

外场中多势垒结构的共振传输

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[摘要] 利用艾里(Airy)函数和转移矩阵方法精确求解了存在电场的一维多势垒结构的电子一维定态薛定谔方程,求出了在一维多势垒结构中电子共振透射系数的表达式,并进一步研究了多势垒结构的共振透射系数与有效质量和势垒宽度及外加偏压的关系.

[关键词] Airy 函数,共振透射系数,外加偏压的多势垒结构

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The Resonance Transmission of Multi-Barrier Structure in a Constant Electric Field

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Abstract: The resonance transmission coefficient of multi-barrier structure in a constant electric field is presented based on an exact solution of the Schrödinger equation by using Airy function and the transfer matrix approach; Furthermore ,we have also studied the relationship between the resonance transmission coefficient and the effective mass ,the barrier width ,the bias voltage.

Key words: Airy function ,the resonance transmission coefficient ,bias voltage of multi-barrier structure

超晶格^[1]是一种由两种材料交替生长而成具有周期性的半导体结构,窄带隙的材料构成势阱,宽带隙的材料构成势垒^[2].一维多势垒结构由周期性的势垒势阱相互排列组成,在半导体超晶格研究中起着非常重要的作用,电子和空穴在多势垒结构中的性质和理论以及表现出一些新的物理现象,在某些情况下会有重要的技术应用,同时由于分子束外延(MBE)、金属有机化合物化学气相沉积(MOCVD)^[3]等制备超晶格技术的不断完善,极大推动了现代半导体器件的发展,多势垒结构是组成这些半导体器件的基础.

超晶格电子态的研究取得了很大进展,利用一维紧束缚模型计算 InAs/GaSb 的能带结构^[4],将有效质量近似理论^[5]推广到超晶格,建立包络函数模型^[6]求解电子和空穴的微带结构,但是包络函数对短周期超晶格不适用,由于有效质量理论要求微扰势在空间变化缓慢.夏建白等人^[7]在经验赝势的基础上提出了用赝势方法计算长周期超晶格能带的方法,从而摆脱了超晶格周期长短的限制. Altarelli 等人采用变分法计算 InAs/GaSb 和 GaAs/Ga_{0.79}Al_{0.21}As 的价带结构^[8,9]及研究了强弱电场中的量子阱结构^[10].多势垒结构的电子输运主要是电子受到外加电场的作用被束缚在结构中的隧穿问题,近年来,还利用光学方法研究了超晶格的微带输运^[11],验证和确定了超晶格中存在电子、空穴通过微带的垂直输运及在微带输运中的扩散系数和迁移率.研究了单势垒双层和双势垒单层石墨烯结构的共振传输问题^[12,13],电子的相干输运和非相干输运之间的转变问题^[14].

本文通过电子在一定能量和波矢下入射外加外场的多势垒结构,利用 Airy 函数和转移矩阵方法求解一维定态薛定谔方程,然后进一步推导出透射系数.研究了透射系数与入射电子能量特性曲线及有效质量、势垒宽度及外加偏压对透射系数的影响,其中计算透射系数采用了转移矩阵方法^[15,16].

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1 模型与理论

本文采用的模型如图 1 所示, 其中 N 为势垒的个数, v_0 为势垒的高度, 势垒和势阱中电子的有效质量分别为 m_b^* 和 m_w^* , 势垒和势阱的宽度分别为 a, b , 另外 v_B 是对势垒结构所加的外电压.

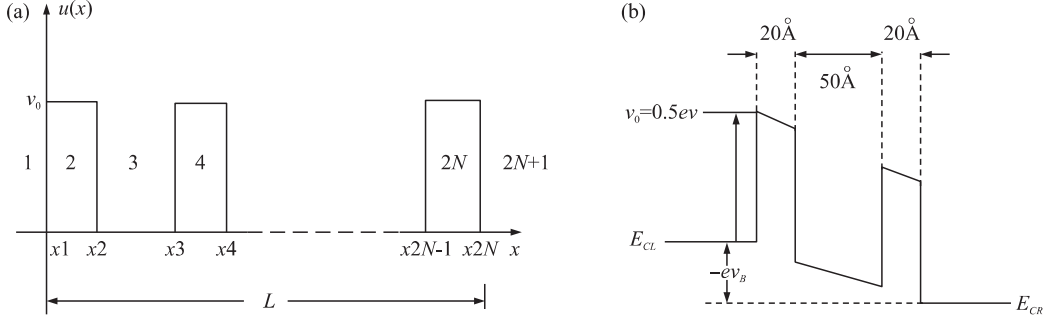


图 1 (a) 多势垒结构 (b) 外场下的多势垒结构

Fig. 1 (a) Multi-barrier structure (b) Multi-barrier structure in external electric field

现考虑将 GaAs/Ga_{0.5}Al_{0.5}As 导带简化成多势垒结构, GaAs 形成势阱, GaAlAs 形成势垒, 如图 1(a) 所示, 且假定该多势垒结构中势垒和势阱不含杂质, 对该势垒结构从左向右施加一个正向电压 v_B , 势垒结构发生倾斜如图 1(b) 所示, 电子从左向右入射, 形成透射隧穿.

在势垒和势阱区中直接求解一维薛定谔方程:

$$\text{在 1 区: } \psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \quad k_1 = \sqrt{\frac{2m_1^* E}{\hbar^2}},$$

$$\text{在 2 区: } \psi_2 = A_2 \text{Ai}(y_2) + B_2 \text{Bi}(y_2) \quad \text{其中: } y_2 = \left(-\frac{2m_2^* e v_B}{L \hbar^2} \right)^{\frac{1}{3}} \left(\frac{E - v_0}{e v_B} L + x \right), \text{ 现令: } l_2 = \left(-\frac{2m_2^* e v_B}{L \hbar^2} \right)^{\frac{1}{3}} g_2 = \frac{E - v_0}{e v_B} L,$$

$$\text{则 } y_2 = l_2 (g_2 + x),$$

⋮

$$\text{在 } 2N \text{ 区: } \psi_{2N} = A_{2N} \text{Ai}(y_{2N}) + B_{2N} \text{Bi}(y_{2N}),$$

$$\text{其中: } y_{2N} = \left(-\frac{2m_{2N}^* e v_B}{L \hbar^2} \right)^{\frac{1}{3}} \left(\frac{E - v_0}{e v_B} L + x \right),$$

$$\text{现令: } l_{2N} = \left(-\frac{2m_{2N}^* e v_B}{L \hbar^2} \right)^{\frac{1}{3}} g_{2N} = \frac{E - v_0}{e v_B} L,$$

$$\text{则 } y_{2N} = l_{2N} (g_{2N} + x).$$

$$\text{在 } 2N+1 \text{ 区: } \psi_{2N+1} = A_{2N+1} e^{ik_{2N+1} x} + B_{2N+1} e^{-ik_{2N+1} x} \quad k_{2N+1} = \sqrt{\frac{2m_{2N+1}^* (E + e v_B)}{\hbar^2}}$$

N 为势垒的个数.

$$m_1^* = m_3^* = \cdots = m_{2N-1}^* = m_{2N+1}^*,$$

$$m_2^* = m_4^* = \cdots = m_{2N-2}^* = m_{2N}^*.$$

由在边界 $x_1, x_2, x_3, x_4, \cdots, x_{2N-1}, x_{2N}$ 处波函数及其一阶导数连续 ($\psi_j = \psi_{j+1}, \frac{1}{m_j^*} \psi_j' = \frac{1}{m_{j+1}^*} \psi_{j+1}'$ [17]) 并由转移矩阵计算可得:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1 x_1} & 0 \\ 0 & e^{-ik_1 x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_1}{m_1^*} & -i \frac{k_1}{m_1^*} \end{pmatrix}^{-1} \times M_1 \times M_2 \times M_3 \times M_4 \times \cdots \times M_{4N-5} \times M_{4N-4} \times M_{4N-3} \times M_{4N-2} \times$$

$$\begin{pmatrix} 1 & 1 \\ i \frac{k_{2N+1}}{m_{2N+1}^*} & -i \frac{k_{2N+1}}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1}x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1}x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix}. \quad (1)$$

其中:

$$\mathbf{M}_1 = \begin{pmatrix} \text{Ai}[l_2(g_2 + x_1)] & \text{Bi}[l_2(g_2 + x_1)] \\ \frac{l_2}{m_2^*} \text{Aid}[l_2(g_2 + x_1)] & \frac{l_2}{m_2^*} \text{Bid}[l_2(g_2 + x_1)] \end{pmatrix} \text{其中 Aid, Bid 分别为 Airy 函数 Ai, Bi 的导数.}$$

$$\mathbf{M}_2 = \begin{pmatrix} M_2(1, 1) & M_2(1, 2) \\ M_2(2, 1) & M_2(2, 2) \end{pmatrix} \text{其中矩阵元 } M_2(1, 1), M_2(1, 2), M_2(2, 1), M_2(2, 2) \text{ 分别为:}$$

$$M_2(1, 1) = \frac{\text{Bid}[l_2(g_2 + x_2)]}{\text{Ai}[l_2(g_2 + x_2)] \text{Bid}[l_2(g_2 + x_2)] - \text{Aid}[l_2(g_2 + x_2)] \text{Bi}[l_2(g_2 + x_2)]},$$

$$M_2(1, 2) = \frac{-\frac{m_2^*}{l_2} \text{Bi}[l_2(g_2 + x_2)]}{\text{Ai}[l_2(g_2 + x_2)] \text{Bid}[l_2(g_2 + x_2)] - \text{Aid}[l_2(g_2 + x_2)] \text{Bi}[l_2(g_2 + x_2)]},$$

$$M_2(2, 1) = \frac{-\text{Aid}[l_2(g_2 + x_2)]}{\text{Ai}[l_2(g_2 + x_2)] \text{Bid}[l_2(g_2 + x_2)] - \text{Aid}[l_2(g_2 + x_2)] \text{Bi}[l_2(g_2 + x_2)]},$$

$$M_2(2, 2) = \frac{\frac{m_2^*}{l_2} \text{Ai}[l_2(g_2 + x_2)]}{\text{Ai}[l_2(g_2 + x_2)] \text{Bid}[l_2(g_2 + x_2)] - \text{Aid}[l_2(g_2 + x_2)] \text{Bi}[l_2(g_2 + x_2)]},$$

⋮
⋮

$$\mathbf{M}_{4N-3} = \begin{pmatrix} \text{Ai}[l_{2N}(g_{2N} + x_{2N-1})] & \text{Bi}[l_{2N}(g_{2N} + x_{2N-1})] \\ \frac{l_{2N}}{m_{2N}^*} \text{Aid}[l_{2N}(g_{2N} + x_{2N-1})] & \frac{l_{2N}}{m_{2N}^*} \text{Bid}[l_{2N}(g_{2N} + x_{2N-1})] \end{pmatrix},$$

$$\mathbf{M}_{4N-2} = \begin{pmatrix} M_{4N-2}(1, 1) & M_{4N-2}(1, 2) \\ M_{4N-2}(2, 1) & M_{4N-2}(2, 2) \end{pmatrix}. \text{其中矩阵元 } M_{4N-2}(1, 1), M_{4N-2}(1, 2), M_{4N-2}(2, 1), M_{4N-2}(2, 2) \text{ 分别为:}$$

$$M_{4N-2}(1, 1) = \frac{\text{Bid}[l_{2N}(g_{2N} + x_{2N})]}{\text{Ai}[l_{2N}(g_{2N} + x_{2N})] \text{Bid}[l_{2N}(g_{2N} + x_{2N})] - \text{Aid}[l_{2N}(g_{2N} + x_{2N})] \text{Bi}[l_{2N}(g_{2N} + x_{2N})]},$$

$$M_{4N-2}(1, 2) = \frac{-\frac{m_{2N}^*}{l_{2N}} \text{Bi}[l_{2N}(g_{2N} + x_{2N})]}{\text{Ai}[l_{2N}(g_{2N} + x_{2N})] \text{Bid}[l_{2N}(g_{2N} + x_{2N})] - \text{Aid}[l_{2N}(g_{2N} + x_{2N})] \text{Bi}[l_{2N}(g_{2N} + x_{2N})]},$$

$$M_{4N-2}(2, 1) = \frac{-\text{Aid}[l_{2N}(g_{2N} + x_{2N})]}{\text{Ai}[l_{2N}(g_{2N} + x_{2N})] \text{Bid}[l_{2N}(g_{2N} + x_{2N})] - \text{Aid}[l_{2N}(g_{2N} + x_{2N})] \text{Bi}[l_{2N}(g_{2N} + x_{2N})]},$$

$$M_{4N-2}(2, 2) = \frac{\frac{m_{2N}^*}{l_{2N}} \text{Ai}[l_{2N}(g_{2N} + x_{2N})]}{\text{Ai}[l_{2N}(g_{2N} + x_{2N})] \text{Bid}[l_{2N}(g_{2N} + x_{2N})] - \text{Aid}[l_{2N}(g_{2N} + x_{2N})] \text{Bi}[l_{2N}(g_{2N} + x_{2N})]}.$$

$$\text{令: } \mathbf{M} = \mathbf{M}_1 \times \mathbf{M}_2 \times \cdots \times \mathbf{M}_{4N-3} \times \mathbf{M}_{4N-2} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \text{则式(1)变为:}$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{ik_1x_1} & 0 \\ 0 & e^{-ik_1x_1} \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_1}{m_1^*} & -i \frac{k_1}{m_1^*} \end{pmatrix}^{-1} \times \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \times \begin{pmatrix} 1 & 1 \\ i \frac{k_{2N+1}}{m_{2N+1}^*} & -i \frac{k_{2N+1}}{m_{2N+1}^*} \end{pmatrix} \times \begin{pmatrix} e^{ik_{2N+1}x_{2N+1}} & 0 \\ 0 & e^{-ik_{2N+1}x_{2N+1}} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix}, \quad (2)$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2} \times \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \times \begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix}, \quad (3)$$

其中:

$$\begin{aligned} S_{11} &= \left[\left(H_{11} + \frac{H_{21}}{i \frac{k_1}{m_1^*}} \right) + i \frac{k_{2N+1}}{m_{2N+1}^*} \left(H_{12} + \frac{H_{22}}{i \frac{k_1}{m_1^*}} \right) \right] e^{-ik_1 x_1} e^{ik_{2N+1} x_{2N+1}}, \\ S_{12} &= \left[\left(H_{11} + \frac{H_{21}}{i \frac{k_1}{m_1^*}} \right) - i \frac{k_{2N+1}}{m_{2N+1}^*} \left(H_{12} + \frac{H_{22}}{i \frac{k_1}{m_1^*}} \right) \right] e^{-ik_1 x_1} e^{-ik_{2N+1} x_{2N+1}}, \\ S_{21} &= \left[\left(H_{11} - \frac{H_{21}}{i \frac{k_1}{m_1^*}} \right) + i \frac{k_{2N+1}}{m_{2N+1}^*} \left(H_{12} - \frac{H_{22}}{i \frac{k_1}{m_1^*}} \right) \right] e^{ik_1 x_1} e^{ik_{2N+1} x_{2N+1}}, \\ S_{22} &= \left[\left(H_{11} - \frac{H_{21}}{i \frac{k_1}{m_1^*}} \right) - i \frac{k_{2N+1}}{m_{2N+1}^*} \left(H_{12} - \frac{H_{22}}{i \frac{k_1}{m_1^*}} \right) \right] e^{ik_1 x_1} e^{-ik_{2N+1} x_{2N+1}}. \end{aligned}$$

现我们假定具有一定能量的粒子由多势垒结构的最左边 ($x < 0$) 向右方入射, 则在 1 区有入射波和反射波, 在 $2N+1$ 区中由于没有由右向左运动的粒子, 因此只有透射波 ($A_{2N+1} \neq 0$), 没有向左传播的波 ($B_{2N+1} = 0$) 且我们根据透射系数的定义^[18]可得:

$$T = \frac{J_T}{J} = \frac{\frac{k_{2N+1}}{m_{2N+1}^*}}{\frac{k_1}{m_1^*}} \left| \frac{A_{2N+1}}{A_1} \right|^2. \quad (4)$$

由 $k_{2N+1} \neq k_1$, $m_1^* = m_{2N+1}^*$ 得:

$$T = \frac{k_{2N+1}}{k_1} \frac{4}{H_{11}^2 + \left(\frac{k_{2N+1}}{m_{2N+1}^*} H_{12} \right)^2 + \left(\frac{1}{k_1} H_{21} \right)^2 + \left(\frac{k_{2N+1}}{k_1} H_{22} \right)^2 + 2 \frac{k_{2N+1}}{k_1} H_{11} H_{22} - 2 \frac{k_{2N+1}}{k_1} H_{12} H_{21}}. \quad (5)$$

2 计算结果和分析

2.1 有效质量的影响

由图 2 知: 随着有效质量的增大, 产生共振透射的共振能量向低能量方向移动, 当共振能量低于零以下, 此时发生共振的透射峰消失, 共振透射峰减少. 两个微带之间的间距随着有效质量的增大而减小, 且势阱中的有效质量对共振透射的影响起主要作用.

2.2 势垒宽度的影响

由图 3 知: 随着势垒宽度的增大, 微带的宽度衰减、各相邻量子阱之间的束缚能级间的耦合作用降低, 从而使微带逐渐转变为量子化能级, 形成尖锐的透射峰. 同时当势垒宽度增大到某一个值后, 透射系数随势垒宽度的增大逐渐减小、完全共振透射峰消失, 在低能量位置不再发生完全共振透射, 高能量位置的微带随着势垒宽度的增加逐渐向低能量方向移动.

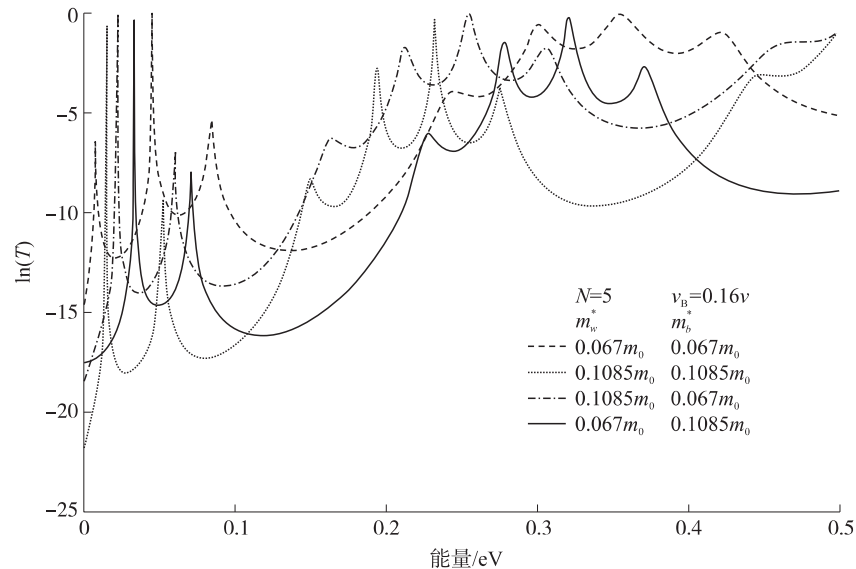


图2 外场中的五势垒结构的透射系数的自然对数与能量的关系图

有效质量为参数, 势垒宽度($a=2$ nm)、势阱宽度($b=5$ nm)、势垒高度($v_0=0.5$ eV)、外加偏压($v_B=0.16$ V) 保持不变

Fig.2 Nature log of transmission coefficient as a function of incident electron energy for a five-barrier structure in a constant electric field.

The effective mass as a parameter. The barrier width($a=2$ nm) , the well width($b=5$ nm) , the barrier height($v_0=0.5$ eV) , bias voltage($v_B=0.16$ V) remain unchanged

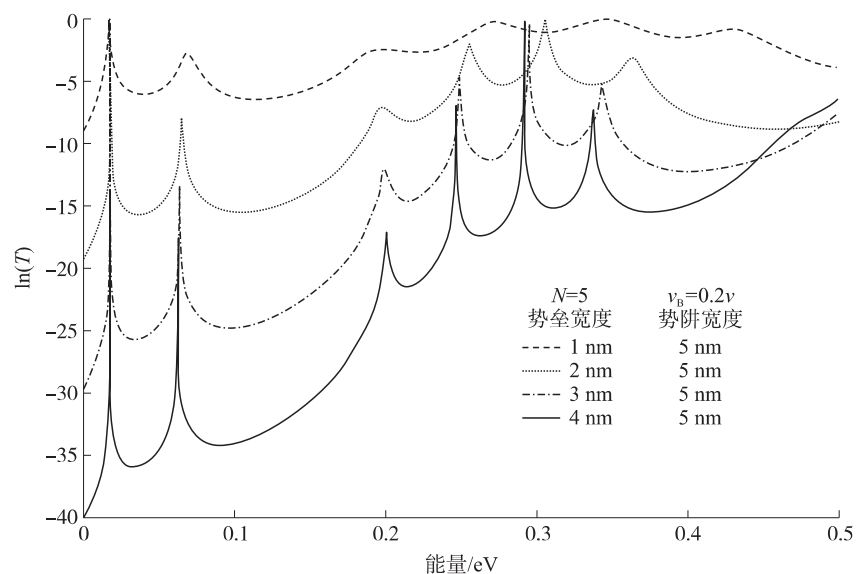


图3 外场中的五势垒结构的透射系数的自然对数与能量的关系图

势垒宽度为参数, 有效质量($m_b^*=0.1085 m_0$, $m_w^*=0.067 m_0$)、势阱宽度($b=5$ nm)、势垒高度($v_0=0.5$ eV)、外加偏压($v_B=0.2$ V) 保持不变

Fig.3 Nature log of transmission coefficient as a function of incident electron energy for a five-barrier structure in a constant electric field

The barrier width as a parameter. The effective mass($m_b^*=0.1085 m_0$, $m_w^*=0.067 m_0$) , the well width($b=5$ nm) , the barrier height($v_0=0.5$ eV) , the bias voltage($v_B=0.2$ V) remain unchanged

2.3 外加偏压对共振传输的影响

由图4知: 随着外加偏压的增大, 发生共振透射的共振能量(准束缚能级) 向低能量方向移动, 这是由于电场势的作用, 多势垒结构发生倾斜(图1b), 使多势垒结构中的电子能级向势能低方向移动. 同时随着偏压增大, 透射系数逐渐降低, 低能量位置的透射峰逐渐减少, 2个透射带之间的间距逐渐减小直到消失,

最后只有一个透射带(图 4g h). 但高能量位置的共振透射能量之间的间距却随着偏压增大而逐渐增大. 这些特性在某种程度上对电子的电导率和正负微分电阻之间的转变和振荡具有一定的影响.

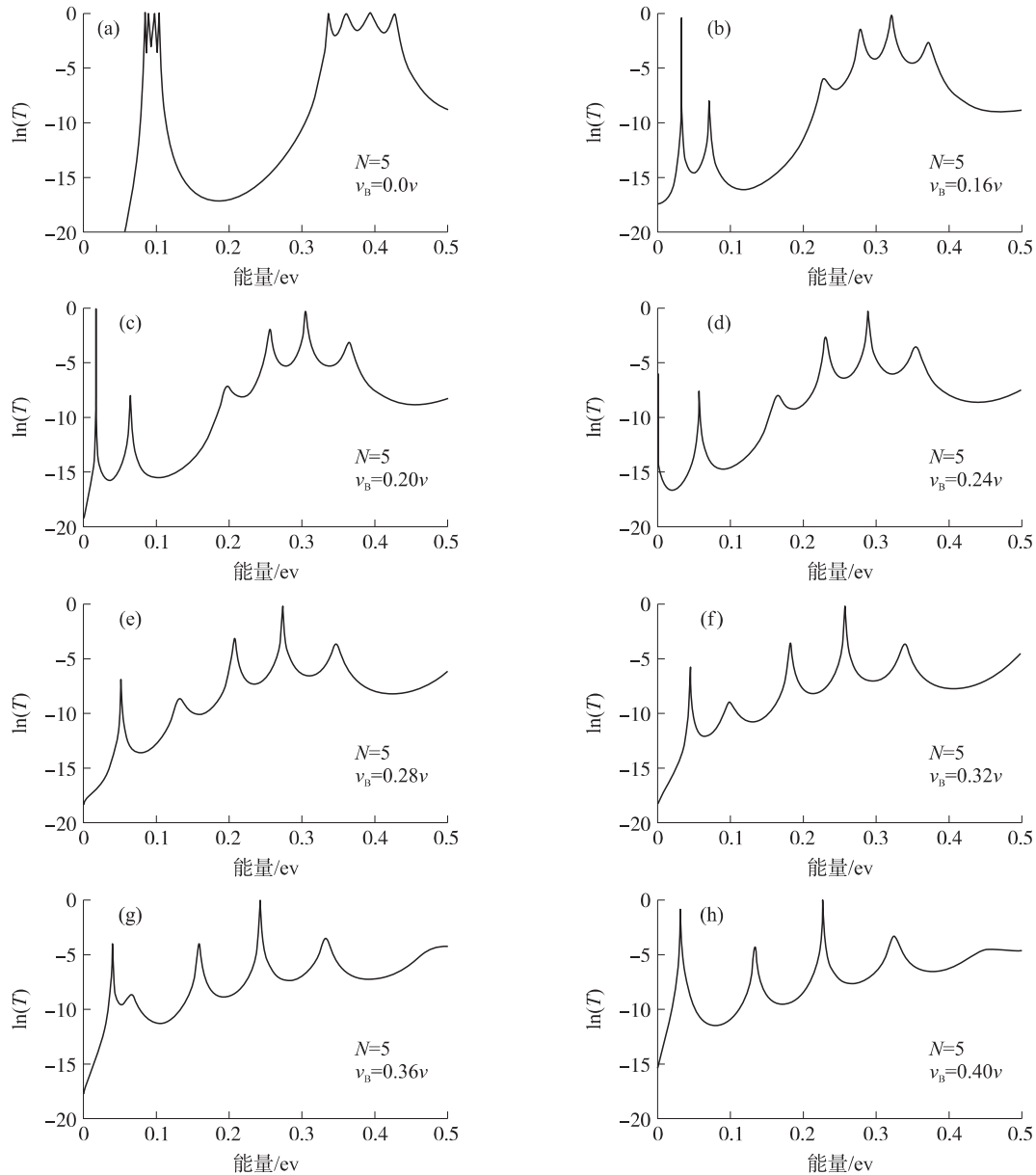


图 4 外场中五势垒结构的透射系数的自然对数与能量的关系图

外加偏压为参数, 有效质量 ($m_b^* = 0.1085m_0$, $m_w^* = 0.067m_0$)、势垒宽度 ($a = 2 \text{ nm}$)、势阱宽度 ($b = 5 \text{ nm}$)、势垒高度 ($v_0 = 0.5 \text{ eV}$) 保持不变

Fig. 4 Nature log of transmission coefficient as a function of incident electron energy for a five-barrier structure in a constant electric field

Bias voltage as a parameter. The effective mass ($m_b^* = 0.1085m_0$, $m_w^* = 0.067m_0$), the barrier width ($a = 2 \text{ nm}$), the well width ($b = 5 \text{ nm}$), the barrier height ($v_0 = 0.5 \text{ eV}$) remain unchanged

3 总结和分析

利用艾里 (Airy) 函数和转移矩阵方法精确求解了存在外场的一维多势垒结构的电子一维定态薛定谔方程, 求出了在一维多势垒结构中电子共振透射系数的表达式, 采用 GaAs/Ga_{1-x}Al_xAs 的参数, 计算了存在偏压情况下五势垒结构的透射系数, 并分析了势垒结构参数及偏压与共振能量之间的关系. 计算结果表明: (a) 发生共振透射的能量随 m_b^* 和 m_w^* 的增加逐渐向低能方向移动, 当共振能量低于零以下, 此时发生

共振的透射峰消失,共振透射峰减少,且 m_w^* 对共振能量的影响比 m_b^* 对其影响大;(b)当势阱宽度一定时,随着势垒宽度的增大,微带的宽度衰减、各相邻量子阱之间的束缚能级间的耦合作用降低,从而使微带逐渐转变为量子化能级,形成尖锐的透射峰。高能量位置的微带随着势垒宽度的增加逐渐向低能量方向移动;(c)随着外加偏压的增大,发生共振透射的共振能量(准束缚能级)向低能量方向移动,透射系数逐渐降低,高能量位置的共振透射能量之间的间距却随着偏压增大而逐渐增大。

这些研究结果有利于我们对电子在多势垒结构中的传导和共振透射物理现象的理解,同时对实验和器件研究也具有一定的参考和指导作用。

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