Ground state energy of a polaron in a superlattice

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The ground state energy of a polaron in a superlattice was calculated using the double-time Green functions. The effective mass of the polaron along the planes perpendicular to the superlattice axis was also calculated. The dependence of the ground state energy and the effective mass along the planes perpendicular to the superlattice axis on the electron–phonon coupling constant α and on the superlattice parameters (i.e. the superlattice period d and the bandwidth Δ) were studied. It was observed that if an infinite square-well potential is assumed, the ground state energy of the polaron decreases (i.e. becomes more negative) with increasing α and d, but increases with increasing Δ. For small values of α, the polaron ground state energy varies slowly with Δ, becoming approximately constant for large Δ. The effective mass along the planes perpendicular to the superlattice axis was found to be approximately equal to the mass of an electron for all typical values of α, d and Δ.

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1. Introduction

Polarons in bulk materials have been extensively investigated for several years now, and many mathematical techniques have been used to solve the polaron problem. Mitra, Chatterjee, and Mukhopadhyay [1] and Peeters and Devreese [2] have given good reviews on polarons in bulk materials.

It is well known that when an electron moves slowly in a heterostructure, such as superlattices (SLs), heterojunctions, dielectric slabs, quantum wires, quantum box, and quantum-well (QW) structures of polar crystals, it may cause a distortion of the lattice, establishing a polarization field which acts back on the

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electron, modifying its properties; in particular, the electron acquires a self-energy and an enhancement of its Bloch effective mass. The single electron, together with its accompanying distortion, is called a polaron. For example, some SLs, such as GaAs/Al$_x$Ga$_{1-x}$As SLs, are made up of polar compounds in which the interaction of an electron with optical phonons is an important mechanism that strongly influences the optical and transport properties of the SL.

Due to the presence of heterofaces in heterostructures, polaron effects in polar semiconductor heterostructures are very different from those in bulk materials, and the polaron problem in this case is much more complicated than the case in bulk materials. Hence approximate methods such as the perturbation theory, the Lee–Low–Pines (LLP) variational method [3], the Landau and Pekar variational calculation, and the Green function method are required for its solution.

A number of works have been done on the effects of polarons in heterostructures and we mention a few of them here. Lin, Chen and George [4] and Hai, Peeters and Devreese [5] investigated the electron–phonon interaction and the polaron states in a symmetric single QW. Hai, Peeters and Devreese [6] further studied magnetopolarons in a GaAs/AlAs symmetric QW. Polarons in a symmetric single QW within an electric field have been investigated by Chen, Liang and Li [7]. Shi *et al.* [8] investigated the ground state polaron energy and the effective mass in asymmetric single and step QWs by using the second-order perturbation theory and the modified LPP variational method. Magnetopolarons in quantum dots were investigated in [9]. Zhou and Gu [10] investigated magnetopolarons in cylindrical quantum wires. Magnetopolarons in a QW have been studied in the case of a weak external magnetic field in [11]. Haupt and Wendler [12] studied the resonant magnetopolaron effects in parabolic QWs. Magnetopolarons in a heterojunction were investigated by means of the Green function method in [13] and [14]. Licari [15], and Liang, Gu and Lin [16] studied the polaron states in a polar slab using second-order perturbation theory. The self-trapping energy of a polaron in a polar-crystal slab in a magnetic field has been obtained by Wei, Zhao, and Gu [17] using the Larsen perturbation theory. Lu and Li [18] studied the properties of a polaron in a polar slab. The polaron effects in a heterojunction were investigated by Degani and Hipólito [19]. The interface polaron in a heterojunction in a magnetic field was investigated by Ban, Liang and Zheng [20]. Farias, Degani and Hipólito [21] studied bound polarons in a heterojunction. Surface polarons in a bilayer system are given in [22]. Thilagam and Singh [23] investigated, in the infinite square-well approximation, polarons in quasi-two-dimensional structures in which only confined bulk-like longitudinal optical (LO) phonons were considered. In addition, Zheng, Ban and Liang [24] studied confined bulk-like LO and interface phonons, and investigated the properties of a polaron in an infinite QW. Using the Landau–Pekar theory, a strong coupling theory of quasi-two-dimensional polarons, in which the contribution of the interface modes to the polaron effect is ignored, was proposed in [25]. The binding energies of bound polarons in strong magnetic fields in a QW, a quantum-well wire and a quantum box were given in [26]. Zhou and Gu [27] also studied impurity bound polarons in a QW. Bound magnetic polarons in a QW were studied in [28].

Though quite a number of works have been done on polarons in bulk materials and heterostructures, to the best of our knowledge, little work has been done on polaron effects in SLs in particular. In our present work, we shall calculate the ground state energy and the effective mass of a polaron in a SL, using the double-time Green functions. This approach provides a relatively easier and more convenient way of calculating the shift in the ground state energy of a polaron formed as a result of electron–phonon interaction in a superlattice.

In this paper it will be indicated that the ground state energy of the polaron depends on d and Δ, if an infinite square-well potential is assumed. The ground state energy of the polaron will be shown to decrease (becomes more negative) with increasing α and d, but increases with increasing Δ. For small values of α, the polaron ground state energy varies slowly with Δ, becoming approximately constant for large Δ. On the other hand, the effective mass along the plane perpendicular to the SL axis will be found to be approximately equal to the mass of an electron for all typical values of α, d and Δ.

The present work is organized as follows. In Sections 2 and 3, we present the theory and the calculation of

the shift in the ground state energy of a polaron in a superlattice. The results and its discussion are presented in Section 4. The conclusion is given in Section 5.

2. Theory

The Hamiltonian for an electron–phonon interaction in the second quantization formalism is

$$H = H_o + H_{\text{int}} \tag{1}$$

$$\text{with } H_o = \sum_{p,s} \varepsilon_p^s a_p^{s\dagger} a_p^s + \sum_q \omega_q b_q^\dagger b_q \tag{2}$$

$$H_{\text{int}} = \sum_{pp'} \sum_{qss'} \langle s, p | V(r) | s', p' \rangle a_p^{s\dagger} a_{p'}^{s'} (b_q + b_{-q}^\dagger) \tag{3}$$

$$\varepsilon_p^s = \frac{p_\perp^2}{2m} + \varepsilon_s - \Delta_s \cos(p_z d), \qquad s = 1, 2, \ldots \tag{4}$$

$$p_\perp^2 = p_x^2 + p_y^2 \tag{5}$$

ε_s and Δ_s are determined by SL parameters [29]; p_z and $p_\perp$ are, respectively, the components of the crystal momentum along and perpendicular to the SL axis; d is the SL period, $a_p^{s\dagger}$, a_p^s are the creation and the annihilation operators of an electron in the sth miniband; ω_q is the phonon frequency with wavevector q; and $b_q^\dagger$, b_q are the phonon creation and annihilation operators.

The matrix element in eqn (3) is given in [30] as

$$\langle s, p | V(r) | s', p' \rangle = \int \psi_p^{s*}(r) V(r) \psi_{p'}^{s'}(r) dr \tag{6}$$

where

$$\psi_p^s = \frac{1}{L} \exp[i(p_x x + p_y y)] \frac{1}{N} \sum_j \psi_s(z - fd) \exp(ip_z fd), \tag{7}$$

L is the normalized length, N is the number of periods in the SL, $\psi_s(z)$ is the wavefunction of an electron in the sth state in one of the one-dimensional potential wells which composes the SL potential. In particular, the matrix element for a scattering potential $V(r)$ is

$$\langle s, p | V(r) | s', p' \rangle = \sum_{n=-\infty}^{\infty} C_q M_{ss'}(q_z) \delta_{q_x, p_x - p_x'} \delta_{q_y, p_y - p_y'} \delta_{q_z, p_z - p_z' + ng} \tag{8}$$

where $g = (0, 0, 2\pi/d)$ is a reciprocal SL vector. C_q are the Fourier components of $V(r)$ and

$$M_{ss'}(q_z) = \int \psi_s^*(z) \psi_{s'}(z) e^{iq_z z} dz. \tag{9}$$

Using eqns (8) and (9), eqn (3) can be written as

$$H_{\text{int}} = \sum_{pqn} \sum_{ss'} C_q M_{ss'}(q_z) a_p^{s\dagger} a_{p-q+ng}^{s'} (b_q + b_{-q}^\dagger). \tag{10}$$

In order to obtain the dispersion relation for electrons we write the equations of motion for $a_p^{s\dagger}$, a_p^s, $b_q^\dagger$, b_q.

$$i \frac{da_p^s}{dt} = \varepsilon_p^s a_p^s + \sum_{qns'} C_q M_{ss'}(q_z) a_{p-q+ng}^{s'} (b_q + b_{-q}^\dagger) \tag{11}$$

$$-i \frac{da_p^{s\dagger}}{dt} = \varepsilon_p^s a_p^{s\dagger} + \sum_{qns'} C_q M_{ss'}(q_z) a_{p+q-ng}^{s'\dagger} (b_q + b_{-q}^\dagger) \tag{12}$$

$$i\frac{db_q}{dt} = \omega_q b_q + \sum_{pnss'} C_q M_{ss'}(-q_z) a_{p-q-ng}^{s^\dagger} a_p^{s'}$$ (13)

$$-i\frac{db_{-q}^\dagger}{dt} = \omega_q b_{-q}^\dagger + \sum_{pnss'} C_q M_{ss'}(-q_z) a_{p-q-ng}^\dagger a_p^{s'}.$$ (14)

The single particle Green functions of the electron type $G_p(t - t')$ are defined as

$$G_p(t - t') = -i\theta(t - t')\langle\{a_p^s(t), a_p^{s'\dagger}(t')\}\rangle = \langle\langle a_p^s(t); a_p^{s'\dagger}(t')\rangle\rangle$$ (15)

where $\{A, B\}$ is the anticommutator of A and B,

$$\{A, B\} = AB + BA$$ (16)

and

$$\theta(t - t') = \begin{cases} 1 & t > t' \\ 0 & t < t' \end{cases}$$ (17)

is called the Heaviside step function. Using eqns (11)–(14) the following equation of motion for $G_p(t - t')$ is obtained,

$$i\frac{dG_p(t - t')}{dt} = \delta(t - t') + G_p(t - t') + \sum_{qnl} C_q M_{sl}(q_z)$$
$$\times (\Gamma_{p-q,p,q}(t - t') + \Gamma'_{p-q,p,q}(t - t'))$$ (18)

where $\Gamma_{p-q,p,q}$ and $\Gamma'_{p-q,p,q}$ are mixed types of Green functions defined, respectively, as

$$\Gamma_{p-q,p,q}(t - t') = \langle\langle a_{p-q+ng}^l b_q|_t; a_p^{s'\dagger}(t')\rangle\rangle$$ (19)

$$\Gamma'_{p-q,p,q}(t - t') = \langle\langle a_{p-q+ng}^l b_{-q}^\dagger|_t; a_p^{s'\dagger}(t')\rangle\rangle.$$ (20)

By constructing equations of motion for $\Gamma_{p-q,p,q}$ and $\Gamma'_{p-q,p,q}$ and decoupling the higher-order Green functions occurring in these equations, we obtain the following equations for $\Gamma_{p-q,p,q}$ and $\Gamma'_{p-q,p,q}$, respectively:

$$i\frac{d\Gamma_{p-q,p,q}(t - t')}{dt} = (\varepsilon_{p-q}^s + \omega_q)\Gamma_{p-q,p,q}$$
$$+ C_q M_{ss}(q_z)(N_q + 1 - f_{p-q}^s)G_p(t - t')$$ (21)

$$i\frac{d\Gamma'_{p-q,p,q}(t - t')}{dt} = (\varepsilon_{p-q}^s + \omega_q)\Gamma'_{p-q,p,q}$$
$$+ C_q M_{ss}(q_z)(f_{p-q}^s + N_q)G_p(t - t')$$ (22)

where $N_q = \langle b_q^\dagger b_q\rangle$ and $f_{p-p}^s = \langle a_{p-q}^{s\dagger} a_{p-q}^s\rangle$ are the number density of phonons and electrons respectively.

Writing eqns (18), (21) and (22) in terms of Fourier components of the Green functions, with

$$G_p(t) = \int_{-\infty}^\infty G_p(E)e^{-iEt}dt$$ (23)

$$\Gamma_{p-q,p,q}(t) = \int_{-\infty}^\infty \Gamma_{p-q,p,q}(E)e^{-iEt}dt$$ (24)

$$\Gamma'_{p-q,p,q}(t) = \int_{-\infty}^\infty \Gamma'_{p-q,p,q}(E)e^{-iEt}dt$$ (25)

$$\delta(t) = \frac{1}{2\pi}\int_{-\infty}^\infty e^{-iEt}dt,$$ (26)

one finds that

$$(E - \varepsilon_{\boldsymbol{p}}^s)G_{\boldsymbol{p}}(E) = \frac{1}{2\pi} + \sum_{\boldsymbol{q}ns} C_{\boldsymbol{q}}M_{ss}(q_z)(\Gamma_{\boldsymbol{p}-\boldsymbol{q},\boldsymbol{p},\boldsymbol{q}}(E) + \Gamma'_{\boldsymbol{p}-\boldsymbol{q},\boldsymbol{p},\boldsymbol{q}}(E)) \tag{27}$$

where

$$\Gamma_{\boldsymbol{p}-\boldsymbol{q},\boldsymbol{p},\boldsymbol{q}}(E) = \frac{C_{\boldsymbol{q}}M_{ss}(q)(N_{\boldsymbol{q}} + 1 - f_{\boldsymbol{p}-\boldsymbol{q}}^s)G_{\boldsymbol{p}}(E)}{E - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}}^s - \omega_{\boldsymbol{q}}} \tag{28}$$

$$\Gamma'_{\boldsymbol{p}-\boldsymbol{q},\boldsymbol{p},\boldsymbol{q}}(E) = \frac{C_{\boldsymbol{q}}M_{ss}(qz)(f_{\boldsymbol{p}-\boldsymbol{q}}^s + N_{\boldsymbol{q}})G_{\boldsymbol{p}}(E)}{E - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}}^s + \omega_{\boldsymbol{q}}}, \tag{29}$$

and hence

$$G_{\boldsymbol{p}}(E) = \frac{1}{2\pi(E - \varepsilon_{\boldsymbol{p}}^s - M_{\boldsymbol{p}}(E))} \tag{30}$$

where

$$M_{\boldsymbol{p}}(E) = \sum_{\boldsymbol{q}s} |C_{\boldsymbol{q}}M_{ss}(q_z)|^2 \left(\frac{N_{\boldsymbol{q}} + 1 - f_{\boldsymbol{p}-\boldsymbol{q}}^s}{E - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}}^s - \omega_{\boldsymbol{q}}} + \frac{N_{\boldsymbol{q}} + f_{\boldsymbol{p}-\boldsymbol{q}}^s}{E - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}}^s + \omega_{\boldsymbol{q}}} \right) \tag{31}$$

is called the mass operator. Equation (30) is the dispersion equation. Assuming the bandgaps are to be wide such that there are no interband transitions, the band label s can be dropped.

Green functions can also be used to obtain the correlation functions [31],

$$\langle a_{\boldsymbol{p}}^{\dagger}(t'); a_{\boldsymbol{p}}(t) \rangle = \int_{-\infty}^{\infty} J_{\boldsymbol{p}}(\omega)e^{-i\omega(t-t')}d\omega \tag{32}$$

where $J_{\boldsymbol{p}}$ is the spectral intensity given by

$$G_{\boldsymbol{p}}(\omega + i\epsilon) - G_{\boldsymbol{p}}(\omega - i\epsilon) = -J_{\boldsymbol{p}}(\omega)(e^{\beta\omega} + 1). \tag{33}$$

Inserting eqn (30) into eqn (32), we obtain

$$M_{\boldsymbol{p}}(\omega \pm i\epsilon) = M_{\boldsymbol{p}}(\omega) \mp i\gamma_{\boldsymbol{p}}(\omega) \tag{34}$$

where

$$\gamma_{\boldsymbol{p}}(\omega) = \pi \sum_{\boldsymbol{q}} |C_{\boldsymbol{q}}M(q_z)|^2 \{(N_{\boldsymbol{q}} + 1 - f_{\boldsymbol{p}-\boldsymbol{q}})\delta(\omega - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}} - \omega_{\boldsymbol{q}})$$
$$+ (f_{\boldsymbol{p}-\boldsymbol{q}} + N_{\boldsymbol{q}})\delta(\omega - \varepsilon_{\boldsymbol{p}-\boldsymbol{q}} + \omega_{\boldsymbol{q}})\}$$

is the coefficient of absorption for electrons.

In order to obtain the shift in the ground state energy of an electron as a result of its interaction with phonons, the mass operator $M_{\boldsymbol{p}}(\omega)$ is expanded in a power series in ω at $\omega = \bar{\varepsilon}_{\boldsymbol{p}}$, taking into account that $\gamma_{\boldsymbol{p}}(\omega)$ is a slowly varying function, i.e. $\gamma_{\boldsymbol{p}}(\omega) \approx \gamma_{\boldsymbol{p}}(\bar{\varepsilon}_{\boldsymbol{p}})$. This implies that

$$\bar{\varepsilon}_{\boldsymbol{p}} - \varepsilon_{\boldsymbol{p}} - M_{\boldsymbol{p}}(\bar{\varepsilon}_{\boldsymbol{p}}) = 0, \tag{35}$$

i.e.

$$\bar{\varepsilon}_{\boldsymbol{p}} - \varepsilon_{\boldsymbol{p}} - P \sum_{\boldsymbol{q}} |C_{\boldsymbol{q}}M(q_z)|^2 \left(\frac{N_{\boldsymbol{q}} + 1 - f_{\boldsymbol{p}-\boldsymbol{q}}}{\bar{\varepsilon}_{\boldsymbol{p}}^o - \bar{\varepsilon}_{\boldsymbol{p}-\boldsymbol{q}}^o - \omega_o} + \frac{f_{\boldsymbol{p}-\boldsymbol{q}} + N_{\boldsymbol{q}}}{\bar{\varepsilon}_{\boldsymbol{p}}^o - \bar{\varepsilon}_{\boldsymbol{p}-\boldsymbol{q}}^o + \omega_o} \right) = 0. \tag{36}$$

For weak electron–optical phonon interactions, where $N_{\boldsymbol{q}} \ll 1$ and $f_{\boldsymbol{p}} \ll 1$, we obtain

$$\bar{\varepsilon}_{\boldsymbol{p}} - \varepsilon_{\boldsymbol{p}} = \Delta\varepsilon_{\boldsymbol{p}} = P \sum_{\boldsymbol{q}} C_{\boldsymbol{q}}^2 |M(q_z)|^2 \frac{1}{\bar{\varepsilon}_{\boldsymbol{p}}^o - \bar{\varepsilon}_{\boldsymbol{p}-\boldsymbol{q}}^o - \omega_o}. \tag{37}$$

3. Calculation

Using the expression in eqn (37) we calculate the change in the ground state energy of the polaron. Changing the summation over $\boldsymbol{q}$ to integration, using cylindrical polar coordinates, and making the following change of variables,

$$
\left.
\begin{aligned}
&\frac{q_\perp}{q_p} = x; \qquad \frac{q_z d}{2} = \chi; \qquad\qquad \frac{p_x}{q_p} = \eta_x; \qquad \frac{p_y}{q_p} = \eta_y \\
&-\frac{2\Delta}{\omega_o} \sin \frac{q_z d}{2} \sin\left(p_z - \frac{q_z}{2}\right) d = y; \quad \left(\frac{2}{q_p d}\right)^2 = k; \quad q_p = \sqrt{2m^*\omega_o}
\end{aligned}
\right\},
\tag{38}
$$

the shift in ground state energy, $\Delta\varepsilon_{\boldsymbol{p}} = \bar{\varepsilon}_{\boldsymbol{p}} - \varepsilon_{\boldsymbol{p}}$, then becomes

$$
\Delta\varepsilon_{\boldsymbol{p}} = -\frac{\alpha}{\pi^2 d}\left(\frac{\omega_o}{2m^*}\right)^{\frac{1}{2}} P \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |m(\chi)|^2 d\chi \int_0^\infty \frac{x\,dx}{k\chi^2 + x^2}
$$
$$
\times \int_0^{2\pi} \frac{d\theta}{1 + y + x^2 - 2x(\eta_x \cos\theta + \eta_y \sin\theta)}.
\tag{39}
$$

On evaluation of the integrals with respect to θ and x, one finds that

$$
\Delta\varepsilon_{\boldsymbol{p}} = -\frac{\alpha}{\pi d}\left(\frac{\omega_o}{2m^*}\right)^{\frac{1}{2}} P \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{|m(\chi)|^2 d\chi}{\sqrt{(y+1-k\chi^2)^2 + 4k\chi^2(\eta_x^2+\eta_y^2)}}
$$
$$
\times \ln\left[\frac{\sqrt{(y+1-k\chi^2)^2 + 4k\chi^2(\eta_x^2+\eta_y^2)} \cdot (y+1) + (y+1)^2 - k\chi^2(1+y-2(\eta_x^2+\eta_y^2))}{k\chi^2\left\{\sqrt{(y+1-k\chi^2)^2 + 4k\chi^2(\eta_x^2+\eta_y^2)} + y + 1 - k\chi^2 - 2(\eta_x^2+\eta_y^2)\right\}}\right].
\tag{40}
$$

At low temperatures, when electron–optical phonon interactions result in polaron effects, the electron momentum is less than that of the phonon, i.e. $\boldsymbol{p} < \boldsymbol{q}$. This implies that

$$
\left|\frac{k\chi^2(\eta_x^2+\eta_y^2)}{(y+1-k\chi^2)^2}\right| \ll 1.
\tag{41}
$$

Therefore, the expression $\dfrac{1}{\sqrt{(y+1-k\chi^2)^2 + 4k\chi^2(\eta_x^2+\eta_y^2)}}$ in eqn (40) can be expanded in binomial series, retaining only first- and lower-order terms, i.e.

$$
\frac{1}{\sqrt{(y+1-k\chi^2)^2 + 4k\chi^2(\eta_x^2+\eta_y^2)}} \cong \frac{1}{y+1-k\chi^2}\left[1 - \frac{2k\chi^2(\eta_x^2+\eta_y^2)}{(y+1-k\chi^2)^2}\right].
\tag{42}
$$

Using this approximation in eqn (40), with

$$
a = k\chi^2 \qquad \text{and} \qquad b = y + 1,
\tag{43}
$$

$\Delta\varepsilon_{\boldsymbol{p}}$ is found to be

$$
\bar{\varepsilon}_{\boldsymbol{p}} - \varepsilon_{\boldsymbol{p}} = -\frac{p_x^2 + p_y^2}{2m^*}\left(\frac{Y_1}{\pi q_p d}\right)\alpha - \left(\frac{Y_2}{\pi q_p d}\right)\alpha\omega_o
\tag{44}
$$

$$
= -\frac{p_\perp^2}{2m^*}\beta_1(d)\alpha - \beta_2(d)\alpha\omega_o
\tag{45}
$$

where

$$Y_1 = P \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |m(\chi)|^2 d\chi \left(\frac{a+b}{(a-b)^2 b} - \frac{2a}{(a-b)^3} \ln \frac{a}{b} \right) \tag{46}$$

$$Y_2 = P \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |m(\chi)|^2 d\chi \frac{1}{a-b} \ln \frac{a}{b} \tag{47}$$

$$\beta_1(d) = \frac{Y_1}{\pi q_p d} \tag{48}$$

$$\beta_2(d) = \frac{Y_2}{\pi q_p d}. \tag{49}$$

The effective mass m_{pol}^* of the polaron in the planes perpendicular to the SL axis is the reciprocal of the second derivative of its energy with respect to the component of momentum in the planes perpendicular to the SL axis. Thus

$$\frac{1}{m_{\text{pol}}^*} = \frac{\partial^2 \bar{\varepsilon}_p}{\partial p_\perp^2} = \frac{1}{m^*}(1 - \alpha\beta_1(d))$$

or

$$m_{\text{pol}}^* = m^*(1 - \alpha\beta_1(d))^{-1} \tag{50}$$

and for $\alpha \ll 1$,

$$m_{\text{pol}}^* = m^*(1 + \alpha\beta_1(d)). \tag{51}$$

4. Results and discussions

It is observed from eqn (44) that the shift in energy, as a result of the formation of a polaron, depends on the integrals Y_1 and Y_2. The effective mass of the polaron also depends on Y_1 only. Both Y_1 and Y_2 depend on the matrix element of the potential trough or well which appears as a result of the electron–phonon interaction. Hence one must know the form of the potential in order to evaluate these integrals. In the case of an infinite square-well potential ($U_o \to \infty$), the model proposed by Shik [30] can be used to show that the matrix element $|m(\chi)|$ of the infinite square-well potential is

$$|m(\chi)|^2 = \frac{\sin^2 \chi}{\chi^2}. \tag{52}$$

With this form of the matrix element, Y_1 and Y_2 are not analytically integrable, therefore these integrals were evaluated numerically.

Assuming that $\omega_o = 10^{14}$ s^{-1}, $m^* = 8.0 \times 10^{-31}$ kg, $p_\perp = 10^{-9}$ kg m s^{-1}, $\hbar = 1.05 \times 10^{-34}$ J s, and considering that for slow electrons ($p < q$), p_z can be assumed to be negligible, the shift in energy $\Delta\varepsilon_p$ was obtained as a function of d and Δ. Typical values of d and Δ are in the order of 10^{-8} m (few hundreds of Å) and 10^{-19} J, respectively. Typical values of α for III–V compounds lie within 0.015–0.080, and for II–VII compounds from 0.39 to 0.65 [32]. The aforementioned limits of the α values for these semiconductor compounds were used in all our calculations. In particular, $d = 10^{-8}$ m, $\Delta = 0.5 \times 1.6 \times 10^{-19}$ J and $\alpha = 0.39$ yielded $\Delta\varepsilon_p/\hbar\omega_o = -0.070$ or $\Delta\varepsilon_p = -0.0046$ eV.

In Fig. 1, $\Delta\varepsilon_p/\hbar\omega_o$ was plotted against d for $\alpha = 0.015, 0.080, 0.39, 0.65$ and $\Delta = 0.5$ eV. Straight lines which become steeper as α increases were obtained. This means that the shift in the energy decreases (becomes more negative) with increasing electron–phonon coupling constant. If the coupling constant is fixed at 0.39, and $\Delta\varepsilon_p/\hbar\omega_o$ is plotted against d for $\Delta = 0.05, 0.5, 1.0$ and 2.0 eV (Fig. 2), the lines become less steep as Δ increases. Thus the shift in energy increases (becomes more positive) with increasing bandwidth.
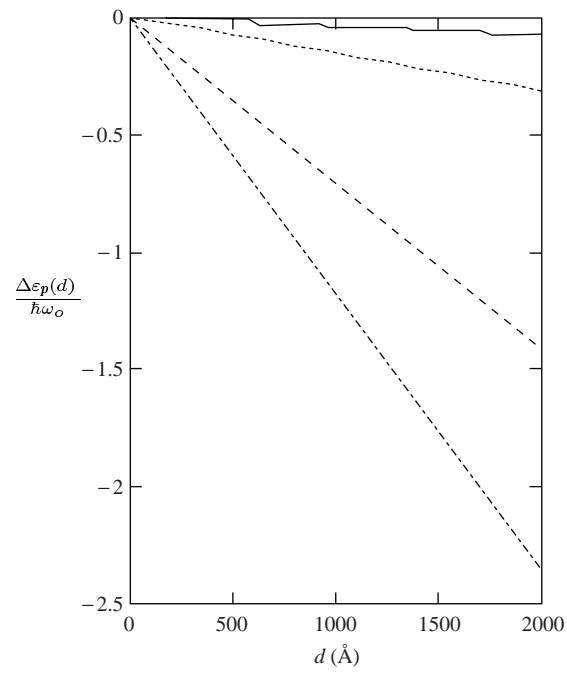
Fig. 1. The dependence of $\Delta\varepsilon_{\boldsymbol{p}}/\hbar\omega$ on d for $\Delta = 0.5$ eV and $\alpha = 0.015$ (——), 0.080 (- - -), 0.39 (– –) and 0.65 (– - –).
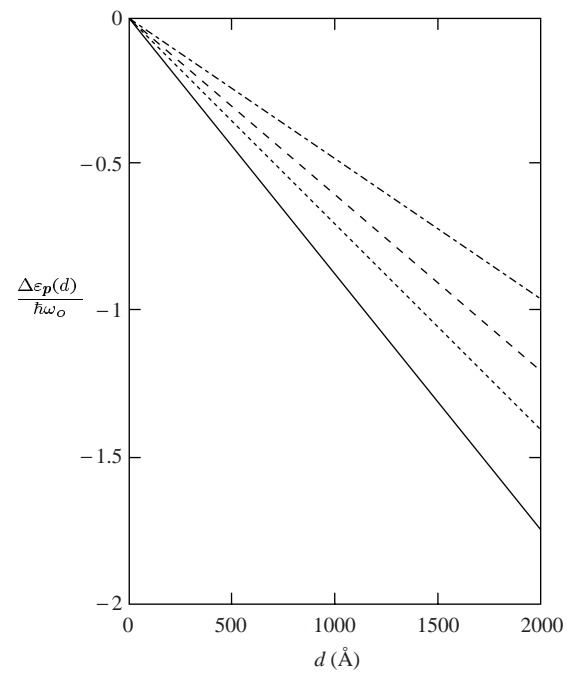

Fig. 2. The dependence of $\Delta\varepsilon_{\boldsymbol{p}}/\hbar\omega_o$ on d for $\alpha = 0.39$ and $\Delta = 0.05$ eV (——), 0.50 eV (- - -), 1.00 eV (– –) and 2.00 eV (– - –).
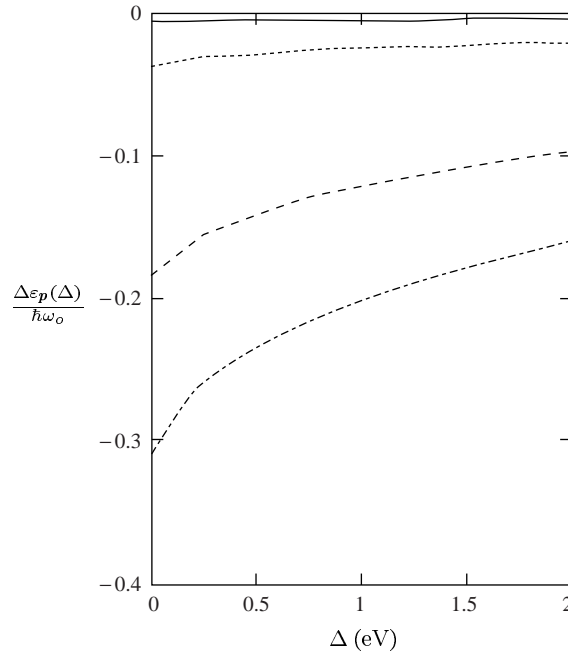
Fig. 3. The dependence of $\Delta\varepsilon_p/\hbar\omega_o$ on Δ for $d = 200$ and $\alpha = 0.015$ (——), 0.080 (- - -), 0.39 (– –) and 0.65 (–·–·).

$\Delta\varepsilon_p/\hbar\omega_o$ was plotted against Δ for $\alpha = 0.015$, 0.080, 0.39, 0.65 and $d = 200$ Å. The curves obtained are shown in Fig. 3. First, we observed that the curves shift down the $\Delta\varepsilon_p/\hbar\omega_o$ axis as α was increased. This again confirms the observation made in Fig. 1 that $\Delta\varepsilon_p$ decreases with increasing coupling constant. Secondly, we observed that for small α ($\alpha = 0.015$) $\Delta\varepsilon_p/\hbar\omega_o$ varies slowly and is almost constant for large values of Δ. If α is fixed at $\alpha = 0.39$ and $\Delta\varepsilon_p/\hbar\omega_o$ is plotted against Δ for $d = 200$, 500, 700 and 1000 Å, the curves, as observed in Fig. 4, shift down the $\Delta\varepsilon_p/\hbar\omega_o$ axis as d increases. Thus $\Delta\varepsilon_p$ depends on the SL parameters d and Δ.

The surface plot shown in Fig. 5 is a plot of $\Delta\varepsilon_p(d, \Delta)/\hbar\omega_o$ against (d, Δ) for $\alpha = 0.39$. This plot and similar plots for $\alpha = 0.015$, 0.080 and 0.65 (not shown) indicate that the shift in energy decreases with increasing α or increasing d, but increases with increasing Δ, summarizing the observations made in Figs 1–4.

Surface plots of the effective polaron mass $m^*_{\text{pol}}(d, \Delta)$ against (d, Δ) for $\alpha = 0.015$, 0.080, 0.39 and 0.65 gave surfaces through 1 and parallel to the d–Δ plane. Thus, the effective mass varies very little with the coupling constant α and SL parameters, d and Δ; and the ratio of the polaron effective mass to electron mass is *almost* 1 for all values of α, d and Δ. To have an idea of the smallness of the difference between the polaron effective mass and the electron mass, the ratio of the polaron effective mass to electron mass was evaluated, assuming $\alpha = 0.65$, $d = 100$ Å and $\Delta = 0.5$ eV. The result obtained is

$$\frac{m^*_{\text{pol}}}{m^*} = 1 + 1.96657 \times 10^{-33} \tag{53}$$

which is approximately equal to 1, so that $m^*_{\text{pol}} \simeq m^*$. Thus the polaron effective mass along the plane perpendicular to the SL axis is approximately equal to electron mass.
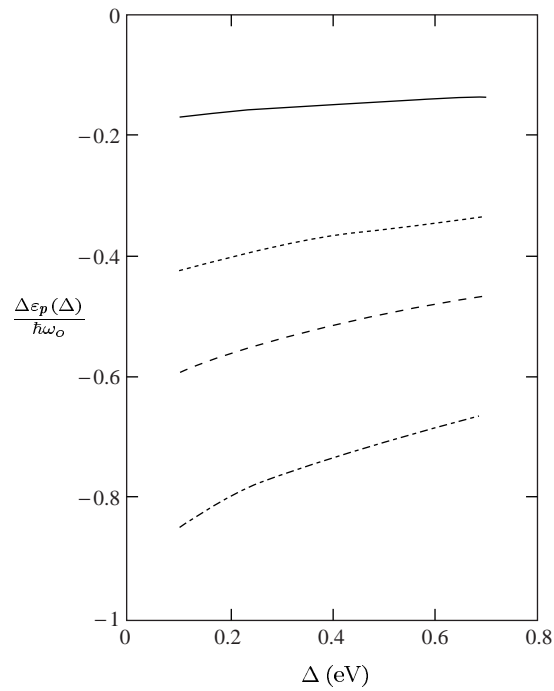
Fig. 4. The dependence of $\Delta\varepsilon_p/\hbar\omega_o$ on Δ for $\alpha = 0.39$ and $d = 200$ (——), 500 (- - -), 700 (– –) and 1000 (–·–).
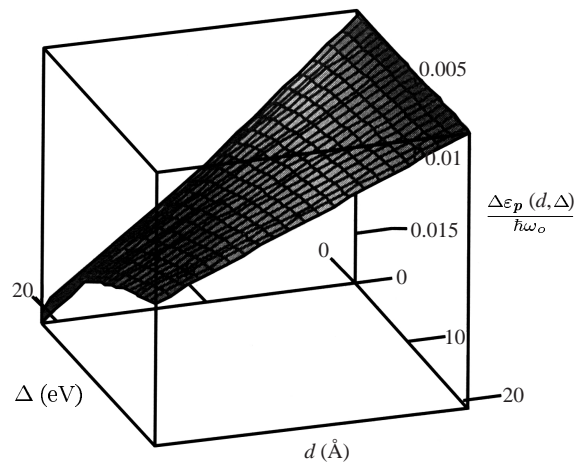

Fig. 5. Surface plot of $\Delta\varepsilon_p(d, \Delta)/\hbar\omega_o$ for $\alpha = 0.39$. M is a 21 × 21 array of points (d, Δ). On the d-axis, 1 unit: 0.12 Å; on the Δ-axis, 1 unit: 0.95 eV.

5. Conclusion

The shift $\Delta\varepsilon_p$ in the ground state energy of an electron whose interaction with a phonon results in the formation of a polaron is dependent on the SL parameters d and Δ, and the coupling constant α, if the potential well in which the electron is trapped is assumed to be an infinite square well. The shift in the

ground state energy decreases with increasing d and α, but increases with increasing Δ. For small values of α, the shift in the ground state energy as a function of Δ varies slowly with Δ, and is approximately constant for large Δ.

The effective mass along the planes perpendicular to the SL axis was found to be approximately equal to the electron mass for all typical values of d, Δ and α, the difference between the effective mass and the electron mass being of the order 10^{-33}.

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