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The pinning effect in a parabolic quantum dot

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Abstract

Using improved Wigner–Brillouin perturbation theory we study resonant electron–phonon interaction in a semiconductor quantum dot. We predict pinning of the excited energy levels to the ground state level plus one optical phonon as a function of the strength of the confinement potential. This effect should be observable through optical spectroscopic measurements.

1. Introduction

Recent years have witnessed an enormous amount of interest in the area of quantum dots. Quantum dots are ultrasmall structures in which the motion of the charge carriers is confined in all spatial directions. The natural length scales in a quantum dot are of the order of a few nanometres and because of this reduced dimensionality it contains a discrete number of electrons and has a discrete energy spectrum. In this sense quantum dots can be regarded as ideal quantum systems and are expected to exhibit pronounced quantum effects. Quantum dot systems, in fact, offer an excellent ground for testing quantum mechanics and therefore they have an intrinsic appeal from the point of view of fundamental physics. Because of the quantum size effect quantum dot structures exhibit many new physical properties that are very interesting and are quite different from those of bulk systems [1]. Furthermore, quantum dots can be fabricated in both two and three dimensions and can also be prepared in different geometrical shapes and sizes. This design flexibility together with very many novel physical effects have made quantum dots technologically highly promising for potential applications in optical and semiconductor-based microelectronic devices. An issue of recent interest has been the role of electron–phonon interaction in the electronic properties of quantum dots [2–5]. The electron–phonon interaction energy scale is comparable to the other relevant energy scales involved in a quantum dot and therefore it is expected that the electron–phonon interaction will play an important role in determining the energy relaxation and other properties of quantum dots. In this connection a number of authors have investigated the polaronic effects in quantum dots [6]. Since most quantum dots available today are made of polar semiconductors, it is natural to expect the formation of polarons in these systems as was recently demonstrated experimentally [6, 7]. Several theoretical calculations have revealed that polaronic effects in semiconductor quantum dots are considerably enhanced if the dot sizes are reduced below a

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few nanometres. Recently, Mukhopadhyay and Chatterjee [8] showed that the phonon-induced Zeeman splitting in a two-dimensional parabolic quantum dot is strongly size dependent for small dots and decreases very rapidly with decreasing dot size. In the present paper we suggest another important polaronic effect in a quantum dot, namely, the pinning effect, which should be experimentally observable.

The phenomenon of the pinning effect is quite well known in bulk polar materials in the presence of a large magnetic field (see [9] and references therein). For example, it has been observed both theoretically and experimentally that in the case of bulk systems the first excited Landau state level gets pinned to the ground state (GS) Landau level plus one longitudinal optical (LO) phonon energy if the strength of the externally applied magnetic field is increased to a sufficient large value. Since the magnetic field behaves in some sense like a harmonic oscillator potential, one would also expect to observe a pinning effect in a quantum dot (even in the absence of an external magnetic field) just on increasing the lateral parabolic confinement which is equivalent to increasing the frequency of the confining parabolic potential. The aim of the present paper is to show theoretically the existence of such a pinning effect in a parabolic quantum dot.

We consider a single electron moving in a symmetric parabolic quantum dot and interacting with the bulk LO phonons of the host lattice. We perform our calculations for both two- and three-dimensional quantum dots. The assumption of parabolic confinement is consistent with far-infrared optical spectroscopic measurements and the generalized Kohn theorem [10]. We shall however neglect in our calculation the effect of the interface phonon modes for the sake of mathematical simplicity. A recent microscopic study by Rücker *et al* [11] has shown that electron–LO-phonon coupling in a quantum wire does not significantly differ from that obtained from the bulk phonon model. We believe that this conclusion should also apply to our quantum dot system. Of course, one would certainly expect some quantitative changes in the results if confined phonon modes [12] were included but the qualitative features are expected to remain the same. Since most semiconductor quantum dots have a weak electron–phonon coupling, perturbative calculations should in general be acceptable. However, it turns out that the Rayleigh–Schrödinger perturbation theory (RSPT) [13] can be used only for the GS energy calculation, if one is interested in the entire range of the confinement length. For the excited states (ESs) of a parabolic quantum dot, RSPT would fail for certain values of the confinement length for which the ESs become unstable with respect to the emission of LO phonons. One should therefore use degenerate perturbation theory or Wigner–Brillouin perturbation theory (WBPT) for such cases. We will employ in the present work an improved version of WBPT which is known as the 'improved Wigner–Brillouin perturbation theory' (IWBPT) and has been found to give the correct pinning behaviour in bulk systems.

2. Theoretical formalism

The Hamiltonian for our system is given by

$$H' = -\frac{\hbar^2}{2m}\nabla'^2_{r'} + \frac{1}{2}m\omega_h^2 r'^2 + \hbar\omega_{LO}\sum_{\vec{q}'} b^\dagger_{\vec{q}'}b_{\vec{q}'} + \sum_{\vec{q}'}(V'_{q'}\mathrm{e}^{-\mathrm{i}\vec{q}'\cdot\vec{r}'}b^\dagger_{\vec{q}'} + \mathrm{h.c.}), \quad (1)$$

where m is the effective mass of the electron, ω_{LO} is the optical phonon frequency, ω_h measures the confining strength of the parabolic potential, $b^\dagger_q(b_q)$ is the creation (annihilation) operator for a LO phonon of wavevector q and V_q is the electron–phonon coupling coefficient. The Hamiltonian in units where $\hbar = m = 1$ reads

$$H = H_0 + H_{ep} = H_e + H_p + H_{ep}, \quad (2)$$

with

$$H_e = -\tfrac{1}{2}\nabla_r^2 + \tfrac{1}{2}\omega^2 r^2, \tag{3a}$$

$$H_p = \sum_{\vec{q}} b_{\vec{q}}^{\dagger} b_{\vec{q}}, \tag{3b}$$

$$H_{ep} = \sum_{\vec{q}} (V_q \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}} b_{\vec{q}}^{\dagger} + \mathrm{h.c.}), \tag{3c}$$

where everything is in dimensionless units and $\omega = \omega/\omega_{LO}$, and $|V_q|^2 = 2\sqrt{2}\pi\alpha/Vq^2$ for 3D and $|v_q|^2 = \sqrt{2}\pi\alpha/qA$ in 2D, α being the electron–phonon constant. The second-order perturbative correction to the electron self-energy due to the electron–phonon interaction is given by

$$\Delta E_n = -\sum_j \sum_{\vec{q}} \frac{|\langle\phi_j^0(\vec{r})|V_q \exp(-\mathrm{i}\vec{q}\cdot\vec{r})|\phi_n^0(\vec{r})\rangle|^2}{E_j^0 - E_n^0 - \Delta_n + 1}, \tag{4}$$

where the energy of the whole system is given by $E_n = E_n^0 + \Delta E_n$. The energy of the electronic part will be $E_j^0 = (j_1 + \cdots + j_N + N/2)\omega$, where $N = 2$ for 2D and $N = 3$ for 3D systems.

Here $\Delta_n = 0$ leads to the RSPT which gives accurate results for the GS and for $\omega \ll 1$. In the case of WBPT $\Delta_n = \Delta E_n$ which can account for the splitting of the degenerate energy levels. $\Delta_n = \Delta E_n - \Delta E_0^{RSPT}$ gives an IWBPT which leads to the correct pinning behaviour [9, 14] for small α. ΔE_0^{RSPT} is the correction for the electron–phonon interaction to the GS energy using the RSPT method. It is easy to see that $\Delta E_0^{IWBPT} = \Delta E_0^{RSPT}$ for all ω.

The wavefunction of the unperturbed harmonic oscillator problem is given by

$$|\phi_j^{ND}\rangle = \left(\frac{\omega}{\pi}\right)^{3/4} \left[\frac{\omega^{N/2}}{\pi^{N/2} 2^{(j_1+\cdots+j_N)} j_1! \cdots j_N!}\right]^{1/2} \exp\left(-\frac{\omega r^2}{2}\right) H_{j_1}(\sqrt{\omega}x_1) \cdots H_{j_N}(\sqrt{\omega}x_N). \tag{5}$$

To perform the summation in equation (4) we follow [9] and insert

$$\frac{1}{E_j - E_n - \Delta_n + 1} = \int_0^{\infty} \mathrm{e}^{-(E_j - E_n - \Delta_n + 1)t}\, \mathrm{d}t, \tag{6}$$

and after using the transformation function of the N-dimensional harmonic oscillator one finds the following expression for the energy correction [13]:

$$\Delta E_n = -\frac{\alpha}{\sqrt{2}} \left(\frac{\omega}{2\pi}\right)^{N/2} \int \phi_n(\vec{r}) \phi_n^*(\vec{r}\,') \frac{\mathrm{e}^{(E_n^0 + \Delta_n - 1)t}}{|\vec{r} - \vec{r}\,'|} \left(\frac{1}{\sinh \omega t}\right)^{N/2} \times \exp\left[-\left(\frac{\omega}{4}\right)\left\{(\vec{r} + \vec{r}\,')^2 \tanh\frac{\omega t}{2} + (\vec{r} - \vec{r}\,')^2 \coth\frac{\omega t}{2}\right\}\right] \mathrm{d}\vec{r}\, \mathrm{d}\vec{r}\,'\, \mathrm{d}t. \tag{7}$$

After integrating over $\vec{r}$ and $\vec{r}\,'$ the following expressions for the energy corrections of the GS and the first ES can be obtained:

$$\Delta E_{GS}^{ND} = -\frac{\alpha}{2\sqrt{\omega}} \frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)} B\left(\frac{1}{\omega}, \frac{1}{2}\right), \tag{8a}$$

$$\Delta E_{ES}^{ND} = -\frac{\alpha}{\sqrt{\omega} 4N} \frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)} \left[(2N-1) B\left(\frac{1 - \Delta_1}{\omega}, \frac{1}{2}\right) + B\left(\frac{1 - \Delta_1}{\omega} - 1, \frac{1}{2}\right)\right], \tag{8b}$$

where $B(x, y)$ is the beta function.

To study the splitting and pinning of the energy level E_n we are interested in the region where $n\omega \approx 1$ and $\omega \to \infty$. The electronic GS plus one phonon is degenerate with the electron

in the first ES. When $n\omega \simeq 1$, the RSPT method is no longer applicable and one has to use degenerate perturbation theory, i.e. WBPT or its improved version (IWBPT), to calculate the energy of the system self-consistently. In the region $1 - \Delta_n \simeq n\omega$, the dominant contribution comes from the second term of equation (8*b*) and we obtain

$$\Delta E_1 = -\frac{\alpha}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\frac{\sqrt{\omega}}{1-\Delta_1-\omega}. \tag{9}$$

When $\omega = 1$, the electron–phonon interaction lifts the degeneracy of the energy level E_1 and E_0 + (one phonon). The splitting of the first ES at $\omega = 1$ is twice

$$|\Delta E_1| = \sqrt{\alpha}\left[\frac{1}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right]^{1/2}. \tag{10}$$

In the large-ω limit, we found to lowest order in α

$$E_1 = \frac{N}{2}\omega + 1 + \Delta E_0^{RSPT} - \alpha\sqrt{\omega}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\frac{1}{4N(\omega - 1 - \Delta E_0^{RSPT})}, \tag{11}$$

and ΔE_0^{RSPT} is given by [13]

$$\Delta E_0^{RSPT} = -\frac{\alpha}{2}\sqrt{\omega}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(1 + \frac{2\ln 2}{\omega}\right). \tag{12a}$$

For large confinement frequency the energy levels are pinned to E_0+1. This is the so-called pinning effect which should be observable experimentally.

In the limit $\omega \to 0$, non-degenerate perturbation theory, i.e. RSPT, has to be used. The energy correction due to the electron–phonon interaction is given by [13]

$$\Delta E_0^{RSPT} = -\frac{\alpha}{2}\sqrt{\pi}\,\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(1 + \frac{1}{8}\omega\right). \tag{12b}$$

3. Numerical results and discussion

In figure 1 we show the unperturbed energy spectrum (dotted lines) together with the energy of an electron in a parabolic GaAs quantum dot ($\alpha = 0.07$) in the presence of the electron–LO-phonon interaction as a function of the confinement frequency ω. We have presented our results for both 2D (full curves) and 3D (dashed curves) quantum dots. The modified energies for the 2D and 3D systems have been obtained from the self-consistent solution of equation (8*b*) for ω less than 1 for the first ES. To obtain the modified energies for ω-values larger than the above value, we have used equation (9) in order to reduce the numerical error.

One can easily see that in the presence of the electron–phonon interaction the electronic energy levels are shifted to lower energies and this is a clear manifestation of the polaronic effect in a quantum dot. It is also clear that the polaronic effect is more pronounced in a 2D quantum dot than in a 3D dot. One can furthermore notice that at $\omega \approx 1$, the first ES energy level does not cross the GS energy plus one LO phonon energy; rather it bends downward because of the polaronic effect. A similar behaviour is observed for the second ES at $\omega \approx 1/2$. These behaviours, in fact, follow from Von Neumann's non-crossing theorem and lead to resonant splittings of the degeneracies that exist in the unperturbed system. We would like to emphasize that these splittings should be observable through far-infrared optical spectroscopic measurements at the right values of the confinement frequency or the effective dot size. Finally, the most interesting observation that one can make from figure 1 is that when the confinement frequency becomes very large, all the energy levels get pinned to the GS energy level plus one

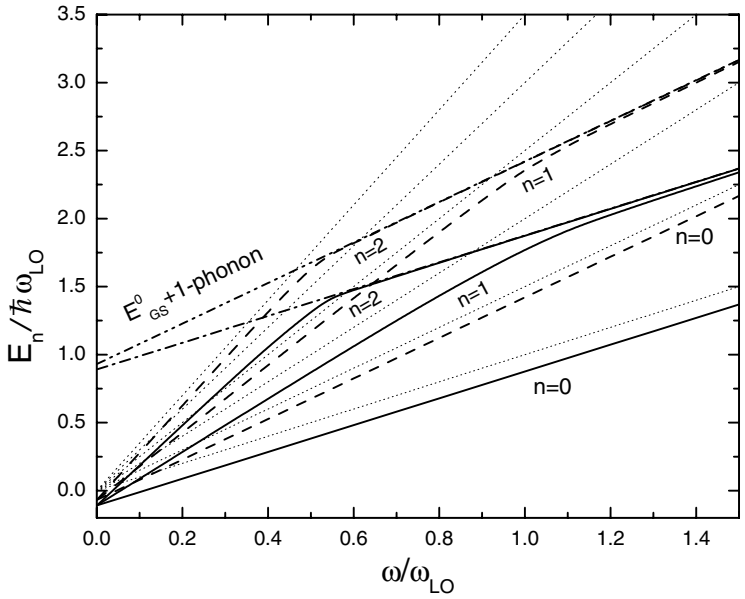

Figure 1. Energy levels ($E_n/\hbar\omega_0$) of an electron in a parabolic quantum dot in both two (solid curves) and three dimensions (thick dashed curves) as a function of the confinement frequency ω/ω_{L0} for $\alpha = 0.07$. The dotted curves are the energy levels of the non-interacting electron.

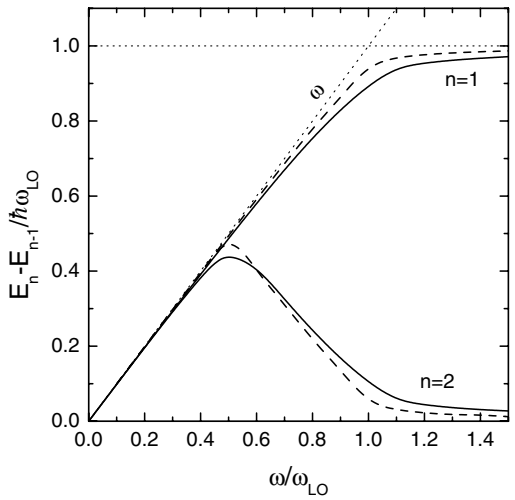

Figure 2. The energy difference between two consecutive energy levels $(E_n - E_{n-1})/\hbar\omega_0$ of an electron in a 2D (solid curves) and in a 3D (thick dashed curves) parabolic dot as a function of the confinement frequency ω/ω_{L0} for $\alpha = 0.07$.

LO phonon energy. This pinning effect is quite well known in the case of bulk polar materials in the presence of an externally applied magnetic field. However, the interesting point that we would like to emphasize here is that it is possible to observe the pinning effect in a quantum dot even in the absence of any external magnetic field just by increasing the lateral confinement.

In figure 2, we have shown the energy difference between two consecutive electronic energy levels both for 2D (solid curves) and for 3D (dashed curves) as a function of the

confinement frequency of the dot. One can clearly see that the difference between the first ES energy and the GS energy becomes equal to the LO phonon energy in the limit where the confinement frequency becomes very large, while the difference between the second excited energy and the first ES energy goes to zero in the same limit. This is again a clear manifestation of the pinning effect.

4. Conclusions

In conclusion, we calculated the energy levels for an electron in a parabolic quantum dot in the presence of electron–LO-phonon interaction using the 'improved WBPT' to second order in the electron–phonon coupling constant. We showed that the electronic energy levels are lowered in energy by the polaronic effect and there are resonant splittings of the ES energy levels at certain values of the confinement frequency. In the limit of strong confinement we found that all the ES energy levels are pinned to the GS energy level plus one LO phonon energy. We applied our results to a GaAs quantum dot for the cases of both two- and three-dimensional confinement. In our opinion, the pinning effect proposed here for a parabolic quantum dot is a very interesting theoretical observation and should be experimentally verified through far-infrared intraband optical spectroscopic measurements, which would give clear and direct evidence of the polaronic effect in a quantum dot. Such a study would give information on the *position* of the polaron energy levels, which provides information complementary to the recent polaron *lifetime* measurements of Sauvage *et al* [7].

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