Comment on "Effects of the localized state inside the barrier on resonant tunneling in double-barrier quantum wells"

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It is shown that the split of the highest-energy peak observed by He and Gu [Phys. Rev. B **41**, 2906 (1990)] in the intermediate- and strong-coupling regions, when $|\Omega_b|$ is very large, is only an artifact.

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Since the work of Beltram and Capasso,[1] effects of the localized state inside the barrier on resonant tunneling in single barrier,[2,3] double-barrier,[4–7] and multibarrier structures[8,9] have been investigated extensively. In a previous publication by He and Gu [Phys. Rev. B **41**, 2906 (1990)], the doping effects on resonant tunneling of a defect-layer sheet inserted in one barrier of the double-barrier quantum well were analyzed by using the effective-mass approximation and transfer-matrix approach. The model potential of defects was taken to be a δ function. It was reported that when $|\Omega_b|$ was very large, i.e., the defect state energy level was very deep, similar to a strong attraction source in the barrier, the defect-layer sheet in the barrier would lead to the split of the highest-energy peak and make a new quasibound state. This effect was observed in both the intermediate- and strong-coupling regions, and it was also reported that the stronger the coupling was, the more obvious this effect was [see Figs. 5(b) and 5(c) of Ref. 5]. These peculiar findings are not only controversy to the results of Arsenault and Meunier[4] given in Figs. 2 and 3 of Ref. 4, but also inconsistent with their own results shown in Figs. 2–4 of Ref. 5. However, the authors of Ref. 5 overlooked this discrepancy and failed to give any explanation, even though this feature is strange and hard to understand. We have recalculated those resonant peaks by using analytical expressions of the transmission probability and the resonance condition. It is found that the split of the highest-energy peak when $|\Omega_b|$ was very large, as observed by He and Gu in intermediate- and strong-coupling regions, is an artifact of their numerical procedure.

The transmission probability can be written as

$$T_{\text{tot}} = \{T_1^{-1}T_2^{-1} + (T_1^{-1}-1)(T_2^{-1}-1) + 2[T_1^{-1}T_2^{-1}(T_1^{-1}-1) \times (T_2^{-1}-1)]^{1/2}\cos\Phi\}^{-1} \tag{1}$$

with

$$\Phi = \phi_1 + \phi_2 + \delta_1 - \delta_2 + 4k_w a, \tag{2}$$

$$T_1 = \left\{\left(\cosh(k_b b) - \frac{k_0}{k_b}\sinh(k_b b)\right)^2 + \left[\frac{k_0}{2k_b}\left(X + \frac{1}{X}\right)\cosh(k_b b - 2k_b x_b) - \frac{1}{2}\left(\frac{1}{X} - X\right)\left(\sinh(k_b b) - \frac{k_0}{k_b}\cosh(k_b b)\right)\right]^2\right\}^{-1}, \tag{3}$$

$$\phi_1 = \arctan\left[\frac{\frac{k_0}{2k_b}\left(X + \frac{1}{X}\right)\cosh(k_b b - 2k_b x_b) - \frac{1}{2}\left(\frac{1}{X} - X\right)\left(\sinh(k_b b) - \frac{k_0}{k_b}\cosh(k_b b)\right)}{\cosh(k_b b) - \frac{k_0}{k_b}\sinh(k_b b)}\right], \tag{4}$$

$$\delta_1 = \arctan\left[\frac{\frac{1}{2}\left(X + \frac{1}{X}\right)\left(\sinh(k_b b) - \frac{k_0}{k_b}\cosh(k_b b)\right) - \frac{k_0}{2k_b}\left(\frac{1}{X} - X\right)\cosh(k_b b - 2k_b x_b)}{-\frac{k_0}{k_b}\sinh(k_b b - 2k_b x_b)}\right], \tag{5}$$

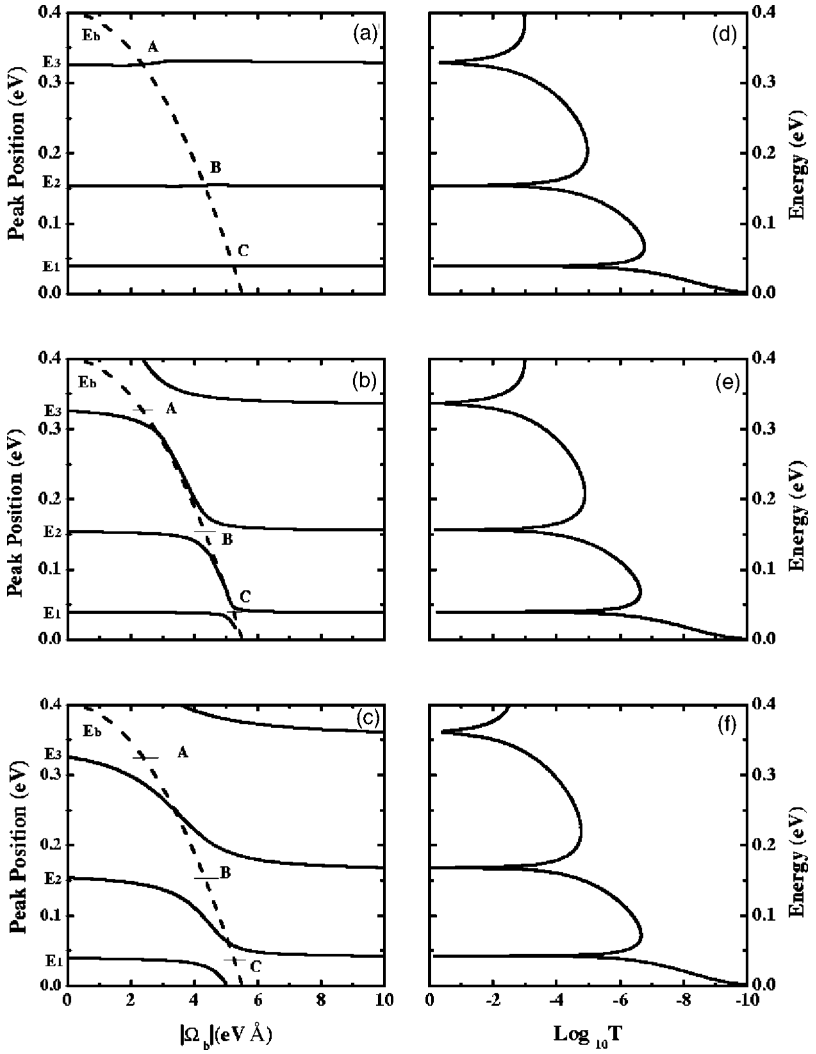

FIG. 1. The dependence of the transmission probability peak position in energy on the strength $|\Omega_b|$ of the δ function. Dashed curves describe the parabolic relation between E_b and Ω_b for the defect state. The cross points A, B, and C are defined by the condition $E_b = E_3, E_2$, and E_1, respectively. (a)–(c) The cases of the weak, intermediate, and strong couplings. The location of the defect layer is $3b/4, b/2$, and $b/4$, respectively. All the parameters are taken the same as those in Ref. 5. (d)–(f) The corresponding logarithmic transmission probability as a function of energy at $\Omega = -10$ eV Å, respectively.

$$T_2 = \left\{ 1 + \left[\frac{1}{2}\left(X + \frac{1}{X} \right) \sinh(k_b b) \right]^2 \right\}^{-1};$$

$$\phi_2 = \arctan\left\{ \frac{1}{2}\left(X - \frac{1}{X} \right) \tanh(k_b b) \right\}, \quad (6)$$

$$\delta_2 = \frac{\pi}{2}, \quad (7)$$

$$k_w = \left(\frac{2m_w^* E}{\hbar^2} \right)^{1/2}, \quad k_b = \left[\frac{2m_b^*(V_0 - E)}{\hbar^2} \right]^{1/2},$$

and

$$X = \frac{m_b^* k_w}{m_w^* k_b}, \quad k_0 = -\frac{m_b^* \Omega_b}{\hbar^2}. \quad (8)$$

When both transmission probabilities are slowly varying functions of energy, the resonance state energies can be determined by

$$\Phi = (2n+1)\pi \quad (n = 0, 1, 2, \ldots). \quad (9)$$

Here m_w^* and m_b^* are the effective masses of the well and barrier regions, respectively. It is seen clearly that Eqs. (1) and (7) reduced to the corresponding result for a symmetrical double-barrier structure without doping by assuming $\Omega_b = 0$. When both barriers are doped symmetrically, one only needs to replace T_2, ϕ_2, and δ_2 in Eq. (1) by T_1, ϕ_1, and δ_1, respectively.

We have recalculated those resonant peaks by using analytical expressions of the transmission probability equation (1) and the resonance condition equation (9). Our results are shown in Figs. 1(a)–1(c). The transmission probability with $\Omega_b = -10$ eV Å at the weak-, intermediate-, and strong-coupling cases are also given in Figs. 1(d)–1(f), respectively. It is clearly seen that there is no split of the highest-energy peak and no new quasibound state for all three cases when $|\Omega_b|$ is very large. This can be easily understood by considering the facts that (1) the defect state energy level becomes very deep below zero when $|\Omega_b|$ is very large and (2) the local-state level for the defects is far from any of the quasi-bound state levels in the quantum well (QW); thus only weak coupling between them occurs, which makes the resonant

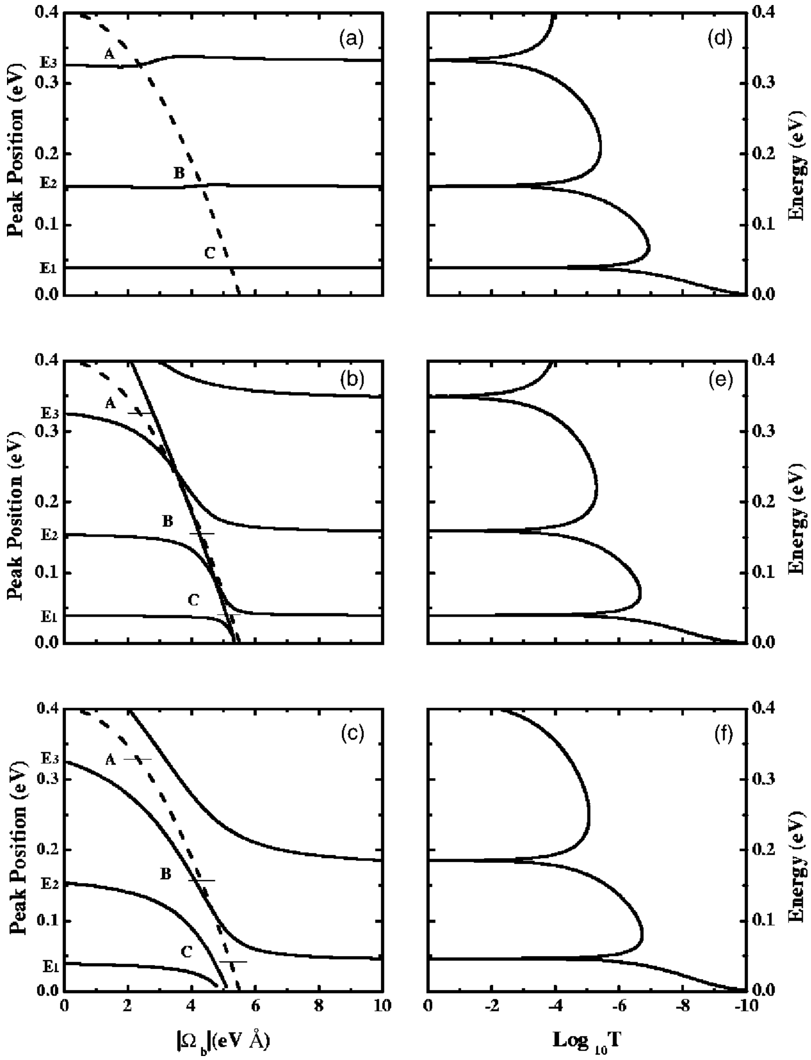

FIG. 2. The same as in Fig. 1 except here both barriers were symmetrically doped.

peaks shift to higher energy levels. The energy shift depends on the energy level and on the position of the defect layer relative to the barrier-well interface. The higher the energy level, the more obviously the energy level shifts to higher energy. The closer the defect layer to the interface, the more the energy shift appears.

It is found that the split of the highest energy peak observed by He and Gu[5] in the intermediate- and strong-coupling regions, when $|\Omega_b|$ was very large, is an artifact of their numerical procedure. Their mistake can be traced back to the problem of their computation of the transmission probability from the direct numerical calculation of the 2×2 transfer matrices, where the good numerical convergence near the turning points is difficult to achieve and leads to a significant error in such a multilayer stack. As can be seen clearly from Ref. 5, the authors of Ref. 5 had adopted the point-to-point transfer matrices in their numerical calculations, which leads to more matrices consisting of exponential elements of opposite exponential factors being multiplied in their calculations, as shown in Eqs (1)–(8) of Ref. 5. The exponential element in the calculations for a multilayer stack always brings about the convergence problem, even though these kinds of matrices are the direct results of the wave function continuity requirement at the boundaries. In fact, this convergence problem can be avoided by changing the point-to-point transfer matrix to the layer-to-layer transfer matrix (or density matrix) after some simple analytical operations. Then the elements of all the matrices will be reduced to trigonometric functions (sine and cosine) or corresponding parabolic functions.

For comparison, we have also shown the corresponding results when both barriers are doped symmetrically in Fig. 2. Again, we cannot see any split of the highest-energy peak or any new quasibound state for all three cases when $|\Omega_b|$ is very large. However, the stronger coupling between the quasibound states in the QW and the defect state energy level shifts the resonant peaks more obviously than those when only one barrier is doped. Other features are also found: an energy state that corresponds to the resonant tunneling energy level in each barrier, resulting from $T_1 = T_2 = 1$, appears for the intermediate-coupling case, as shown in Fig. 2(b). For the strong-coupling case, the interaction lifts the highest excited state up into the quasicontinuous states. On the other hand, the interaction forces not only the ground state but also the second state to fall into the gap near the cross point C, as shown in Figs. 2(c) and 2(f).

In conclusion, we have analytically and numerically recalculated the doping effects on resonant tunneling of a defect-layer sheet inserted in one or two barriers of the double-barrier quantum well. It is revealed that there is no split of the highest-energy peak and no new quasi-bound state for all three cases when $|\Omega_b|$ is very large. It is pointed out that the split of the highest-energy peak, as observed by He and Gu in the intermediate- and strong-coupling regions, is an artifact of their numerical procedure.

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