

Interface-phonon-mediated magnetopolaronic effect on impurity transition energies in quantum wells

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(Received 21 May 1990)

Electron interactions with interface phonon modes and strictly confined bulk phonon modes are considered to calculate the resonant magnetopolaronic $1s-2p_+$ transition energy of a hydrogenic impurity in the quantum well of a double heterostructure. An interaction gap is predicted between the bulk LO and TO frequencies, in contrast to the Fröhlich-type interaction. These results are in good agreement with recent experimental data.

The interface and confined bulk phonon modes in heterostructures and superlattices have been discussed theoretically¹ and observed experimentally² in the past. Only recently, optical-phonon modes supported by a semiconductor double heterostructure (DHS) have been solved independently in the long-wavelength limit by two groups.^{3,4} It is found that there exist two types of phonon modes, confined bulk modes and interface modes. The confined modes can be either longitudinal optical (LO) or transverse optical (TO) with frequencies ω_L and ω_T identical to those of the bulk excitations, while the interface (IN) modes can have frequencies between ω_L and ω_T . Eigenvectors and dispersion relations for all these modes can be found in Refs. 3 and 4. The Hamiltonian operator describing the electron-optical-phonon interaction has also been derived to study the polaron mobility and magnetophonon resonance spectra,⁴ and the polaronic states in a DHS.⁵ The importance of interface modes is clearly demonstrated in these calculations.

The resonant magnetopolaron effect on the $1s-2p_+$ transition energy is found to be well below ω_L in far-infrared photoconductivity measurements⁶ carried out for a donor impurity doped at the center of GaAs quantum wells in a GaAs/Al_xGa_{1-x}As multiple-quantum-well (MQW) structure, in contrast to the bulk case which has been quantitatively accounted for.⁷ As the electron does not couple to TO phonons, the data have been regarded as a significant deviation from reasonable expectations based on the Fröhlich model of interaction with the bulk GaAs zone-center LO phonons, both in magnitude and field dependence. The experiment has been improved and extended recently in a series of measurements.⁸ The data appear to deviate smoothly from the calculated transition energy in the absence of electron-phonon interactions, and the deviation is generally smaller than what is reported in Ref. 6. In addition, two gaps are observed and many more points are measured above the first gap in qualitative agreement with our theoretical results.

We report, in this Rapid Communication, a calculation of the $1s-2p_+$ transition energy as a function of the applied magnetic field for a magnetopolaron bound to a hydrogenic impurity in a double heterostructure, i.e., a single quantum well with finite barriers. The electron-phonon interaction Hamiltonian derived in Refs. 4 and 5 is treated as a perturbation on the hydrogen-like atom confined in a quantum well under strong magnetic fields. Since the unperturbed system cannot be solved exactly, a variational calculation has been performed with properly chosen trial wave functions. The calculation is actually quite complicated and we can only present the results along with a brief outline of the procedures. Detailed account of this work will be published elsewhere.⁹

Consider a donor impurity at the center of the GaAs quantum well of width d in a GaAs/Al_xGa_{1-x}As DHS system. A magnetic field is applied along the growth direction. For convenience, we introduce the two-dimensional vectors κ and ρ such that $\mathbf{k}=(\kappa, q)$ and $\mathbf{r}=(\rho, z)$ for the phonon momentum and electron position, respectively. The electron momentum is denoted by $\mathbf{k}_e=(k_{||}, k_z)$. In the absence of electron-phonon interactions, the Hamiltonian of the impurity is given by

$$H_e = \frac{1}{2m_e} \left[\mathbf{p} - \frac{e}{c} \mathbf{A} \right]^2 - \frac{e^2}{\epsilon_0 r} + V_B(z) \quad (1a)$$

$$V_B(z) = \begin{cases} 0, & |z| \leq d/2 \\ V_0, & |z| > d/2. \end{cases} \quad (1b)$$

The interaction Hamiltonian H_{e-ph} is taken directly from Ref. 5. It consists of two terms: the electron interaction with confined LO modes, and the interaction with interface modes. As has been shown in Ref. 5, contributions of lattice vibrations outside the well to the polaron effect are significant only when the well width d is extremely small. For $d \gtrsim 100 \text{ \AA}$, they are completely negligible. Therefore we have

$$H_{e-ph} = H_{e-LO} + H_{e-IN}, \quad (2a)$$

$$H_{e-LO} = - \sum_{\kappa} e^{i\kappa \cdot \rho} \left[\sum_{m=1,3,\dots} B_m(\kappa) \cos \left(\frac{m\pi}{d} z \right) [a_m(\kappa) + a_m^\dagger(-\kappa)] + \sum_{m=2,4,\dots} B_m(\kappa) \sin \left(\frac{m\pi}{d} z \right) [a_m(\kappa) + a_m^\dagger(-\kappa)] \right], \quad (2b)$$

$$H_{e\text{-IN}} = - \sum_{\kappa, j} e^{i\kappa \cdot \rho} \left[B_{sj}(\kappa) \frac{\cosh(\kappa z)}{\cosh(\kappa d/2)} [a_{s,j}(\kappa) + a_{sj}^\dagger(-\kappa)] - B_{aj}(\kappa) \frac{\sinh(\kappa z)}{\sinh(\kappa d/2)} [a_{a,j}(\kappa) + a_{aj}^\dagger(-\kappa)] \right], \quad (2c)$$

where $H_{e\text{-LO}}$ represents the electron interaction with confined bulk LO phonon modes in the quantum well where $q = m\pi/d$ is quantized, and $H_{e\text{-IN}}$ represents the electron interaction with interface phonon modes in the well. We have introduced in Eqs. (2) the creation and annihilation operators $a_m^\dagger(\kappa)$ and $a_m(\kappa)$ for the confined modes and $a_{sj}^\dagger(\kappa)$ and $a_{sj}(\kappa)$ for the symmetric and antisymmetric interface phonon modes, respectively. They obey the commutation relations

$$[a_\alpha(\kappa), a_\beta^\dagger(\kappa')] = \delta_{\alpha\beta} \delta(\kappa - \kappa'), \quad (3a)$$

$$[a_\alpha^\dagger(\kappa), a_\beta^\dagger(\kappa')] = [a_\alpha(\kappa), a_\beta(\kappa')] = 0. \quad (3b)$$

The normalization constants are given by

$$|B_m(\kappa)|^2 = \frac{1}{Ad} \frac{4\pi e^2 \hbar \omega_L}{\kappa^2 + (m\pi/d)^2} \left[\frac{1}{\epsilon_{\infty 1}} - \frac{1}{\epsilon_{01}} \right], \quad (4a)$$

$$|B_{sj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa} \frac{\hbar \omega_{sj}(\kappa)}{\bar{\epsilon}_1 \tanh(\kappa d/2) + \bar{\epsilon}_2}, \quad (4b)$$

$$|B_{aj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa} \frac{\hbar \omega_{aj}(\kappa)}{\bar{\epsilon}_1 \coth(\kappa d/2) + \bar{\epsilon}_2}, \quad (4c)$$

where A stands for the interface area, $\epsilon_{\infty \nu}$ and $\epsilon_{0\nu}$ denote the optic and static dielectric constants of material ν ($\nu=1$ for the well and $\nu=2$ for the barrier), and $\bar{\epsilon}_\nu(\omega)$ is defined by

$$\frac{1}{\bar{\epsilon}_\nu(\omega)} = \frac{1}{\epsilon_\nu(\omega) - \epsilon_{0\nu}} - \frac{1}{\epsilon_\nu(\omega) - \epsilon_{\infty\nu}}, \quad (5)$$

with the dielectric function of material ν given by

$$\epsilon_\nu(\omega) = \epsilon_{\infty\nu} (\omega_{L\nu}^2 - \omega^2) / (\omega_{T\nu}^2 - \omega^2). \quad (6)$$

We now proceed to calculate the transition energy by perturbation theory. For the unperturbed system, we take the hydrogenic impurity in the well with a magnetic field applied normal to the interfaces. Thus $H_0 = H_e$ and $H_{e\text{-ph}}$ is treated as a perturbation. It is noted, however, that even the unperturbed problem is not exactly solvable. Thus we employ the variational method to determine the unperturbed energy levels. The trial wave function is taken to be

$$\psi = f(z) G(\rho, z, \phi), \quad (7)$$

$$f(z) = \begin{cases} \cos(k_z z), & |z| \leq \frac{d}{2}, \\ A \exp(-k_z' |z|), & |z| > d/2, \end{cases} \quad (8)$$

$$G(\rho, z, \phi) = \rho^{|m|} \exp(im\phi - \gamma\rho^2/4 - \gamma\xi^2 z^2/4), \quad (9)$$

where we have defined $k_z = (2m_e E_1 / \hbar^2)^{1/2}$ and k_z'

$= [2m_e(V_0 - E_1)/\hbar^2]^{1/2}$ with the first electron subband energy E_1 , the parameter $\gamma = \hbar\omega_c/2R_y$ with the cyclotron frequency $\omega_c = eB/m_e c$, and the effective Rydberg $R_y = m_e e^4 / 2\hbar^2$ for the impurity. The quantum number m specifies the impurity levels such that $m=1, 0, -1$ for the $2p_+, 1s, 2p_-$ levels, respectively. The variational parameter ξ is determined by minimizing the energy of the level in question. All the other levels, for particular samples used in these measurements,⁸ can be neglected. Hence the Hilbert space in our perturbation calculation is truncated to only the three states, $1s, 2p_+$, and $2p_-$.

The energy levels are calculated by means of Wigner-Brillouin perturbation theory to second order. The result is

$$\epsilon_i(B) = E_i(B) + \frac{1}{(2\pi)^2} \sum_{n \neq i} \int d^2\kappa \frac{|\langle n | H_{e\text{-ph}} | i \rangle|^2}{\epsilon_i(B) - E_n(B) - \hbar\omega(\kappa)}, \quad (10)$$

where $E_i(B)$ stands for the corresponding unperturbed energy. As the matrix element is generally small compared to the transition energy, the perturbation energy in (10) becomes appreciable only when the electronic energy-level difference in the denominator matches the phonon energy $\hbar\omega(\kappa)$. This implies immediately that the electron-phonon coupling has negligible influence on the $1s$ energy level. Hence it is sufficient to calculate $\Delta E = \epsilon_{2p_+} - E_{1s}$ for the transition energy. Furthermore, we note that significant contribution from the second term in (10) is expected around $\Delta E \approx E_{2p_-} - E_{1s} + \hbar\omega_L$ for the three-level resonance, as well as around $\Delta E \approx \hbar\omega_L$ for the two-level resonance.

As can be seen from Eqs. (2), the calculation of energy levels involves the evaluation of four matrix elements

$$\begin{aligned} M_1(\gamma) &= \langle 2p_+, 0_m | H_{e\text{-LO}} | 1s, 1_m \rangle, \\ M_2(\gamma) &= \langle 2p_+, 0_j | H_{e\text{-IN}} | 1s, 1_j \rangle, \\ M_3(\gamma) &= \langle 2p_+, 0_m | H_{e\text{-LO}} | 2p_-, 1_m \rangle, \\ M_4(\gamma) &= \langle 2p_+, 0_j | H_{e\text{-IN}} | 2p_-, 1_j \rangle, \end{aligned} \quad (11)$$

where the states $|nl, N_m\rangle$ are specified by the atomic level nl and the number N of phonons of mode m . The explicit expressions for these matrix elements have been worked out in Ref. 9. Here we just present the results as functions of the applied field in Fig. 1. It is observed that in both the two-level and three-level resonance cases, the interface phonon modes generally result in larger matrix elements, and that M_4 is the largest and is generally 3–4 times larger than the others. This is understandable, since the Bohr radius of the impurity is of the same order as the well width, and since the p -state wave functions extend out much farther in the xy plane than the s -state wave function.

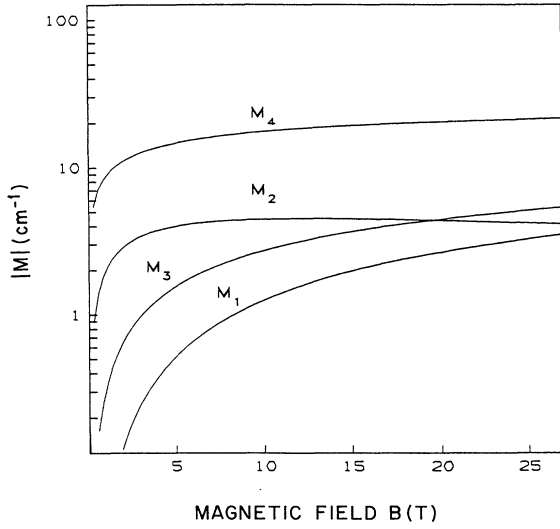


FIG. 1. Absolute values of the matrix elements of the electron-phonon interactions calculated as functions of the applied magnetic field in the GaAs well of a GaAs/Ga_{1-x}Al_xAs double heterostructure.

The energy of the $2p_+$ level is then given by

$$\varepsilon_{2p_+}(\gamma) = E_{2p_+}(\gamma) + T(\gamma), \quad (12a)$$

$$T(\gamma) = \frac{1}{(2\pi)^2} \int d^2\kappa \left[\frac{|M_1|^2}{\varepsilon_{2p_+} - E_{1s} - \hbar\omega_L} + \frac{|M_2|^2}{\varepsilon_{2p_+} - E_{1s} - \hbar\omega(\kappa)} + \frac{|M_3|^2}{\varepsilon_{2p_+} - E_{1s} - (E_{2p_-} - E_{1s} + \hbar\omega_L)} + \frac{|M_4|^2}{\varepsilon_{2p_+} - E_{1s} - [E_{2p_-} - E_{1s} + \hbar\omega(\kappa)]} \right]. \quad (12b)$$

The evaluation of (12) is still very difficult. We adopt a numerical iteration procedure to compute the transition energy. Let $X(\gamma) = \varepsilon_{2p_+} - E_{1s}$ and $\Gamma(\gamma) = E_{2p_+} - E_{1s}$. Then Eq. (12) can be rewritten as

$$X(\gamma) = \Gamma(\gamma) + T(\gamma, X). \quad (13)$$

The function $\Gamma(\gamma)$ represents the transition energy in the absence of the electron-phonon interactions and is already known from the variational calculations. Therefore, we start the iteration with $X = \Gamma(\gamma)$ in T for a fixed B which determines the parameter γ . A new X value is obtained from (13) and employed to compute a new T . The procedure goes on until self-consistency is achieved. The iteration procedure repeats when B changes and eventually the transition energy is found as a function of B .

Results of our numerical computation are presented in Fig. 2 in which the $1s$ - $2p_+$ transition energy is plotted as a function of B . The parameters used in the numerical work are $d = 125 \text{ \AA}$, $m_e = 0.067m_0$, $a_0 = 98.7 \text{ \AA}$, $R_y = 5.83 \text{ meV}$, and $V_0 = 230 \text{ meV}$. The solid line includes the effect of the nonparabolic band mass¹⁰ and the dash-dotted line does not. The dashed line represents the transition energy from unperturbed energy levels. It is computed from Greene-Bajaj wave functions¹¹ with the nonparabolicity effect included. The horizontal lines are drawn only to in-

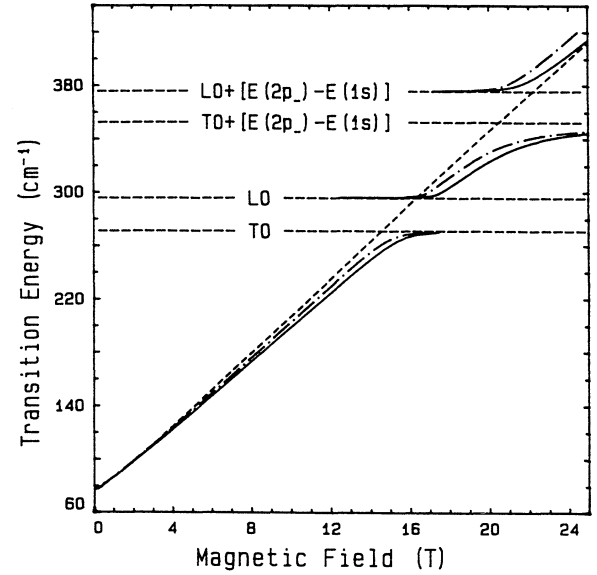


FIG. 2. $1s$ - $2p_+$ transition energy as a function of the applied field B . The solid line represents results from the present theory including nonparabolic band mass, and the dash-dotted line does not. The dashed line is the transition energy in the absence of electron-phonon interactions. It is calculated from Greene-Bajaj wave functions with the nonparabolicity correction.

dicating the gap positions. It is remarkable that the theoretical curve breaks into three branches separated by two gaps, in good qualitative agreement with experimental data. A comparison of the theory with experiments can be found in Ref. 8. The pinning effect, or the unperturbed energy-level repulsion, is apparently a result of the strong resonance interaction when the denominator of the second-order perturbation energy vanishes. As the electron does not interact with TO phonons, the appearance of the gaps can only be attributed to the coupling of the electron with interface phonons which oscillate at frequencies between the bulk ω_T and ω_L .

Further studies, both theoretical and experimental, are necessary for a complete understanding of the problem. The determination of the transition frequency from experimental data is difficult, as the observed intensity distribution in the resonance region deviates greatly from the Lorentz shape. Theoretical study of the influence of electron-phonon interactions on the transition probability is needed for detailed comparison with the experimental line shapes and observed rapid decrease in intensity in this energy region. Furthermore, as we have noted previously, the trial function (9) has only one adjustable parameter. More accurate functions must be constructed, for more accurate results.

In conclusion, we assert that it is the interaction of the electron with interface phonon modes that changes the polaronic properties in the reduced geometry. These modes should always be included in the interpretation of such experiments. Since the coupling constant of the bulk Fröhlich type cannot be clearly defined for the interface modes, polaronic phenomena observed in the reduced

dimensionality should not be analyzed by varying the coupling strength in terms of the bulk Fröhlich interaction.

We are grateful to B. D. McCombe and J. P. Cheng for providing us with experimental data prior to publication. This research was supported in part by the U.S. Office of Naval Research.

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