a composite particle consisting of a bare electron and the accompanying polarization of the lattice was introduced by Fröhlich.[1] Much of the work on the polaron theory is based on the Fröhlich model. The earlier work is mainly devoted to polaronic properties in three-dimensional crystals, but more recent work deals with polarons in two dimensions. This new development is attributed to technological progress in the production of systems in which electronic motion is restricted to two dimensions. In a recent paper Peeters, Xiaoguang, and Devreese[4] have developed a polaronic model for an arbitrary space of n dimensions. The treatment is consistent with the results of two- and three-dimensional polaronic results when the appropriate limit is considered. The present paper deals with the polaron in n dimensions but the approach followed in this paper is considerably different from the approach followed by Peeters *et al.*[4] While Peeters and collaborators derive their result by extending the Fröhlich Hamiltonian to n dimensions, in this paper we follow the dispersion-energy formalism appropriate to the n-dimensional polaron. Apart from the difference between our approach and that of the earlier authors, specifically we calculate the ground-state energy as well as the energy of a slow moving polaron within the linear approximation in the electron-lattice coupling, while Peeters *et al.* calculate only the ground-state energy—up to second-order terms in the electron-lattice coupling. Where comparison is possible, our results agree with the results of Peeters *et al.*

To generalize the Frölich Hamiltonian, Peeters *et al.* make use of the idea that it is possible to obtain the polaron Hamiltonian in lower dimensions from the Hamiltonian in higher dimensions by integrating out one or more dimensions. Furthermore, these authors assume that the electron interaction which causes the polarization is the same as in three dimensions, but that the electron motion is assumed to be in n-dimensional space. Thus, if we define by x_n the nth position coordinate and by k_n the nth wave number of the electron, then the position vector $\mathbf{r}$ and the wave vector $\mathbf{k}$ are, respectively, given by

$$|\mathbf{r}| = \left[\sum_{n=1} (x_n)^2\right]^{1/2}, \tag{1}$$

$$|\mathbf{k}| = \left[\sum_{n=1} (k_n)^2\right]^{1/2}, \tag{2}$$

and

$$\mathbf{k}\cdot\mathbf{r} = \sum_{n=1} k_n x_n . \tag{3}$$

Making use of Eqs. (1)—(3), Peeters *et al.* are able to generalize the Fröhlich Hamiltonian to n-dimensional space. By combining the generalized Fröhlich Hamiltonian and Feynman path integral method these authors have calculated the ground-state energy (i.e., an electron at the bottom of the conduction band) for the polaron up to quadratic terms in α, the Fröhlich coupling constant.

Our approach is different from that of the earlier authors. Most importantly it is not based on the Fröhlich Hamiltonian. We follow the dispersion-theory formalism and using Eqs. (1)—(3) generalize this approach to the n-dimensional space. The basic idea in our formalism is that the polaron energy is given by the difference in the zero-point energy of the radiation field of the electron-lattice system when the interaction energy between the electron and the lattice is present and when it is absent. We believe that this approach is simple and physically transparent. Moreover, it provides a valid alternative approach to the polaron in n-dimensional space. The application of this approach to the polaron theory in three dimensions was proposed by Hawton and Paranjape[5] and by Mahanty and Paranjape.[6] The generalization of this to n dimensions is proposed in this paper. Using this approach we have obtained the polaron energy in n-dimensional space for a slow moving electron. Our calculations are restricted to linear terms in α—the Fröhlich coupling constant. Our results agree with the results of Peeters *et al.* for the ground-state energy up to linear terms in the coupling constant.

The sketch of the dispersion theory is given in the following section since the details of the theory can be found in the earlier papers.[5,6] The generalization procedure of the dispersion theory to n dimensions is also provided in this section. The comparison of our work with that of Peeters *et al.* is given in the concluding section.

II. DISPERSION THEORY

In the dispersion theory the interaction energy between a particle and a given medium can be obtained if the dielectric response of the medium is given. For a polar crystal the frequency-dependent dielectric constant can be expressed by

$$\epsilon(\omega)=\epsilon(\infty)+\frac{\epsilon(0)-\epsilon(\infty)}{1-\omega^2/\omega_T^2}\ , \tag{4}$$

where $\epsilon(\infty)$ and $\epsilon(0)$ are the dielectric constants for infinite and zero frequency, respectively, and ω_T^2 is the transverse-optical-mode frequency of the polar lattice. The longitudinal-optical-mode frequency ω_0 is related to ω_T by the well-known Lyddane-Sachs-Teller relation[7]

$$\frac{\omega_0^2}{\omega_T^2}=\frac{\epsilon(0)}{\epsilon(\infty)}\ . \tag{5}$$

Consider a frequency-dependent field $\mathbf{E}(\mathbf{r}',\omega)$ at point $\mathbf{r}'$ in the crystal. The field causes polarization of the electron-lattice system, producing a polarization-induced field $\mathbf{E}(\mathbf{r},\omega)$ at point $\mathbf{r}$. If the generating and generated fields are the same, then a self-consistent equation for the fields at $\mathbf{r}$ and $\mathbf{r}'$ is given by

$$\mathbf{E}(\mathbf{r},\omega)=\int \overleftrightarrow{\mathrm{F}}(\mathbf{r},\mathbf{r}',\omega)\cdot\mathbf{E}(\mathbf{r}',\omega)\,d^3r'\ , \tag{6}$$

where $\overleftrightarrow{\mathrm{F}}(\mathbf{r},\mathbf{r}',\omega)$, the nonlocal tensor, is determined by the polarizing properties of the electron and the medium. Thus $\overleftrightarrow{\mathrm{F}}(\mathbf{r},\mathbf{r}',\omega)$ depends on the electronic state and the state of the lattice. In an extreme case $\overleftrightarrow{\mathrm{F}}(\mathbf{r},\mathbf{r}',\omega)$ is equal to $\delta(\mathbf{r}-\mathbf{r}')$ if the electron lattice is replaced by an empty space. In this calculation we consider the electron state to be a plane-wave state $|\,k_0\rangle$ and the lattice whose dielectric response, given by (4), is assumed to be at temperature $T=0$. The form of $F(\mathbf{r},\mathbf{r}',\omega)$ for a three-dimensional crystal is given earlier by Hawton and Paranjape.[5] Its generalization to n dimensions is required. Assuming for the time being that $\overleftrightarrow{\mathrm{F}}(\mathbf{r},\mathbf{r}',\omega)$ is known, it is possible to rewrite Eq. (6) in terms of its Fourier components according to

$$\mathbf{E}(\mathbf{k},\omega)=\sum_{\mathbf{k}'}\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k}',\omega)\cdot\mathbf{E}(\mathbf{k}',\omega)\ . \tag{7}$$

Clearly the eigenvalues of the frequencies for the system are given by the roots of the secular determinant, $D(\omega)$, given by

$$D(\omega)=|\,\overleftrightarrow{\mathrm{I}}\delta_{\mathbf{k},\mathbf{k}'}-\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k}',\omega)\,|=0\ . \tag{8}$$

If the interaction between the electron and the lattice is neglected, then the frequencies of the system are determined by the roots of the secular determinant

$$D^0(\omega)=|\,\overleftrightarrow{\mathrm{I}}\delta_{\mathbf{k},\mathbf{k}'}-\overleftrightarrow{\mathrm{F}}_0(\mathbf{k},\mathbf{k}',\omega)\,|=0\ . \tag{9}$$

The self-energy of the electron, in the dispersion theory,[8] is given by the difference in the zero-point energies with and without the interaction according to

$$\Delta E_s=-\frac{\hbar}{4\pi i}\oint d\omega\,\mathrm{Tr}\ln\left[\frac{D(\omega)}{D^0(\omega)}\right]\ , \tag{10}$$

where the contour encloses the real positive axis of the complex ω plane. Expanding the ln term in (10) and restricting ourselves to the first term in the expansion which corresponds to the linear effect of the electron-lattice coupling, we get

$$\Delta E_s=-\frac{\hbar}{4\pi i}\oint d\omega\,\mathrm{Tr}[\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k}',\omega)-\overleftrightarrow{\mathrm{F}}_0(\mathbf{k},\mathbf{k}',\omega)]\ . \tag{11}$$

We now obtain $\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k}',\omega)$ for our system as follows. Consider a frequency-dependent potential $\phi(\mathbf{r},\omega)$. Using the time-dependent perturbation theory it is possible to calculate the effect of the potential on the state $|\,k_0\rangle$. We may then write the expectation value of any physical quantity $\hat{0}$ for the perturbed state. It is given by

$$\langle\Delta O\rangle=\sum_{\mathbf{k}'}\left[\frac{\langle\mathbf{k}_0\,|\,\hat{0}\,|\,\mathbf{k}'\rangle\langle\mathbf{k}'\,|\,-e\phi(\mathbf{r},\omega)\,|\,\mathbf{k}_0\rangle}{E_{\mathbf{k}'}-E_{k_0}-\hbar\omega}+\frac{\langle\mathbf{k}_0\,|\,-e\phi(\mathbf{r},\omega)\,|\,\mathbf{k}'\rangle\langle\mathbf{k}'\,|\,\hat{0}\,|\,\mathbf{k}_0\rangle}{E_{k'}-E_{k_0}+\hbar\omega}\right]\ , \tag{12}$$

where $\hat{0}$ is the operator corresponding to the physical quantity O and E_k is the energy of the particle in plane-wave state $|\,k\rangle$. The self-consistent equation for the electric field $\mathbf{E}$ in the form given by Eq. (7) is obtained as follows. Let

$$\hat{0}=\nabla_{\mathbf{r}'}\frac{e}{|\,r'-r'\,|\,\epsilon(\omega)}\ , \tag{13}$$

where $\hat{0}$ is the electric field at $\mathbf{r}'$ due to a charge e at $\mathbf{r}$ and the screening due to the lattice polarization is considered in (13) through $\epsilon(\omega)$. We also express $\phi(\mathbf{k},\omega)$ in terms of $\mathbf{E}(\mathbf{k},\omega)$ using Poisson's equation, as

$$i\,\mathbf{k}\cdot\mathbf{E}(\mathbf{k},\omega)=k^2\phi(\mathbf{k},\omega)\ . \tag{14}$$

Substituting (13) and (14) in (12) and writing $1/|\,\mathbf{r}-\mathbf{r}'\,|$ in n-dimensional space as

$$\frac{1}{|\,\mathbf{r}-\mathbf{r}'\,|}=\frac{\Gamma((n-1)/2)}{2\pi^{(n+1)/2}}\int\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^{n-1}}d^nk\quad\text{for } n\geq 2\ , \tag{15}$$

then by comparison between the resultant Eqs. (12) and (7), we obtain

$$\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k}',\omega)=\frac{(2\pi)^n e^2}{L^n\hbar\epsilon(\omega)}\frac{\Gamma((n-1)/2)}{2\pi^{(n+1)/2}}\sum_{\mathbf{k}''}\frac{\mathbf{k}\mathbf{k}'}{k^2(\mathbf{k}')^{n-1}}\left[\frac{\langle\mathbf{k}_0|e^{-i\mathbf{k}\cdot\mathbf{r}'}|\mathbf{k}''\rangle\langle\mathbf{k}''|e^{i\mathbf{k}\cdot\mathbf{r}}|\mathbf{k}_0\rangle}{\omega_{\mathbf{k}'',\mathbf{k}_0}-\omega}+\frac{\langle\mathbf{k}_0|e^{i\mathbf{k}\cdot\mathbf{r}}|\mathbf{k}''\rangle\langle\mathbf{k}''|e^{-i\mathbf{k}'\cdot\mathbf{r}'}|\mathbf{k}_0\rangle}{\omega_{\mathbf{k}'',\mathbf{k}_0}+\omega}\right], \tag{16}$$

where $\omega_{\mathbf{k}'',\mathbf{k}_0}=(E_{\mathbf{k}''}-\mathbf{E}_{\mathbf{k}_0})/\hbar$. The expression for $\overleftrightarrow{\mathrm{F}}_0(\mathbf{k},\mathbf{k},\omega)$ follows from Eq. (16) by substituting $\epsilon(\omega)=1$. This substitution is equivalent to neglecting the interaction between the electron and lattice. Straightforward evaluations of the matrix elements in (16) lead to

$$\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k},\omega)=\frac{(2\pi)^n e^2}{L^n\hbar\epsilon(\omega)}\frac{\Gamma((n-1)/2)}{2\pi^{(n+1)/2}}\frac{\mathbf{k}\mathbf{k}}{k^{n+1}}\times\left[\frac{1}{\omega_{\mathbf{k}+\mathbf{k}_0,\mathbf{k}_0}-\omega}+\frac{1}{\omega_{\mathbf{k}+\mathbf{k}_0,\mathbf{k}_0}+\omega}\right], \tag{17}$$

where L^n is the periodic volume in n-dimensional space.

To obtain the polaron energy we now substitute $\overleftrightarrow{\mathrm{F}}(\mathbf{k},\mathbf{k},\omega)$ and $\overleftrightarrow{\mathrm{F}}_0(\mathbf{k},\mathbf{k},\omega)$ into (11). The result is

$$\Delta E_s=\frac{e^2}{2}\omega_0\left[\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right]\frac{\Gamma((n-1)/2)}{2\pi^{(n+1)/2}}\times\int\int\frac{dk\,d\Omega_n}{\left[\omega_0+\frac{\hbar k^2}{2m}+\frac{\hbar k k_0\cos(\theta_{n-1})}{m}\right]}, \tag{18}$$

where $d\Omega_n$ is the solid angle in n dimensions and θ_{n-1} is the angle between $\mathbf{k}$ and $\mathbf{k}_0$ in n-dimensional space. The volume element in n-dimensional k space is taken to be $k^{n-1}dk\,d\Omega_n$. Following Hooft and Veltman[9] the solid angle $d\Omega_n$ is given by

$$d\Omega_n=\sin^{n-2}(\theta_{n-1})d\theta_{n-1}\sin^{n-3}(\theta_{n-2})d\theta_{n-2}\cdots d\theta_1\,, \tag{19}$$

where

$$0<\theta_i<\pi \text{ for all } i \text{ except } i=1,\quad 0<\theta_1<2\pi\,.$$

For slow electron $\hbar k_0^2/2m<\omega_0$, so that the denominator can be expanded in powers of k_0. Retaining terms up to k_0^2 and integrating Eq. (18), we obtain

$$\Delta E_s=-\alpha\hbar\omega_0\frac{\Gamma((n-1)/2)}{\Gamma(n/2)}\frac{\sqrt{\pi}}{2}\left[1+\frac{\hbar k_0^2}{4m\omega_0 n}\right], \tag{20}$$

where α is the Fröhlich coupling constant given by

$$\alpha=\frac{1}{2}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]e^2\left[\frac{2m\omega_0}{\hbar}\right]^{1/2}\frac{1}{\hbar\omega_0}\,. \tag{21}$$

The interaction energy of the electron in n-dimensional space is given by (20) and represents the main result of this paper.

III. CONCLUDING REMARKS

In this paper the polaron energy in n-dimensional space is obtained using the dispersion theory. The energy given by (20) agrees with the result of the ground-state energy of the polaron as calculated by Peeters *et al.* if we consider only the linear term of their result. Our result gives energy of the slow moving polaron while the work of the earlier authors is restricted to the ground state (i.e., $k_0=0$). The polaron effective mass m_{pol} in n-dimensional space can be obtained from our Eq. (20) as

$$\frac{1}{m_{\mathrm{pol}}}=\frac{1}{m}\left[1-\alpha\hbar\omega_0\frac{\Gamma((n-1)/2)}{\Gamma(n/2)}\frac{\sqrt{\pi}}{\hbar\omega_0}\frac{1}{4n}\right] \tag{22}$$

or

$$m_{\mathrm{pol}}\simeq m\left[1+\alpha\frac{\Gamma((n-1)/2)}{\Gamma(n/2)}\frac{\sqrt{\pi}}{4n}\right]. \tag{23}$$

For $n=3$, $m_{\mathrm{pol}}=m[1+(\alpha/6)]$, and $n=2$; $m_{\mathrm{pol}}=m[1+(\alpha\pi/8)]$. Both these results are consistent with the result of three-dimensional theory and with the result of Das Sarma[10] for a two-dimensional polaron.

The dispersion-theory approach does not depend on the use of the Fröhlich Hamiltonian. On the other hand, Peeters *et al.*[4] derived a recurrence relation between the Fröhlich Hamiltonian in n- and $(n-1)$-dimensional spaces. Using this relation and with the known form of the Fröhlich Hamiltonian in three dimensions they were able to derive results for any arbitrary dimensions. In contrast to this procedure, our method gives the polaronic energy more easily and directly in the n-dimensional space.

The variation of the effective mass for the polaron in n dimensions is given by Eq. (23). It shows that the polaron mass decreases with increasing dimensions. This result, we believe, is not available in the literature.

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