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# ANALYSIS OF KINETIC PROPERTIES AND TUNNEL-COUPLED STATES IN ASYMMETRICAL MULTILAYER SEMICONDUCTOR STRUCTURES

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This study investigates the kinetic properties of both symmetrical and asymmetrical multilayer and nano-sized semiconductor structures. We develop a theoretical framework using various models and mathematical methods to solve the Schrödinger matrix equation for a system of electrons, taking into account the Bastard condition, which considers the difference in the effective masses of current carriers in adjacent layers. We analyze tunnel-coupled electronic states in quantum wells separated by a narrow tunnel-transparent potential barrier. Our findings provide insights into the electronic properties of semiconductor structures, which are crucial for applications in micro- or nanoelectronics and other areas of solid-state physics.
**Keywords:** *Multilayer and nano-sized semiconductor structures; Schrödinger matrix equation; Hamiltonian; Electrons; Quantum wells; Effective mass; Tunneling effect; Electronic transport; Bastard condition*
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## INTRODUCTION

The exploration of electronic properties in semiconductor structures, whether symmetrical or asymmetrical, holds significant relevance for their application in micro- and nanoelectronics, as well as broader fields of solid-state physics. While prior research has delved into the kinetic properties of these multilayer and nanoscale structures, employing a variety of models and mathematical methodologies to tackle the full Schrödinger equation for electron systems, a gap remains. Notably, these investigations have overlooked the Bastard condition, which accounts for the variance in effective masses of charge carriers across adjacent layers. Furthermore, there has been a lack of focus on the study of tunnel-coupled electronic states within quantum wells, especially those delineated by narrow, tunnel-permeable potential barriers. Our research is designed to bridge these gaps, offering new insights into the physics of semiconductor structures by incorporating these critical factors.

## METHODS

In structures featuring two or more closely spaced potential wells, the wave functions from adjacent wells significantly overlap within the barrier region. This overlap leads to a substantial probability of detecting an electron within this barrier region, thereby enabling charge carriers to transition from one well to another, even without their energies surpassing the barrier height. This quantum mechanical phenomenon, known as the tunneling effect [9-10], is particularly notable in quantum wells where the tunneling probability is considerable, rendering these wells tunnel-coupled.

The phenomenon of tunnel coupling, which becomes more pronounced as the wells draw nearer to each other, significantly affects both the positioning of energy levels and the characteristics of the wave functions within the wells. To accurately determine the levels of size quantization and their corresponding wave functions, it's essential to solve the Schrödinger equation under a specific potential while adhering to Bastard boundary conditions. These conditions necessitate the continuity of the wave function $\psi(x)$ and its derivative with respect to mass $\frac{1}{m}\frac{d\psi}{dx}$ at the interface between the potential well (denoted as Layer A) and the barrier (Layer B). In mathematical terms, this continuity is expressed as:

$$\psi|A = \psi|B, \left.\frac{1}{m}\frac{d\psi(x)}{dx}\right|_A = \left.\frac{1}{m}\frac{d\psi(x)}{dx}\right|_B \quad (1)$$

Following the establishment of the Bastard boundary conditions, as denoted by equation (1), it's imperative to incorporate these conditions into our calculations at each interface between different materials within the nanostructure. This approach is critical for accurately modeling the behavior of charge carriers, especially when considering the real wave vector scenarios that result in the wave functions decaying to zero at the limits of $x \to \pm\infty$. Given a nanostructure composed of two quantum wells, we encounter two distinct interfaces that necessitate the resolution of a system comprising equations for eight variables, reflecting the complexity of electron behavior in these confined spaces.

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To facilitate our analysis, we define $U_1(x)$ and $U_2(x)$ as the potentials for the left and right wells, respectively. These are treated as independent entities within their own spatial domains. For simplicity, and without loss of generality, we position our energy reference at the barrier level, allowing us to consider $U_1(x)$ and $U_2(x)$ as being effective only within their respective wells. Consequently, the potential $(U(z))$ describing the dual-well structure emerges as the summation of $U_1(x)$ and $U_2(x)$.

$$H\psi = E\psi, \tag{2}$$

where $H = H_1 + H_2 + U_1 + U_2$, with $H_1(U_1)$ and $H_2(U_2)$ being the Hamiltonian (potential) operators for the left and right potential wells, respectively. Thus, the general Schrödinger equation takes the form:

$$\left(-\frac{\hbar^2}{2m_1}\vec{\nabla}^2 - \frac{\hbar^2}{2m_2}\vec{\nabla}^2 + U_1 + U_2\right)\psi = E\psi$$

Transitioning to a one-dimensional analysis simplifies our approach to:

$$\left(-\frac{\hbar^2}{2\mu_{12}^+}\frac{\partial^2}{\partial z^2} + U_1 + U_2\right)\psi(x) = \left(E - \frac{\hbar^2 k_\perp^2}{2\mu_{12}^+}\right)\psi(x) \tag{3}$$

Here, $\mu_{12}^+$ represents the effective mass term, accounting for the combined mass effects from both wells, and $k_\perp^2 = k_x^2 + k_y^2$ reflects the transverse component of the wave vector. This nuanced formulation provides a direct pathway to solving the individual Schrödinger equations for each well:

$$\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial z^2} + U_1\right)\psi_1 = \left(E_1 - \frac{\hbar^2 k_\perp^2}{2m_1}\right)\psi_1, \quad \left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial z^2} + U_2\right)\psi_2 = \left(E_2 - \frac{\hbar^2 k_\perp^2}{2m_2}\right)\psi_2. \tag{4}$$

Leveraging the principle of superposition, we express the system's wave function as a linear combination of the well-specific wave functions:

$$\psi(x) = C_1\psi_1(x) + C_2\psi_2(x) \tag{5}$$

Substituting equation (5) into equation (3) and reconciling this with equation (4), we arrive at a composite equation that encapsulates the interaction between the two wells through the coefficients $C_1$ and $C_2$, manifesting in:

$$C_1\left(\frac{m_1}{\mu_{12}^+}\left[-\frac{\hbar^2}{2m_1}\frac{\partial^2\psi_1(x)}{\partial z^2} + U_1\psi_1(x)\right] + \left(1 - \frac{m_1}{\mu_{12}^+}\right)U_1\psi_1(x) + U_2\psi_1(x)\right) +$$

$$+C_2\left(\frac{m_2}{\mu_{12}^+}\left[-\frac{\hbar^2}{2m_2}\frac{\partial^2\psi_2(x)}{\partial z^2} + U_2\psi_2(x)\right] + U_1\psi_2(x) + \left(1 - \frac{m_2}{\mu_{12}^+}\right)U_2\psi_2(x)\right) =$$

$$= C_1\left(E - \frac{\hbar^2 k_\perp^2}{2\mu_{12}^+}\right)\psi_1(x) + C_2\left(E - \frac{\hbar^2 k_\perp^2}{2\mu_{12}^+}\right)\psi_2(x) \tag{6}$$

To delve deeper into the system's quantum mechanics, we apply integration by multiplying equation (6) from the left with $\psi_2^*(x)$, and similarly with $\psi_1^*(x)$, to integrate over the spatial domain. This operation is crucial for isolating the coefficients $C_1$ and $C_2$, facilitating the extraction of meaningful physical parameters:

$$\int \psi_2^*(x)\,[Equation\ (6)]dx\ and\ similarly\ for\ \psi_1^*(x)]$$

Through this process, we obtain a system of homogeneous equations that encapsulate the interaction dynamics between the quantum wells, structured as follows:

$$\begin{cases} C_1\left[\tilde{E}_1\sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right)U_1^{(21)} + U_2^{(21)} - \tilde{E}\sigma\right] + C_2\left[\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right)U_2^{(22)} - \tilde{E}\right] = 0, \\ C_1\left[\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right)U_1^{(11)} + U_2^{(11)} - \tilde{E}\right] + C_2\left[\tilde{E}_2\sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right)U_2^{(12)} - \tilde{E}\sigma\right] = 0. \end{cases} \tag{7}$$

The overlaps $U_1^{(ij)}$ and $U_2^{(ij)}$ are integrals representing the interaction terms between the wells, and $\sigma$ symbolizes the overlap integral between $\psi_2^*$ and $\psi_1$. This configuration allows us to calculate the adjusted energies $\tilde{E}_1$ and $\tilde{E}_2$, reflecting the modified energy levels due to the coupling between the wells.

$$U_1^{(21)} = \int \psi_2^*(x) U_1 \psi_1(x) \cdot dx, U_2^{(21)} = \int \psi_2^*(x) U_2 \psi_1(x) \cdot dx, \quad U_1^{(22)} = \int \psi_2^*(x) U_1 \psi_2(x) \cdot dx,$$
$$U_2^{(22)} = \int \psi_2^*(x) U_2 \psi_2(x) \cdot dx, \; U_1^{(11)} = \int \psi_1^*(x) U_1 \psi_1(x) dx, U_2^{(11)} = \int \psi_1^*(x) U_2 \psi_1(x)\, dx,$$
$$U_1^{(12)} = \int \psi_1^*(x) U_1 \psi_2(x)\, dx, \; U_2^{(12)} = \int \psi_1^*(x) U_2 \psi_2(x)\, dx, \sigma = \int \psi_2^*(x) \psi_1(x) \cdot dx, \; \tilde{E}_a = E_a - \frac{\hbar^2 k_1^2}{2\mu_{12}^+},$$
$$\tilde{E} = E - \frac{\hbar^2 k_1^2}{2m_a}, \tilde{E}_1 = \frac{m_1}{\mu_{12}^+}\left(E_1 - \frac{\hbar^2 k_1^2}{2m_1}\right), \tilde{E}_2 = \frac{m_2}{\mu_{12}^+}\left(E_2 - \frac{\hbar^2 k_1^2}{2m_2}\right).$$

For a non-trivial solution of equation (7), the determinant of the system must be set to zero, leading us to:

$$\begin{bmatrix} \tilde{E}_1\sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)} - \tilde{E}\sigma & \tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)} - \tilde{E} \\ \tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)} - \tilde{E} & \tilde{E}_2\sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)} - \tilde{E}\sigma \end{bmatrix} = 0. \tag{8}$$

From this, we derive a second-degree algebraic equation for the variable $\tilde{E}$, which can be represented in the general form:

$$a\tilde{E}^2 - b \cdot \tilde{E} + c = 0\,, \tag{9}$$

which has two roots, $\tilde{E}_\pm$, representing the sought-after energy levels of the electron in the double-well potential $U(x)$

$$\tilde{E}_+ = \frac{b}{2a}\left(-1 + \sqrt{1 - 4\frac{ac}{b^2}}\right), \tilde{E}_- = \frac{b}{2a}\left(-1 - \sqrt{1 - 4\frac{ac}{b^2}}\right) \tag{10}$$

where

$a = (1 + \sigma^2), b = (1 + \Xi_6 + \Xi_2 + \Xi_3), c = \Xi_4 - \Xi_1,$

$\Xi_1 = \left(\tilde{E}_1\sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)}\right)\left(\tilde{E}_2\sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)}\right),$

$\Xi_2 = \left(\tilde{E}_2\sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)}\right)\sigma, \Xi_3 = \left(\tilde{E}_1\sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)}\right)\sigma,$

$\Xi_4 = \left(\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)}\right) \cdot \left(\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)}\right),$

$\Xi_5 = \left(\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)}\right), \Xi_6 = \left(\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)}\right)$

By substituting these roots, $\tilde{E}_+$ and $\tilde{E}_-$, back into equation (7) in turn, one can find two solutions of the system, $\left(\frac{C_1}{C_2}\right)_+$ for $\tilde{E}_+$ and another $\left(\frac{C_1}{C_2}\right)_-$ for $\tilde{E}_-$, which according to equation (7) determine the wave functions $\tilde{\psi}_1(z), \tilde{\psi}_2(z)$, corresponding to the energy levels $\tilde{E}_+$ and $\tilde{E}_-$, respectively.

## CONCLUSIONS

Thus, in tunnel-coupled wells, the energy levels are shifted relative to the levels of isolated wells, and the wave functions emerge from the wave functions of isolated wells as a result of their interaction. The system of equations (7) can be simplified, preserving the main features of its solutions, if we neglect the contributions with terms $U_{1,2}^{(nn)}$, where $n = 1,2$ exceeds the considered range. Consequently, equation (7) takes the form:

$$\begin{cases} \Re_1 C_1 + C_2\left(\tilde{E}_2 - \tilde{E}'\right) = 0, \\ C_1\left(\tilde{E}_1 - \tilde{E}'\right) + \Re_2 C_2 = 0, \end{cases} \tag{11}$$

where $\Re_1 = \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)}$, $\Re_2 = U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)}$. Then, by setting the determinant of the system of equations (11) to zero, we obtain a less cumbersome equation instead of (8):

$$\tilde{E}'^2 - \left(\tilde{E}_1 + \tilde{E}_2\right)\tilde{E}' + \tilde{E}_1\tilde{E}_2 + \Re_1\Re_2 = 0, \tag{12}$$

whose roots are equal

$$\tilde{E}'_\pm = \frac{1}{2}\left[\tilde{E}_1 + \tilde{E}_2 \pm \sqrt{\left(\tilde{E}_1 - \tilde{E}_2\right)^2 + 4\Re_1\Re_2}\right]. \tag{13}$$

Analyzing the expression for the energy level gap $\Delta E = \left|\tilde{E}'_{+} - \tilde{E}'_{-}\right|$ from equation (13), the quantity $\Delta E_{asym} = \left|\tilde{E}_1 - \tilde{E}_2\right|$ serves as a measure of the asymmetry between the two quantum wells and equals zero for symmetric wells. If its square dominates under the square root in equation (4), then $\Delta E \approx \Delta E_{asym}$. In this scenario, the solutions of the system (11) correspond to wave functions $\tilde{\psi}_1(z), \tilde{\psi}_2(z)$ that are close to the original functions $\psi_1$,$\psi_2$, indicating that mixing of the wave functions is almost nonexistent. Conversely, when the asymmetry of the wells is negligibly small, the gap between levels (13) in tunnel-coupled wells is given by $\Delta E \approx \sqrt{4\Re_1\Re_2}$, where this quantity characterizes the tunnel splitting of energy levels. In this case, the solutions of the system (11) correspond to a strong mixing of the original wave functions, where the coefficients $C_1$ and $C_2$ are comparable in magnitude.

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**АНАЛІЗ КІНЕТИЧНИХ ВЛАСТИВОСТЕЙ ТА ТУНЕЛЬНО-ЗВ'ЯЗАНИХ СТАНІВ В АСИМЕТРИЧНИХ БАГАТОШАРОВИХ НАПІВПРОВІДНИКОВИХ СТРУКТУРАХ**

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Це дослідження досліджує кінетичні властивості як симетричних, так і асиметричних багатошарових і нанорозмірних напівпровідникових структур. Ми розробляємо теоретичну базу з використанням різних моделей і математичних методів для вирішення рівняння матриці Шредінгера для системи електронів, враховуючи умову Бастарда, яка враховує різницю в ефективних масах носіїв струму в суміжних шарах. Ми аналізуємо тунельно-зв'язані електронні стани в квантових ямах, розділених вузьким тунельно-прозорим потенційним бар'єром. Наші висновки дають змогу зрозуміти електронні властивості напівпровідникових структур, які мають вирішальне значення для застосування в мікро- чи наноелектроніці та інших областях фізики твердого тіла.

**Ключові слова:** *багатошарові та нанорозмірні напівпровідникові структури; матричне рівняння Шредінгера; Гамільтоніан; електрони; умова Бастарда*