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COMMENT

An improved Lamb shift calculation for a bound polaron in a purely two-dimensional quantum well

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Abstract. Using an improved variational wave function the 2s excited state energy of a Coulomb impurity bound polaron in a purely two-dimensional quantum well is calculated and the excitation energies and the phonon-induced Lamb shift corrections are obtained for several polar materials.

Much effort has lately gone into exploring electronic states at surfaces and interfaces, and in quantum wells and heterojunction superlattices of polar semiconductors [1]. These studies are important both from the point of view of fundamental physics and for applications to electronic devices. In a recent paper [2] we have addressed ourselves to the problem of an impurity bound optical polaron in a purely two-dimensional (2D) quantum well. Using a variant of the Lee, Low and Pines (LLP) method [3] as proposed by Huybrechts [4] we have obtained the ground state (GS) energy, the size of the polaron, the average number of virtual phonons in the polaron cloud, the first two internal excited states and the phonon-induced Lamb shift corrections. This Lamb shift calculation, however, suffers from a drawback that one of the excited states, namely the 2s state, was not orthogonal to the GS. The purpose of this comment is to make an improved variational calculation of the 2s state using a better trial function, and to recalculate the Lamb shift corrections. For the sake of completeness we shall also briefly describe the formulation, and the GS and 2p state calculations.

The Hamiltonian for a 2D bound polaron in Feynman units is given by [2]

$$\mathcal{H} = -\frac{1}{2}\nabla_\rho^2 - \frac{\beta}{\rho} + \sum_q (b_q^+ b_q + \tfrac{1}{2}) + \sum_q (\xi_q e^{-iq\cdot\rho} b_q^+ + \text{HC}) \tag{1}$$

where ρ is the 2D position vector of the electron, β is the renormalized Coulomb binding parameter, $b_q^+(b_q)$ is the creation (annihilation) operator for a dispersionless optical phonon of wave vector q and ξ_q is the electron–phonon interaction coefficient which contains the dispersionless electron–phonon coupling constant α.

In the LLP–Huybrechts method the variational energy is written as

$$E = \langle \Phi(\rho) | \langle 0 | \tilde{\mathcal{H}} | 0 \rangle | \Phi(\rho) \rangle \tag{2}$$

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where $\Phi(\rho)$ is the electronic function to be chosen variationally, $|0\rangle$ the unperturbed zero phonon state and $\tilde{\mathcal{H}}$ is a transformed Hamiltonian given by

$$\tilde{\mathcal{H}} = U_2^{-1}U_1^{-1}\mathcal{H}U_1U_2 \tag{3}$$

where

$$U_1 = \exp\left(-ia\sum_q q\cdot\rho b_q^+ b_q\right) \tag{4}$$

$$U_2 = \exp(f_q b_q^+ - f_q^* b_q) \tag{5}$$

'a' and f_q being the variational parameters. From [2] it is clear that for most cases the hydrogenic approximation is a better choice than the Gaussian approximation. We shall therefore work in the hydrogenic approximation. For the GS calculation in [2] the trial function was chosen as

$$\Phi_{1s} = 2^{2/3}(\gamma/\sqrt{\pi})e^{-2\gamma\rho} \tag{6}$$

where γ is a variational parameter. The minimization of (2) with respect to f_q and γ yields

$$E_{1s} = -2[\beta + (\sqrt{2}/4)tF(t)]^2 - F(t) \tag{7}$$

where

$$t = (1-a)/\sqrt{2}a\gamma \tag{8}$$

$$F(t) = (\alpha\pi/8)(3t^2 + 18t + 32)(t+2)^{-3} \tag{9}$$

$$\gamma = \beta + (\sqrt{2}/4)tF(t). \tag{10}$$

Finally E_{1s} is minimized numerically with respect to t. Numerical results have been reported in [2].

For the first two excited states the following functions were chosen in [2]:

$$\Phi_{2s} = (4\lambda/3\sqrt{6\pi})[1-(4\lambda/3)\rho]e^{-(2\lambda/3)\rho} \tag{11}$$

$$\Phi_{2p} = (8\lambda'^2/9\sqrt{3\pi})\rho e^{-(2\lambda'/3)\rho}e^{i\vartheta} \tag{12}$$

where λ and λ' are variational parameters. As we have already mentioned, Φ_{2s} as given in (11) suffers from an orthogonality problem, i.e. it is not orthogonal to Φ_{1s}. The 2p state wave function (equation (12)), however, does not suffer from any such problem. In this comment we therefore modify the 2s state trial function as

$$\Phi_{2s} = A[1-(4\delta/3)\rho]e^{-(2\lambda/3)\rho} \tag{13}$$

where A is the normalization constant, λ is a variational parameter and δ is chosen such that

$$\langle\Phi_{1s}|\Phi_{2s}\rangle = 0. \tag{14}$$

We find that

$$A = (18\pi/16\lambda^2)^{-1/2}(1 - 4\delta/\lambda + 6\delta^2/\lambda^2) \tag{15}$$

and

$$\delta = (\lambda + 3\gamma)/4. \tag{16}$$

The calculation for the 2p state is performed with the same function (12).

We have studied the variation of the excited state energies E_{2s} and E_{2p} as a function of the electron–phonon coupling constant α for three values of the Coulomb binding parameter β ($\beta = 2$, 5, 10). Results are shown graphically in figures 1–3. In figure 1 we plot E_{2s} and E_{2p} versus α for $\beta = 2$. The behaviour is quite interesting and somewhat different from what we observed in [2]. At low values of α, the 2s and 2p states are degenerate and as α increases the degeneracy is slightly lifted with the 2s level coming lower than the 2p level, leading to a small phonon-induced Lamb shift. But interestingly, as α exceeds a certain value there is a cross-over of the 2s and 2p levels and as α increases further a large phonon Lamb shift results with a reversal in sign. In figure 2 we plot the 2s, 2p energies versus α for $\beta = 5$. Again for low α the 2s–2p degeneracy is not lifted and there is no Lamb shift. But for intermediate and large values of α the energy levels do split, giving rise to a Lamb shift which increases monotonically with α and is again negative in sign. In figure 3 we plot our results for $\beta = 10$. The behaviour is similar to that observed for $\beta = 5$, but now there are Lamb shifts even for small values of α.

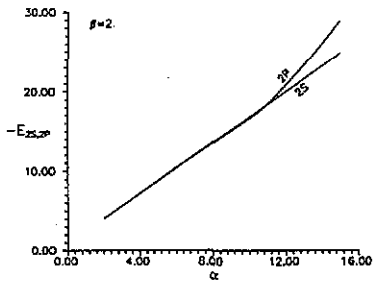

Figure 1. The 2D bound polaron excited state energies E_{2s} and E_{2p} (in Feynman units) versus α for $\beta = 2$ in the hydrogenic approximation.

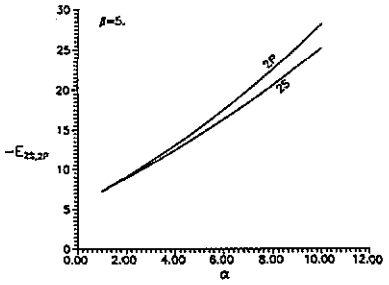

Figure 2. The 2D bound polaron excited state energies E_{2s} and E_{2p} (in Feynman units) versus α for $\beta = 5$ in the hydrogenic approximation.

In table 1 we present the 1s–2s and 1s–2p transition energies and the phonon Lamb shifts for a number of 2D polar materials. The Lamb shifts $E_{2p}-E_{2s}$ are again found to be zero for GaAs, ZnAs, CdS and TiCl, as were found in [1]. For the alkali halides like NaCl, KCl, NaBr, NaI, KI and for Cu_2O we find quite large Lamb shifts which again have a negative sign. For ZnO and MnO, however, we find small positive values for the Lamb shift. It may be noted that for some materials the present values of the Lamb shift may be significantly different from those obtained by the unimproved wave function used in [2]. For example, the Lamb shift for Cu_2O changes by about 10 meV when the improved wave function is used. Figure 4 compares the present improved 2s state energies for $\beta = 5$ with the corresponding values reported in [2]. For several materials, however, the present Lamb shift values may be only slightly different from the unimproved ones, but in some cases even a slight change in the 2s state energy might bring about a qualitative difference in the Lamb shift, such as in the sign of the Lamb shift, as shown in figure 1.

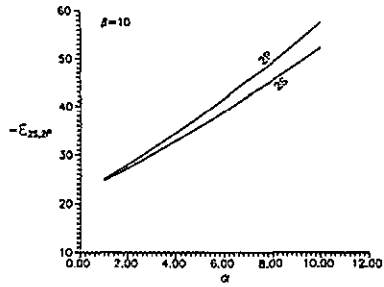

Figure 3. The 2D bound polaron excited state energies E_{2s} and E_{2p} (in Feynman units) versus α for $\beta = 10$ in the hydrogenic approximation.

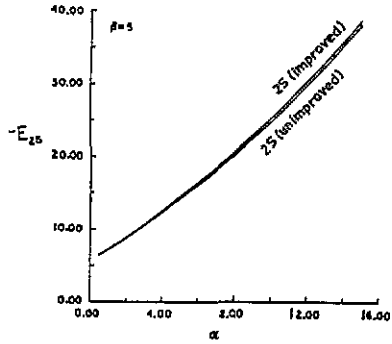

Figure 4. A comparison of the present 2s state energies with those of [2].

Table 1. GS energies (E_{1s}), excited state energies (E_{2s}, E_{2p}), transition energies (E_{1s}–E_{2s}, E_{1s}–E_{2p}) and Lamb shift corrections (E_{2p}–E_{2s}) in meV for the 2D bound polaron in the hydrogenic approximation, for a few polar materials. (See [2] for values for the material parameters.)

Materials	α_s	β_s	E_{1s}	E_{2s}	E_{2p}	E_{1s}–E_{2s}	E_{1s}–E_{2p}	E_{2p}–E_{2s}
GaAs	0.116	1.011	−81.16	−14.91	−14.91	−66.24	−66.24	0
ZnS	0.9	2.264	−594.97	−109.303	−109.303	−485.67	−485.67	0
CdS	0.987	2.334	−553.94	−100.93	−100.93	−453.01	−453.01	0
ZnO	1.472	2.151	−1044.15	−227.98	−226.98	−816.867	−817.172	0.30
MnO	2.052	1.687	−1066.31	−315.25	−315.02	−751.06	−751.19	0.23
TiCl	4.382	1.163	−360.66	−143.134	−143.134	−217.53	−217.53	0
NaCl	11.34	15.47	−23 744.26	−2970.44	−3222.06	−20 774.42	−20 522.20	−258.38
KCl	9.70	16.84	−20 174.69	−2472.68	−2648.30	−17 702.01	−17 526.39	−175.62
NaBr	11.13	16.91	−21 548.71	−2663.31	−2878.315	−18 880.39	−18 670.39	−215.00
NaI	11.625	17.42	−19 978.42	−2475.59	−2672.72	−17 502.83	−17 305.7	−197.33
KI	8.37	19.42	−17 800.71	−2135.41	−2257.69	−15 665.29	−15 543.02	−122.28
Cu_2O	5.079	5.52	−5826.56	−805.39	−858.40	−5021.17	−4968.16	−53.01

In conclusion, we have performed an improved variational calculation for the phonon-induced Lamb shifts for an impurity bound polaron in a purely 2D quantum well. We again find that the 2D phonon Lamb shifts are much larger than the corresponding 3D values and are of negative sign when α and β are both large or one of them is large. When α and β are both small, the Lamb shift corrections are either zero or may have small positive values. This is an interesting theoretical observation and should be tested experimentally.

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