Resonant tunnelling of a composite particle through a single potential barrier

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N Saito and Y Kayanuma

Department of Physics, Faculty of Science, Tohoku University, Sendai 980, Japan

Abstract. Some aspects of quantum tunnelling of a composite particle are clarified by a simple model. We calculate the probability that a couple of point particles bound to each other by a square well potential with a hard core tunnel through a rectangular potential barrier. It is shown that resonance structures appear in the transmission spectrum in some cases, which reflects the existence of quasi-bound-states of the centre of mass motion around the potential barrier. It is also shown that an inelastic tunnelling occurs in which the transitions in the relative motion are induced by the tunnelling of the centre of mass.

1. Introduction

The resonant tunnelling of a particle through a double-potential-barrier structure in one dimension is a striking manifestation of the wave-like feature of quantum mechanical systems [1]. Recent progress in microfabrication techniques has made it possible to observe such a phenomenon in man-made quasi-one-dimensional systems, it has even been proposed that the effect should be utilized in future device technology [2]. The physical mechanism of the resonant tunnelling is quite simple. When the kinetic energy of the incident particle is resonant with one of the energy levels of the quasi-bound-states in the region sandwiched by the two potential barriers, the interference between the paths for multiple reflections works constructively and highly enhances the transmission, just like the case of a Fabry–Perot optical interferometer.

Although a number of theoretical works have studied tunnelling phenomena in various situations, quantum tunnelling of a *composite* particle, in which the particle itself has an internal structure, has yet to be clarified. For example, one may ask what the probability of transmission of a composite particle is if the potential barrier is defined for each component particles and how the internal motion is correlated with the tunnelling of the centre of mass. It should be noted here that the essential condition for the occurrence of resonant tunnelling is not the existence of double (or multiple) potential barriers but the existence of quasi-bound-states localized around the potential barriers. Therefore, it can be expected that a composite particle will also show a resonant tunnelling through a *single* potential barrier if it is momentarily trapped around the barrier†. In the present paper, we investigate some aspects of the quantum tunnelling of a composite particle by a simplified-model calculation.

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† In this connection, Mashkevich [3] recently pointed out that the problem of the quantum tunnelling of N point particles rigidly connected with each other through a single potential barrier is equivalent to that of a point particle through N barriers and thus the maximum probability of transmission is equal to unity.

2. Model and formulation

Consider a homonuclear diatomic molecule which travels in one dimension and hits a rectangular potential barrier as shown in figure 1. If the barrier height is larger than the kinetic energy of the centre of mass, the molecule will be completely reflected classically but will tunnel through the barrier quantum mechanically with some probability. Let us investigate the probability of transmission. Each atom is regarded as a point particle with mass m. The interatomic potential is assumed to be deep enough so that we approximate it by a *square well potential with infinite barrier height which confines the mutual distance of the atoms in the range* $[\ell - d/2, \ell + d/2]$, in which ℓ is the average interatomic distance. The internal motion mimics the molecular vibration. This is a rather crude approximation of real systems but is enough to see some essential features of the problem. By changing d one can control the rigidity of binding.
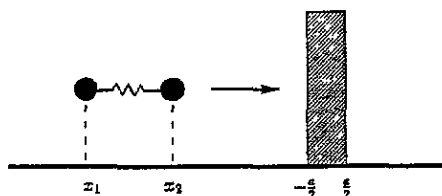

Figure 1. Quantum tunnelling of a diatomic molecule through a rectangular potential barrier.

The Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + V(x_1) + V(x_2) + U(|x_1 - x_2|) \tag{1}$$

where

$$V(x) = \begin{cases} V_0 & -a/2 \leqslant x \leqslant a/2 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

and

$$U(x) = \begin{cases} 0 & \ell - d/2 \leqslant x \leqslant \ell + d/2 \\ \infty & \text{otherwise} \end{cases} \tag{3}$$

in which V_0 is the barrier height and a its width. Without loss of generality, we assume $x_1 \leqslant x_2$ hereafter. Next we introduce the centre of mass coordinate $x \equiv (x_1 + x_2)/2$ and the relative coordinate $y \equiv x_2 - x_1 - \ell + d/2$. Then the Schrödinger equation is written as

$$\left(-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{m}\frac{\partial^2}{\partial y^2} + U(y + \ell - d/2) + W(x, y)\right)\Psi(x, y) = E\Psi(x, y). \tag{4}$$

Here, the potential $W(x, y)$ takes a non-zero value $W(x, y) = V_0$ only in the regions between two pairs of lines, $y = 2x \pm a - \ell + d/2$ and $y = -2x \pm a - \ell + d/2$, except for the area common to these regions where $W(x, y)$ is given by $W(x, y) = 2V_0$. In the case $\ell - d/2 > a$, the problem is thus equivalent to successive tunnelling through the *two* potential barriers by a single particle confined in the two-dimensional strip with width d as shown in figure 2(a). For $\ell - d/2 < a$, the two barriers coalesce (figure 2(b)). Note that the boundaries of the potential barriers are slanted spatially. This means that a coupling occurs between the internal motion and the translational motion as the molecule tunnels through the barriers.
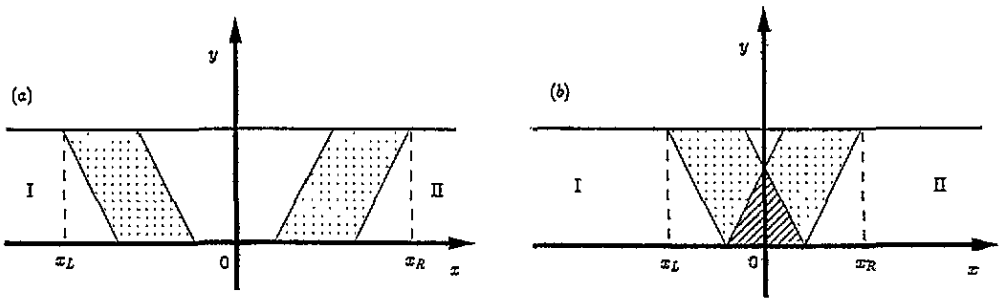
Figure 2. Schematic diagram of the potential-barrier structure in the xy plane in the case of (a) $\ell - d/2 > a$ and (b) $\ell - d/2 < a$. $W(x, y) = V_0$ in the dotted area, $W(x, y) = 2V_0$ in the dashed area and $W(x, y) = 0$ otherwise.

The wave function $\Psi(x, y)$ is expanded in a series of complete sets of eigenfunctions of the internal mode as

$$\Psi(x, y) = \sum_{n=1}^{\infty} \psi_n(x)\varphi_n(y) \tag{5}$$

where

$$\varphi_n(y) = \sqrt{\frac{2}{d}} \sin\left(\frac{n\pi}{d} y\right) \tag{6}$$

which satisfies

$$-\frac{\hbar^2}{m}\frac{d^2}{dy^2}\varphi_n(y) = \varepsilon_n\varphi_n(y) \tag{7}$$

with $\varepsilon_n = (\hbar^2/m)(n\pi/d)^2$ and the boundary condition $\varphi_n(0) = \varphi_n(d) = 0$. We will call the nth eigenstate of the internal mode channel n. For an incident wave with total energy E satisfying the condition $\varepsilon_n < E < \varepsilon_{n+1}$, propagating states can exist in the region out of the potential barrier for channels up to n. The excitation and deexcitation of the internal mode will occur induced by the tunnelling of the centre of mass coordinate. This is somewhat analogous to the multi-channel scattering in atomic and molecular collisions [4]. The transmission probability $T_{n,n'}(E)$ for the incident wave coming from the left-hand side of figure 2 in channel n and going out to the right-hand side in channel n' is calculated by the transfer matrix method as follows.

As shown in figure 2, the strip is divided into three regions; the potential-free region $x < x_L$ (denoted as I) and $x > x_R$ (denoted as II) and the active region $x_L \leqslant x \leqslant x_R$, where $x_L = -(2a + 2\ell + d)/4$, $x_R = (2a + 2\ell + d)/4$. In the regions I and II, the wave function $\Psi(x, y)$ of equation (4) can be written as

$$\Psi_\lambda(x, y) = \sum_{n=1}^{\infty}[a_\lambda(n, +1)e^{ik_n x} + a_\lambda(n, -1)e^{-ik_n x}]\varphi_n(y) \qquad \lambda = \text{I, II} \tag{8}$$

where $k_n = 2\sqrt{m(E - \varepsilon_n)}/\hbar$. Since ε_n takes all the eigenvalues of the internal mode, not only the real values but also the imaginary values of k_n are included. The convention $\sqrt{-1} = +i$ is adopted here and hereafter. Therefore, $a_\lambda(n, +1)$ represents the amplitude of a propagating state towards the right-hand side of figure 2 or an evanescent state which

decays in this direction. The coefficients $a_\lambda(n, \sigma)$ are connected by the transfer matrix $\mathbf{M}_{\mathrm{I, II}}$ as

$$a_{\mathrm{I}}(n, \sigma) = \sum_{n'=1}^{\infty} \sum_{\sigma'=\pm 1} \mathbf{M}_{\mathrm{I, II}}(n, \sigma; n', \sigma') a_{\mathrm{II}}(n', \sigma'), \tag{9}$$

where $\sigma = \pm 1$.

Now we replace the original system by a fictitious one in which the potential barrier in the region $x > 0$ is entirely removed. The wave function $\Psi_{\mathrm{R}}(x, y)$ in the region $x > 0$ is then written as

$$\Psi_{\mathrm{R}}(x, y) = \sum_{n=1}^{\infty} [a_{\mathrm{R}}(n, +1) e^{ik_n x} + a_{\mathrm{R}}(n, -1) e^{-ik_n x}] \varphi_n(y). \tag{10}$$

The transfer matrix $\mathbf{M}_{\mathrm{I, R}}(n, \sigma; n', \sigma')$ from I to the region $x > 0$ is calculated in the following way. We define the Hamiltonian matrix $\mathbf{H}_{n,n'}(x)$ by

$$\mathbf{H}_{n,n'}(x) = \int_0^d \varphi_n^*(y) H(x, y) \varphi_{n'}(y) \, \mathrm{d}y. \tag{11}$$

Then, the Schrödinger equation (4) is cast into a set of simultaneous differential equations for $\psi_n(x)$

$$\sum_{n'=1}^{\infty} [H_{n,n'}(x) - E\delta_{n,n'}] \psi_{n'}(x) = 0 \tag{12}$$

where

$$H_{n,n'}(x) = \left(\varepsilon_n - \frac{\hbar^2}{4m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) \delta_{n,n'} + W_{n,n'}(x) \tag{13}$$

with

$$W_{n,n'}(x) = \int_0^d \varphi_n^*(y) W(x, y) \varphi_{n'}(y) \, \mathrm{d}y. \tag{14}$$

The infinite set of simultaneous equations (12) is truncated into a finite one by taking into account a sufficient number of channels N from the lowest. The N simultaneous second-order differential equations are transformed into $2N$ equations of first order and solved numerically from $x = 0$ to x_{L} under the boundary condition

$$\begin{aligned} \psi_m(0) &= \delta_{m,n} \\ \psi_m'(0) &= i\sigma k_n \delta_{m,n} \qquad m = 1, 2, \ldots, N \end{aligned} \tag{15}$$

where $\sigma = \pm 1$ and the prime indicates the derivative. Then the (n, σ) row of the transfer matrix $\mathbf{M}_{\mathrm{I, R}}(n, \sigma; n', \sigma')$ is obtained by smoothly connecting the solution to that in the region $x \leqslant x_{\mathrm{L}}$ as the solution of simultaneous equations

$$\psi_{n'}(x_{\mathrm{L}}) = \sum_{\sigma'=\pm 1} \mathbf{M}_{\mathrm{I, R}}(n, \sigma; n', \sigma') \exp(i\sigma' k_{n'} x_{\mathrm{L}})$$

$$\psi_{n'}'(x_{\mathrm{L}}) = \sum_{\sigma'=\pm 1} i\sigma' k_{n'} \mathbf{M}_{\mathrm{I, R}}(n, \sigma; n', \sigma') \exp(i\sigma' k_{n'} x_{\mathrm{L}}). \tag{16}$$

The domain of the numerical integration actually needed can be reduced to the region where $V_{n,n'}(x)$ has an off-diagonal component. For $\ell - d/2 > a$ (figure 2(a)), it can be further reduced by using the symmetry property of the barrier structure under spatial inversion.

Next, we consider a second fictitious system in which the potential barrier in the region $x < 0$ is entirely removed. The transfer matrix $M_{L,II}(n, \sigma; n', \sigma')$ from the region $x < 0$ to II is defined in the same way as $M_{I,R}(n, \sigma; n', \sigma')$. From the symmetry argument, one can readily derive the formula $M_{L,II} = \tilde{M}_{I,R}^{-1}$, where $\tilde{M}_{I,R}$ is a matrix defined by $\tilde{M}_{I,R}(n, \sigma; n', \sigma') = M_{I,R}(n, -\sigma; n', -\sigma')$. Then, the transfer matrix $M_{I,II}$ for the original system is given by the matrix multiplication $M_{I,II} = M_{I,R}M_{L,II}$.

The transmission probability $T_{n,n'}(E)$ for $E - \varepsilon_n > 0$ and $E - \varepsilon_{n'} > 0$ is calculated by imposing a suitable asymptotic condition at infinity on the wave function. Namely, in the equation

$$a_I(n, \sigma) = \sum_{n'} \sum_{\sigma'} M_{I,II}(n, \sigma; n', \sigma')a_{II}(n', \sigma') \tag{17}$$

we put $a_I(m, +1) = \delta_{m,n}$ $(m = 1, 2, \ldots, N)$ and $a_{II}(m', -1) = 0$ $(m' = 1, 2, \ldots, N)$ and N simultaneous equations for $a_{II}(n', +1)$ are solved. Then, $T_{n,n'}(E)$ is given by

$$T_{n,n'}(E) = |a_{II}(n', +1)|^2 k_{n'}/k_n. \tag{18}$$

The coefficient $a_I(n', -1)$ can be calculated by putting the obtained $a_{II}(n', +1)$ into the right-hand side of equation (17), by which the reflection probability is given as $|a_I(n', -1)|^2 k_{n'}/k_n$. From the symmetry under the time reversal and the spatial inversion $x \to -x$, the relation $T_{n,n'}(E) = T_{n',n}(E)$ is easily derived. The total transmission probability $T_n(E)$ is given by $T_n(E) = \sum_{n'} T_{n,n'}(E)$.

3. Numerical results and discussion

In figure 3, the transmission probabilities are shown for fixed values of parameters, $a/\lambda_0 = 1$ and $\ell/\lambda_0 = 5$ where $\lambda_0 \equiv \hbar/\sqrt{mV_0}$, against the incident centre of mass kinetic energy $E - \varepsilon_1$ normalized by V_0 with parameter d varying as $d/\lambda_0 = 5, 7, 8$ and 9.5. The solid curve represents $T_{1,1}(E)$, the dashed curve $T_{1,2}(E)$ and the dotted curve $T_{1,3}(E)$. Channels up to $N = 7$ have been taken into account in this calculation. It has been ascertained that numerical results converge well for these parameter values.

Figure 3(a) shows a typical feature of resonant tunnelling. Because the threshold for the excitation of the second channel, $E = \varepsilon_2$, lies above $E = V_0 + \varepsilon_1$, the line shape is almost the same as that of the one-dimensional resonant tunnelling corresponding to the case $d = 0$. The three peaks originate from the resonance with the three quasi-bound-states formed in the trapezoid well between the barriers. Physically, these bound states correspond to the situation where one of the two atoms has transmitted the potential barrier while the other is left behind and thus the molecule is trapped momentarily. Note that the maximum values of $T_{1,1}(E)$ reach unity at resonances.

As d is increased, the threshold energy for the excitation of the internal mode decreases and additional quasi-bound-states appear in the potential well associated with the excited channels. The threshold energies of the second channel are indicated by the small solid arrows on the abscissa and that of third channel by the dotted arrow. Above threshold, the transmission spectrum $T_{1,1}(E)$ becomes a little more complicated with extra peaks and dips. Furthermore, the transmission probabilities $T_{1,2}(E)$ and $T_{1,3}(E)$ appear as shown by the dashed cuves in figures 3(b)–(d) and the dotted curve in figure 3(d) respectively. These inelastic transmissions mean that a diatomic molecule travelling in its ground state hits a potential barrier, tunnels through it and goes away with a velocity slowed down in the excited state of the internal mode.
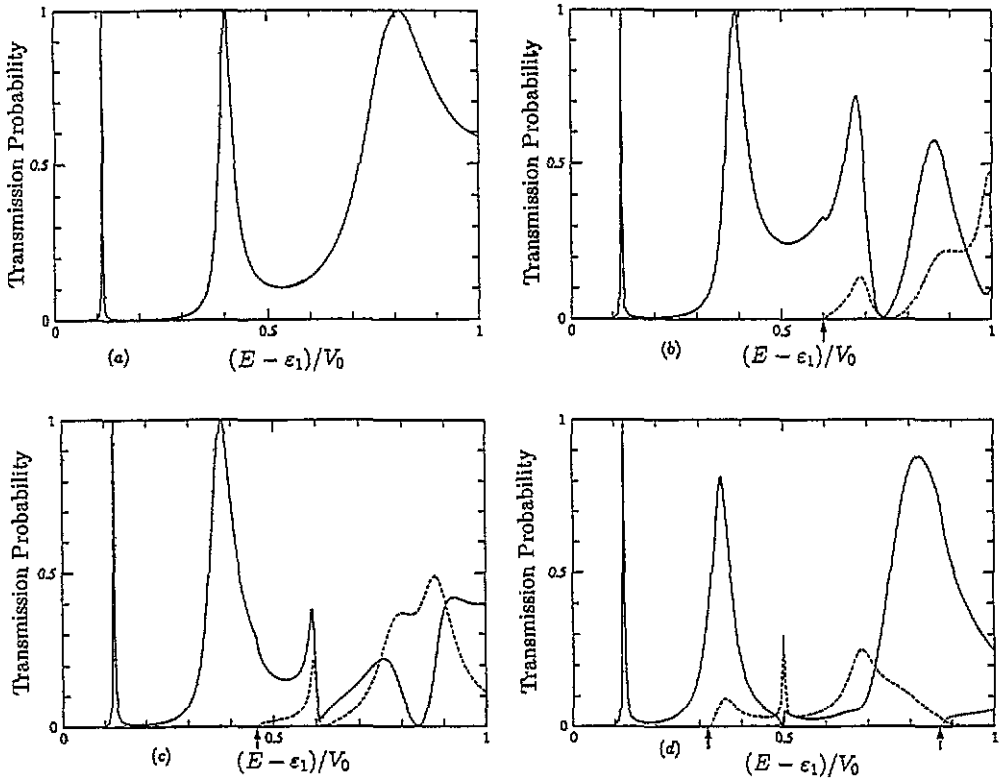
Figure 3. The transmission probabilities plotted against $(E - \varepsilon_1)/V_0$ for parameter values $a/\lambda_0 = 1$, $\ell/\lambda_0 = 5$, and (a) $d/\lambda_0 = 5$, (b) $d/\lambda_0 = 7$, (c) $d/\lambda_0 = 8$, (d) $d/\lambda_0 = 9.5$. The solid curve represents $T_{1,1}$, the dashed line $T_{1,2}$ and the dotted curve $T_{1,3}$. The small solid arrows on the abscissa indicate the threshold energy for the excitation of the second channel. The dotted arrow in (d) indicates that for the third channel.

Although the motional states in the x and y directions are not separable in the trapezoid well, one may roughly assign quantum numbers (m, j) for each quasi-bound-state, which means the jth bound state in the mth channel. This is valid as long as d is relatively small and the trapezoid can be approximated by a rectangle. As d becomes larger for fixed values of a and ℓ, the characterization of the quasi-bound-states in this way would be endangered. However, one may still use the same quantum numbers to denote the resonance peaks in so far as the peaks are isolated from each other. Furthermore, one can assign a *transition path* to each resonance denoted as $(n, k) \rightarrow (m, j) \rightarrow (n', k')$, which means an in-coming state with wave vector k in the nth channel is resonant with the quasi-bound-state (m, j) and is transmitted as an out-going state with wave vector k' in the n'th channel. For example, in figure 3(c), the third peak of the spectrum $T_{1,1}(E)$ (the peak at $(E - \varepsilon_1)/V_0 \simeq 0.59$) corresponds to the path $(1, k) \rightarrow (2, 1) \rightarrow (1, k)$. The interference with the path $(1, k) \rightarrow (1, 3) \rightarrow (1, k)$ gives rise to the strong asymmetry of this peak. At the same energy, the sharp resonance peak appears in the spectrum $T_{1,2}(E)$ which comes from the path $(1, k) \rightarrow (2, 1) \rightarrow (2, k')$. The dip in the spectrum $T_{1,1}(E)$ around $(E - \varepsilon_1)/V_0 \simeq 0.83$ is also due to the destructive interference between the paths $(1, k) \rightarrow (2, 2) \rightarrow (1, k)$ and $(1, k) \rightarrow (1, 3) \rightarrow (1, k)$. Resonance structures of other spectra in figure 3 can be assigned in the same way. Note that the intensity of the extra structure strongly depends on d. We find a general feature that the maximum value of the

total transmission probability $T_1(E) = \sum_n T_{1,n}(E)$ for a resonance peak reaches unity as long as it lies in the energy region where the excitation of the internal mode is not allowed.

In figure 4, $T_{2,2}(E)$ is plotted for the same parameter values as figure 3(*d*), $a/\lambda_0 = 1$, $\ell/\lambda_0 = 5$ and $d/\lambda_0 = 9.5$, against $(E - \varepsilon_1)/V_0$. The lowest two peaks are assigned as due to the resonance with the quasi-bound-states $(2, 1)$ and $(2, 2)$. It is found that the transmission probability is relatively low when the incident wave comes in the excited state of the internal mode.
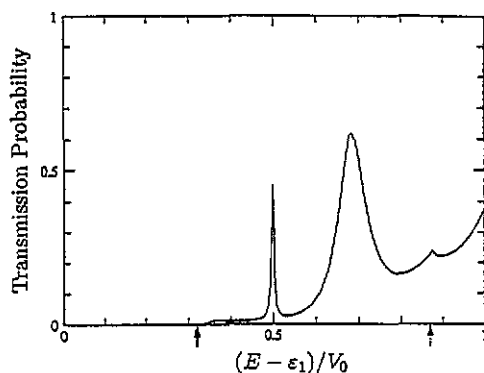

Figure 4. The transmission probability $T_{2,2}$ plotted against $(E - \varepsilon_1)/V_0$ for parameter values $a/\lambda_0 = 1$, $\ell/\lambda_0 = 5$, and $d/\lambda_0 = 9.5$.

We have also investigated the change of the transmission spectrum due to the change of the averaged size of the molecule ℓ for fixed values of a and d. The resonance peaks shift to the higher energy side as ℓ is decreased and, for relatively small values of d, even the lowest peak disappears from the sub-barrier region at a critical value of ℓ. In the case that the molecule is much smaller than the width of the potential barrier, $\ell + d/2 \ll a$, it behaves essentially as a single particle with mass $2m$ which tunnels through the potential barrier with the barrier height $2V_0$.

To summarize, we have clarified some features of quantum tunnelling of a composite particle through a potential barrier. The tunnelling behaviour strongly depends on the ratio of the averaged size of the composite particle to the width of the potential barrier and on the rigidity of binding. It has been demonstrated that resonance structures in the transmission spectrum are expected in some cases even for tunnelling through a single potential barrier. The condition for this is that the parameter values are such that there exists a configuration in which the composite particle is momentarily trapped by the barrier. It has also been shown that an inelastic tunnelling occurs in some cases in which the conversion of the energy is induced between the centre of mass translational mode and the internal mode.

Although actual calculations have been done for a one-dimensional model, one may well expect that essentially the same conclusion will be drawn in higher dimensions as well, since the physical origin of tunnelling resonance is the momentary trapping of the composite particle at the potential barrier, which is independent of dimensionality. A slight complication in higher dimensions is that the internal degrees of freedom consist not only of the vibrational mode but also of the rotational mode. These two modes will couple with each other and also with the translational mode as the particle tunnels through or is reflected by the barrier.

As for the experimental possibility of observing such a phenomenon, we would like to point out that the ballistic exciton which tunnels a hetero-structure such as GaAs–AlGaAs–GaAs may show resonant tunnelling due to a mechanism analogous to that treated here. Part of the AlGaAs provides potential barriers for the electron and the hole. The momentarily trapped configuration in this case is such that either the electron or the hole is transmitted

through the barrier while the other is left on the opposite side and the two particles combine with each other by the attractive Coulomb force. We have recently performed a numerical study of quantum tunnelling of a Wannier exciton in a one-dimensional model [5]. It was found that a series of sharp resonance structures actually appears in the transmission spectrum as a function of incident kinetic energy of the exciton. Experimental verification of such a structure would be possible by optical measurement, namely, by observing the reflectance or the transmittance of light around the excitonic resonance energy in a sample containing a hetero-barrier structure. Details will be presented elsewhere.

References

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