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Dispersion theory of the polaron in a quasi-one-dimensional structure

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Instead of using the Fröhlich Hamiltonian, we have presented in this paper the dispersion-theory approach based on the zero-point energy to discuss the polaron in a quasi-one-dimensional structure. The polaron energy is calculated. The effect of a degenerate electron gas on the phonon frequencies is also presented.

I. INTRODUCTION

In recent years, there has been considerable research activity concerning the properties of quantum wires. The interest is motivated by the expectation of extensive use of these structures in device fabrication.[1] The present day technology allows the construction of quantum wires, using heterojunctions formed by polar semiconductors, such as $\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$-GaAs. The motion of electrons in these structures is unrestricted in one direction and confined within an average radius in the range of 10–200 nm, in the remaining two directions. As in three-dimensional(3D) polar crystals, in quantum wires, which are quasi-one-dimensional structures, the coupling between the electron and the lattice vibrations of the system leads to the formation of a composite particle called the polaron. Introduced by Fröhlich[2] and others in 1950, the polaron in a polar crystal consists of a charged electron surrounded by a phonon cloud. The study of the polaron in 3D crystals is carried out at least for the past 40 years. The polaron in quasi-one-dimensional situations was initially examined by Holstein.[3] With the advances in semiconductor technology, quasi-one-dimensional structures are now easily available and there is renewed interest in these structures. The partial electron confinement in quantum wires gives rise to significant changes in the polaron properties[4] from those encountered in 3D crystals. While the traditional study of the polaron is based on the use of the Fröhlich Hamiltonian, the object of the present paper is to introduce a different approach based on the dispersion theory to study the quasi-one-dimensional polaron. Using this approach, we are able to examine some aspects of the polaron properties, which are not, as yet, well investigated.

The Fröhlich Hamiltonian has been the basis of almost all of the studies of the polaron in 3D and more recently of the polaron in restricted spaces including the quantum wires. For the case of the weak coupling between the electron and the phonons, the perturbative approach based on the use of the Fröhlich Hamiltonian provides the most widely used method for calculating the polaron energy. Within the weak-interaction regime, there is, however, an alternate approach[5] based on the dispersion theory for the study of the polaron that does not depend on the use of the Fröhlich Hamiltonian. In this approach, we obtain the difference in the zero-point energy of the electromagnetic modes of the crystal when the electron is interacting with the lattice vibrations and when it is not. The difference between the two energies provides the polaron energy of the electron, due to its coupling with the lattice phonons. The change in the zero-point energy is expressed in terms of shifts in the electromagnetic frequencies, which are associated with the lattice vibrations and the single-particle excitations of the electron. We have used this approach for calculating the polaron energy in a quasi-one-dimensional quantum wire. In addition, we are able to obtain the shift in the frequency of the polar optical vibrations of the lattice, due to its interaction with the electron. Although the shift in the frequency of a lattice mode interacting with a single electron can be very small, it becomes significant when the lattice mode is in interaction with a large number of electron. We have evaluated the effect of the number density of electrons (per unit length of the wire) on the lattice frequencies of the modes propagating in the direction of the wire.

In quasi-one-dimensional polar crystals, it is known that the electron interacts with surface, confined and unconfined modes of the lattice. Although all of the three modes are needed in the study of the polaron properties, it is found that reasonably accurate results arise[6] if the three modes of vibrations are replaced by the bulk 3D polar lattice modes. This is partly true since a quantum wire is usually embedded in a crystal. Thus, in this assumption, the electron-phonon interaction is assumed to be the same as in 3D. The replacement of the confined modes by 3D modes is shown to be a reasonable assumption,[6] if the electron confinement is achieved by the electrostatic field effect. In a structural confinement, the assumption is, however, valid if the confining radius is greater than 100 nm. In this paper, we assume that the electron interacts with only the 3D modes of the lattice. We also assume for mathematical convenience that the unperturbed polar mode frequencies of the lattice are undispersed and that the unperturbed electron energies along the wire are expressed in terms of a free-electron model with a constant effective mass.

The plan of the paper is as follows. In Sec. II, we describe the elements of the dispersion theory using the zero-point approach. In Sec. III, the results of the theory are applied to the electron in quasi-one-dimensional quantum wire. The polaron energy is also derived in this section. The shifts in the polar optical modes of the lattice, in the presence of a degenerate electron gas, are obtained in Sec. IV. The concluding remarks are given in Sec. V.

II. DISPERSION THEORY

In a polarizable medium, the electric potential at any point $\mathbf{r}$ is determined by the potential at other points in the medium. The electric potential $\varphi(\mathbf{r},\omega)$ oscillating at frequency ω at any point $\mathbf{r}$ in the polar crystal is related to the electric potential $\varphi(\mathbf{r}',\omega)$ at $\mathbf{r}'$, by the relation

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$$\varphi(\mathbf{r},\omega)=\int F(\mathbf{r},\mathbf{r}',\omega)\varphi(\mathbf{r}',\omega)d^3\mathbf{r}', \tag{1}$$

where $F(\mathbf{r},\mathbf{r}',\omega)$ is the kernel that depends on the dielectric properties of the crystal. If the crystal is replaced by free space, then $F(\mathbf{r},\mathbf{r}',\omega)$ is a δ function $\delta(\mathbf{r}-\mathbf{r}')$. The Fourier transform of Eq. (1) is given by

$$\varphi(\mathbf{q},\omega)=\sum_{\mathbf{q}'} F(\mathbf{q},\mathbf{q}',\omega)\varphi(\mathbf{q}',\omega). \tag{2}$$

The secular determinant $D(\omega)$, giving the frequencies of the electromagnetic fields, follows from Eq. (2) as

$$D(\omega)=|I-F(\mathbf{q},\mathbf{q}',\omega)|=0, \tag{3}$$

where I is the unit matrix. For the case of an electron interacting with the medium in a quasi-one-dimensional structure, we will obtain the expression for $F(\mathbf{q},\mathbf{q}',\omega)$. The expression $F_0(\mathbf{q},\mathbf{q}',\omega)$, which differs from $F(\mathbf{q},\mathbf{q}',\omega)$, can be derived for the situation in which the interaction of the electron associated with the infinite frequency response of the medium is only included; in this case, the frequencies of the medium are given by a secular determinant $D_0(\omega)$ as

$$D_0(\omega)=|I-F_0(\mathbf{q},\mathbf{q}',\omega)|=0. \tag{4}$$

The shift in the frequencies, due to the interaction of the electron with the lattice vibrations is obtained, in principle, by solving the secular determinant for electromagnetic frequencies, using Eqs. (3) and (4) and obtaining the difference. Although the zero-point energy of the medium can be obtained from the frequencies shifts, a more direct method for expressing the zero-point energy E is available, following the work of Mahanty and Ninham.^{7} It is given by

$$E=-(\hbar/4\pi i)\oint \ln|I-F(\mathbf{q},\mathbf{q}',\omega)|d\omega, \tag{5}$$

where the counter encloses the positive real axis. By staying restricted to the first order coupling between the electrons and the lattice, Eq. (5) can be approximated by expanding the ln term to give

$$E=(\hbar/4\pi i)\oint \mathrm{tr}F(\mathbf{q},\mathbf{q}',\omega)d\omega. \tag{6}$$

The zero-point energy, when the electron reacts to the infinite frequency response of the medium, is given by

$$E_0=(\hbar/4\pi i)\oint \mathrm{tr}[F_0(\mathbf{q},\mathbf{q}',\omega)]d\omega. \tag{7}$$

The change in the zero-point energy, due to the electron interaction with the lattice vibrations, is then expressed by

$$\Delta E=(\hbar/4\pi i)\oint \mathrm{tr}G(\mathbf{q},\mathbf{q}',\omega)d\omega, \tag{8}$$

where

$$G(\mathbf{q},\mathbf{q}',\omega)=F(\mathbf{q},\mathbf{q}',\omega)-F_0(\mathbf{q},\mathbf{q}',\omega), \tag{9}$$

and ΔE is the interaction energy. In addition to giving the zero-point energy, Eqs. (3) and (4) can be used to obtain the change in the frequency of an individual phonon mode of the medium. This will be discussed in Sec. IV. Results given by Eqs. (1)–(9), valid, in general, to all polar crystals, are now applied in the following section, to the case of an electron in a quantum wire.

III. POLARON IN A QUANTUM WIRE

We describe the parameters defining the quantum wire as follows. The length of the wire is taken to be in the x direction and the potential energy of the electron in this direction is assumed constant. The electron potential energy in the y-z directions is assumed to be that of two identical harmonic oscillators. The quantized energies of the electron in the y-z directions are separated by $\hbar\Omega$. We assume that the energy separations are sufficiently large, so that the electrons occupy the ground state of the two-dimensional harmonic oscillator. The calculations are valid at zero temperature.

The electron wave function in the direction of the wire is a plane wave denoted by $(1/L)^{1/2}\exp(ikx)$, where the one-dimensional wave vector k is in the x direction and the wave functions in the y-z directions are given by the 2D harmonic-oscillator-wave functions. Since we assume that the electrons occupy only the lowest harmonic-oscillator state, we denote the free electron and oscillator states in terms of a composite notation $|0,k\rangle$. If the electronic states are perturbed by a potential $\varphi(\mathbf{r}',\omega)$, then the perturbed electron wave functions can be obtained easily if we neglect the excited states of the oscillator in the second-order perturbation theory. Using the perturbed wave function, we obtain the expectation value at the potential $(-e)/[\varepsilon(\omega)|\mathbf{r}-\mathbf{r}'|]$ at point $\mathbf{r}$, due to the electron of charge $(-e)$ at $\mathbf{r}'$. In calculating the expectation value of the potential, we have taken into account the polarization effect of the medium by using the frequency-dependent dielectric constant $\varepsilon(\omega)$. Denoting the expectation value of the electric potential at r by $\varphi(\mathbf{r},\omega)$, we get

$$\varphi(\mathbf{r},\omega)=\sum_{k'}\left[\frac{\langle k,0|[-e/\varepsilon(\omega)|\mathbf{r}-\mathbf{r}'|]|0,k'\rangle\langle k',0|e\varphi(\mathbf{r}',\omega)|0,k\rangle}{\hbar\omega_{k',k}+\hbar\omega}+\frac{\langle k,0|e\varphi(\mathbf{r}',\omega)|0,k'\rangle\langle k',0|[-e/\varepsilon(\omega)|\mathbf{r}-\mathbf{r}'|]|0,k\rangle}{\hbar\omega_{k',k}-\hbar\omega}\right], \tag{10}$$

where

$$\hbar\omega_{k',k}=\hbar^2k'^2/2m-\hbar^2k^2/2m\,. \tag{11}$$

We take the Fourier transform of the Eq. (10) in 3D after utilizing the identities

$$\frac{1}{|\mathbf{r}'-\mathbf{r}'|}=\frac{1}{2\pi^2}\int\frac{\exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]}{(q)^2}d^3q=\frac{4\pi}{V}\sum\frac{\exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]}{(q)^2} \tag{12}$$

and

$$\varphi(\mathbf{r}',\omega)=\sum_{\mathbf{q}'}\varphi(\mathbf{q}',\omega)\exp(i\mathbf{q}'\cdot\mathbf{r}'), \tag{13}$$

to write

$$\begin{aligned}\varphi(\mathbf{q},\omega)=\frac{-4\pi e^2}{\varepsilon(\omega)V}\sum_{q'}&\left[\frac{1}{(\hbar\omega_{k+q_x,k}+\hbar\omega)(q)^2}\right.\\&\left.+\frac{1}{(\hbar\omega_{k-q_x,k}-\hbar\omega)(q)^2}\right]\\&\times\exp\{-[(q_y^2+q_z^2+q_y'^2+q_z'^2)/2\beta^2]\}\\&\times\delta_{q_x,q_x'}\varphi(\mathbf{q}',\omega),\end{aligned} \tag{14}$$

where V is the periodic volume. In Eq. (14), we have substituted for the matrix elements in Eq. (10) between plane-wave states and between harmonic oscillators, performed the sum over k', and used the definition

$$\beta^2=2m\Omega/\hbar\,. \tag{15}$$

It is important to note that in Eqs. (12)–(14) and in the following, $\mathbf{q}\equiv(q_x,q_y,q_z)$ is a 3D vector, while both k and k' are in 1D. We now multiply the Eq. (14) by $\exp[-(q_y^2+q_z^2)/2\beta^2]$ and sum the resultant expression on both sides of the equation over q_y and q_z. Writing

$$\sum_{q_y,q_z}\varphi(q_x,q_y,q_z,\omega)\exp[-(q_y^2+q_z^2)/2\beta^2]=\phi(q_x,\omega), \tag{16}$$

we get

$$\begin{aligned}\phi(q_x,\omega)=-\frac{4\pi e^2}{V\varepsilon(\omega)}\sum_{q_y,q_z}&\left[\frac{1}{\hbar\omega_{k+q_x,k}+\hbar\omega}+\frac{1}{\hbar\omega_{k-q_x,k}-\hbar\omega}\right]\\&\times\left[\frac{\exp\{-(q_y^2+q_z^2)/\beta^2\}}{q_x^2+q_y^2+q_z^2}\right]\phi(q_x,\omega).\end{aligned} \tag{17}$$

Performing the sum over q_y and q_z allows us to express the secular determinant as

$$\begin{aligned}D(\omega)=\left|1-\frac{e^2}{L\varepsilon(\omega)}\right.&\left[\frac{1}{\hbar\omega_{k+q_x,k}+\hbar\omega}+\frac{1}{\hbar\omega_{k-q_x,k}-\hbar\omega}\right]\\&\left.\times\exp(q_x^2/\beta^2)\mathrm{Ei}\left(-\frac{q_x^2}{\beta^2}\right)\right|,\end{aligned} \tag{18}$$

where for $x>0$, we have used the exponential-integral function defined as

$$\mathrm{Ei}(-x)=-\int_x^\infty\frac{\exp(-t)}{t}dt. \tag{19}$$

The formal expression for the frequency-dependent dielectric constant $\varepsilon(\omega)$ for a polar crystal is expressed by

$$\varepsilon(\omega)=\varepsilon(\infty)+[\varepsilon(0)-\varepsilon(\infty)]/[1-(\omega/\omega_T)^2], \tag{20}$$

where ω_T, the transverse lattice mode frequency, is related to the optical-phonon mode frequency by the relation

$$\omega_T^2/\omega_0^2=\varepsilon(\infty)/\varepsilon(0)\,. \tag{21}$$

The expression $D_0(\omega)$ for the electron interacting with the infinite response part of the medium, is obtained by replacing in Eq. (18) $\varepsilon(\omega)$ by $\varepsilon(\infty)$, so that

$$\begin{aligned}D_0(\omega)=\left|1-\frac{e^2}{L\varepsilon(\infty)}\right.&\left[\frac{1}{\hbar\omega_{k+q_x,k}+\hbar\omega}\right.\\&\left.\left.+\frac{1}{\hbar\omega_{k-q_x,k}-\hbar\omega}\right]\exp(q_x^2/\beta^2)\mathrm{Ei}\left(-\frac{q_x^2}{\beta^2}\right)\right|.\end{aligned} \tag{22}$$

For an electron in an unperturbed plane-wave state k, using Eqs. (18) and (22) in (3)–(9) allows us to express the interaction energy as

$$\begin{aligned}\Delta E=\frac{\hbar}{4\pi i}\sum_{q_x}\oint d\omega\frac{e^2}{L}&\left(\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right)\frac{\omega_0^2}{\omega^2-\omega_0^2}\\&\times\exp(q_x^2/\beta^2)\mathrm{Ei}\left(-\frac{q_x^2}{\beta^2}\right)\left[\frac{1}{\frac{\hbar^2q_x^2}{2m}+\frac{\hbar^2kq_x}{m}+\hbar\omega}\right.\\&\left.+\frac{1}{\frac{\hbar^2q_x^2}{2m}-\frac{\hbar^2kq_x}{m}-\hbar\omega}\right].\end{aligned} \tag{23}$$

After performing the contour integral in Eq. (23), we get

$$\begin{aligned}\Delta E=\frac{\alpha\hbar\omega_0r_0}{\pi}&\int_0^\infty\frac{dq_x}{r_0^2q_x^2+2r_0^2kq_x+1}\\&\times\tfrac{1}{2}\exp(q_x^2/\beta^2)\mathrm{Ei}(-q_x^2/\beta^2),\end{aligned} \tag{24}$$

where we make use of the following definitions: r_0, the polaron radius is given by

$$r_0^2=(\hbar/2m\omega_0), \tag{25}$$

and the Fröhlich coupling constant α by

$$\alpha=\left(\frac{1}{2}\right)\left(\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right)\left(\frac{e^2}{r_0}\right)\left(\frac{1}{\hbar\omega_0}\right). \tag{26}$$

Expression (24) for the change in the polaron energy is exactly the same as obtained by Hai, Peeters, Devreese, and Wendler,[8] but with the important difference that they use the Fröhlich Hamiltonian, while the present treatment is based on the dispersion theory. The exact equivalence between the two results confirms the validity of the alternate approach presented in this paper.

For the electron in state $k=0$, the shift in the ground-state energy ΔE_0 follows from Eq. (24)

$$\Delta E_0=\frac{\alpha\hbar\omega_0}{\pi}\int_0^\infty\frac{dq_x}{r_0^2q_x^2+1}\left(\frac{1}{2}\right)\exp(q_x^2/\beta^2)\mathrm{Ei}(-q_x^2/\beta^2). \tag{27}$$

IV. CALCULATION OF PHONON FREQUENCY SHIFTS

In this section, we calculate the effect of a degenerate electron gas on the phonon vibrational frequencies. When we consider the effect of the electron-phonon interaction, the frequencies of the electromagnetic radiation are given by the secular determinant.

$$D(\omega)=|1-G(\mathbf{q},\mathbf{q}',\omega)|. \tag{28}$$

The result follows from Eqs. (8) and (9). Using Eqs. (3), (4), (18), (22), in (28) allows us to write

$$G(q_x,q_x,\omega)=\frac{e^2}{L}\left(\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right)\frac{\omega_0^2}{\omega^2-\omega_0^2}\times\exp(q_x^2/\beta^2)\mathrm{Ei}(-q_x^2/\beta^2)\times\left[\frac{1}{(\hbar^2q_x^2/2m)+(\hbar^2q_xk/m)+\hbar\omega}+\frac{1}{(\hbar^2q_x^2/2m)-(\hbar^2q_xk/m)-\hbar\omega}\right]. \quad (29)$$

Equation (29) is valid for a single electron in state k and we generalize the result to the case when a large number of electrons are present. To do that, we multiply the first and second term in the square bracket of Eq. (29) by the statistical factors $f(k)[1-f(k+q_x)]$ and $f(k)[1-f(k-q_x)]$. The first of these factors stands for the probability of finding an electron in state k and of finding the electron state $k+q_x$ empty. Similarly, the second factor stands for the probability of finding the electron in state k and of finding the state $k-q_x$ empty. Assuming zero temperature, the $f(k)$ is unity for all $k's$ within $-k_F<k\leqslant k_F$ and zero otherwise. Performing the sum over k and substituting the result in (28) gives the secular determinants in the presence of a degenerate electron gas. It is important to note that the determinant is diagonal. Equating any diagonal term to zero produces an equation for the frequency of a mode (q_x). For the unperturbed frequency $\omega=\omega_0$ associated with the phonon frequencies, the frequencies affected by the electron-phonon interaction are given by

$$\omega^2=\omega_0^2+\frac{e^2}{\pi}\left[\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right]\omega_0^2\exp\left(\frac{q_x^2}{\beta^2}\right)\mathrm{Ei}\left(-\frac{q_x^2}{\beta^2}\right)\frac{m}{\hbar^2q_x}\times\ln\left[\left|\frac{(q_x^2r_0^2-2q_xk_Fr_0^2)^2-1}{(q_x^2r_0^2+2q_xk_Fr_0^2)^2-1}\right|\right]. \quad (30)$$

Rewriting Eq. (30) in terms of a frequency shift $\Delta\omega=\omega-\omega_0$, we get

$$(\Delta\omega_0/\omega_0)=\left[1+\frac{\alpha}{\pi}\exp(q_x^2r_0^2\omega_0/\Omega)\mathrm{Ei}(-q_x^2r_0^2\omega_0/\Omega)\times\left(\frac{1}{q_xr_0}\right)\ln\left|\frac{(q_x^2r_0^2-2q_xk_Fr_0^2)^2-1}{(q_x^2r_0^2+2q_xk_Fr_0^2)^2-1}\right|\right]^{1/2}-1. \quad (31)$$

For small values of q_x, expression (31) can be approximated to give

$$(\Delta\omega_0/\omega_0)=[2\alpha Nr_0(r_0q_x)^2\exp(q_x^2r_0^2\omega_0/\Omega)\times\mathrm{Ei}(-q_x^2r_0^2\omega_0/\Omega)]. \quad (32)$$

In Eq. (31), we have seen the relation $k_F=(N\pi/2)$, which connects the Fermi wave vector k_F with the number density N of electrons per unit range of the wire.

V. CONCLUDING REMARKS

The main object of this paper is to propose the dispersion theory method as an alternative to a more traditional approach, using the Fröhlich Hamiltonian for determining the polaron energy in a quasi-one-dimensional system. It is shown that the two approaches lead to identical results for the polaron energy. In the dispersion theory approach, the polaron energy is expressed in terms of frequency shifts in the electromagnetic modes of the medium. The method allows us to obtain the shift in the phonon mode frequencies in the presence of a degenerate electron gas. For small values of q_x, the frequency shift is linearly proportional tot he number of electrons per unit length of the wire, as seen from Eq. (32).

For the numerical estimate of the frequency shift, we use the approximate relation (32). For GaAs-Ga$_x$Al$_{1-x}$As quantum wire, various parameters occurring in Eq. (32) are readily available in literature.[8,9] The coupling constant $\alpha=0.07$ and the polaron radius $r_0=3.987$ nm. The number of electrons per unit range of the wire vary over a broad range[8,9] (10^6–10^9 per meter). To maximize the frequency shift, we select $N=(1.5)\times10^8$/m, so that $Nr_0=0.6$. The energy levels of the quantum well are kept sufficiently separated, so that only the lowest-energy level is occupied by the electrons. For the electron concentration used in the numerical evaluation, this condition is easily satisfied[8] if we set $(\Omega/\omega_0)=10.0$. As q_xr_0 approaches zero, the frequency shift also goes to zero. Inserting the value of $q_xr_0=0.5$ into Eq. (32) gives $(\Delta\omega_0/\omega_0)=0.14$, and for $q_xr_0=0.2$, the fraction $(\Delta\omega_0/\omega_0)=0.034$. The calculated frequency shifts in units of the unperturbed frequency are not negligible. In view of the fact that the electron number can be varied over a wide range, it will be interesting to measure the dependence of the frequency shift on the electron density.

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