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Eigen-equation of Electronic Energy in Quantum Dot

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Abstract In this paper, we present one simple model of quantum dot to describe the potential. Based on the boundary continuity of wave function and its derivative, using the Chebyshev polynomial of the second kind and matrix theory, we deduced one eigen-equation of electronic energy which can clearly describe the relationship between the energy level and the surface potential in quantum dot. The further study shows that the eigen-equation of electronic energy is different when the material of quantum dot is different.

Keywords Quantum Dot, Eigen-equation, Electronic Energy

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1. Introduction

Semiconductor quantum dot is composed of a small number of atoms. The number of atoms is usually about a few to hundreds of atoms, and the size of the three dimensions is less than 100 nm. In the three dimensions of the quantum dot, because the motion of the carrier is limited by the size effect and the quantum effect is very significant. Because of the special energy, the quantum dot exhibits the unique physical properties, such as quantum size effect and quantum tunneling effect, et, al. it has very important significance in the research of basic physics and new electronic and optoelectronic devices. Now a large number of studies have been reported on the energy level of the quantum dot [1-13]. For example, on the base of the adiabatic approximation, the adiabatic approximation with averaging and full numerical solution, Yiming Li, Jinn-Liang Liu et al solved the three dimensional Schrödinger equation, and gave qualitative as well as quantitative trends in electronic properties with various parameters[14].By the method of integrating directly the Schrödinger equation, Xiao-Yan Gu[15] gave the calculated energy spectra for two electrons in quantum dot given. K G Dvoyan[16] used perturbation theory and limiting potential to study the energy states of electron in ellipsoidal quantum dot. Analytical expressions for particle energy spectrum have been obtained taking into account that electron effective masses are different in medium and in quantum dot. However, few reports completely describe the relationship of energy band or band gap with the surface potential, the interior periodic potential and the structure parameters.

In this paper, we try to study the dependence of the electronic energy on the quantum surface potential and other structure parameters. Our aim is to deduce an eigen-equation theoretical for describing the relationship of electronic energy with the surface potential, the internal periodic potential and structure parameters, which will be used to calculate the electronic energy in quantum dot.

2. Theory

In this paper, one simple model is presented **(**shown Figure.1). In the model, there is the periodic potential of U_0 when $0 \le x \le l = 2Nb$ and the surface potential of $U_1$when $x \le 0, or\, x \ge l$

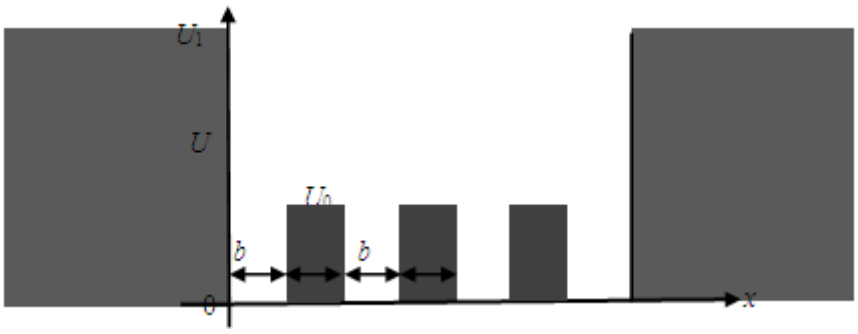

Figure 1. the simplified model of periodic potential in quantum dot

Based on this model in Fig.1, Schrödinger equation:

$$\left(-\frac{\hbar^2 d^2}{2mdx^2}+U\right)\psi(x)=E\psi(x) \tag{1}$$

here $U(x)$ is the potential, $\psi(x)$ is the wave function, E is the energy, m is the electronic mass, $\hbar$ is a Plank **constant.** By solving one-dimensional Schrödinger equation, we can get, respectively

$$\begin{cases} \psi(x)=F_0e^{\beta_0 x} & U=U_1 \quad x\le 0 \\ \psi(x)=A_0e^{i\alpha x}+B_0e^{-i\alpha x} & U=0 \quad 0\le x\le b \\ \psi(x)=C_0e^{i\beta x}+D_0e^{-i\beta x} & U=U_0 \quad b\le x\le 2b \\ \psi(x)=A_1e^{i\alpha x}+B_1e^{-i\alpha x} & U=0 \quad 2b\le x\le 3b \\ \psi(x)=A_Ne^{-\beta_0(x-2Nb)} & U=U_1 \quad x\ge 2Nb \end{cases} \tag{2}$$

Here U_1 is the surface potential, U_0 is the interior periodic potential, $\beta_0=\sqrt{\frac{2m}{\hbar^2}(U_1-E)}$, $\alpha=\sqrt{\frac{2m}{\hbar^2}E}$, $\beta=\sqrt{\frac{2m}{\hbar^2}(E-U_0)}$ and $F_0, A_0, B_0, C_0, D_0, A_1, B_1$ are constant, respectively.

For the above model with the atom layer of $2N+1$ in Fig.1, Using the method in the paper [22], we have

$$\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\left\{\begin{bmatrix}\cos\alpha b & -\frac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}\cos\beta b & -\frac{1}{\beta}\sin\beta b\\ \beta\sin\beta b & \cos\beta b\end{bmatrix}\right\}^N\begin{bmatrix}\cos\alpha b & -\frac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}\psi((Nb+b))\\ \psi'((Nb+b))\end{bmatrix} \tag{3}$$

Based on the property of the transfer matrix, (3) can be changed into

$$\begin{bmatrix}\psi(0)\\ \psi'(0)\end{bmatrix}=\begin{bmatrix}m_{11}U_{N-1}(\chi)-U_{N-2}(\chi) & m_{12}U_{N-1}(\chi)\\ m_{12}U_{N-1}(\chi) & m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\end{bmatrix}\begin{bmatrix}\cos\alpha b & -\frac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}\psi(Nb+b)\\ \psi'(Nb+b)\end{bmatrix} \tag{4}$$

Here $m_{11}=\cos\alpha b\cos\beta b-\frac{\beta}{\alpha}\sin\alpha b\sin\beta b, m_{12}=-\frac{1}{\beta}\cos\alpha b\sin\beta b-\frac{1}{\alpha}\sin\alpha b\cos\beta b$

$$m_{21}=\alpha\sin\alpha b\cos\beta b+\beta\cos\alpha b\sin\beta b, m_{22}=-\frac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b$$

$$U_N(\chi)=\frac{\sin\left[(N+1)\arccos\chi\right]}{\sqrt{1-\chi^2}} \text{ (defined as chebyshev polynomials)} \tag{5}$$

$$\text{and } \chi=\frac{1}{2}\left[\left(\cos\alpha b\cos\beta b-\frac{\beta}{\alpha}\sin\alpha b\sin\beta b\right)+\left(-\frac{\alpha}{\beta}\sin\alpha b\sin\beta b+\cos\alpha b\cos\beta b\right)\right] \tag{6}$$

By substituting both $x=0$ and $x=l=2Nb+b$ into（2）and it's derivative, we have, respectively,

$$\begin{cases}\frac{\psi'(0)}{\psi(0)}=-\frac{1}{\beta_0}\\ \frac{\psi'(l)}{\psi(l)}=\frac{A_Ne^{-\beta_0 l}}{-\beta_0A_Ne^{-\beta_0 l}}=\frac{1}{-\beta_0}\end{cases} \tag{7}$$

Thus, the substitution of (7) into (4) produces

$$\begin{bmatrix}1\\ \beta_0\end{bmatrix}=\begin{bmatrix}m_{11}U_{N-1}(\chi)-U_{N-2}(\chi) & m_{12}U_{N-1}(\chi)\\ m_{21}U_{N-1}(\chi) & m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\end{bmatrix}\begin{bmatrix}\cos\alpha b & -\frac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}1\\ -\beta_0\end{bmatrix} \tag{8}$$

Now by multiplying (8) with $\begin{bmatrix}-\beta_0A_1 & A_1\end{bmatrix}$, and using $\begin{bmatrix}-\beta_0A_1 & A_1\end{bmatrix}\begin{bmatrix}A_1\\ \beta_0A_1\end{bmatrix}=0$, we easily obtain

$$\begin{bmatrix}-\beta_0 & 1\end{bmatrix}\begin{bmatrix}m_{11}U_{N-1}(\chi)-U_{N-2}(\chi) & m_{12}U_{N-1}(\chi)\\ m_{21}U_{N-1}(\chi) & m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\end{bmatrix}\begin{bmatrix}\cos\alpha b & -\frac{1}{\alpha}\sin\alpha b\\ \alpha\sin\alpha b & \cos\alpha b\end{bmatrix}\begin{bmatrix}1\\ -\beta_0\end{bmatrix}=0 \tag{9}$$

The expansion of (9) can be changed into

$$\begin{aligned}&\left[-\beta_0\cos\alpha b\left(m_{11}U_{N-1}(\chi)-U_{N-2}(\chi)\right)-\beta_0 m_{12}U_{N-1}(\chi)\alpha\sin\alpha b\right]\\&+\left[m_{21}U_{N-1}(\chi)\cos\alpha b+\left(m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\right)\alpha\sin\alpha b\right]\\&+\left[\left(-\frac{\beta_0^2}{\alpha}\sin\alpha b\right)\left(m_{11}U_{N-1}(\chi)-U_{N-2}(\chi)\right)+\beta_0^2 m_{12}U_{N-1}(\chi)\alpha\cos\alpha b\right]\\&-\left[m_{21}U_{N-1}(\chi)\left(-\frac{\beta_0}{\alpha}\sin\alpha b\right)+\beta_0\left(m_{22}U_{N-1}(\chi)-U_{N-2}(\chi)\right)\alpha\cos\alpha b\right]=0\end{aligned} \tag{10}$$

After the expansion, we have

$$\begin{aligned}&\sin\left(\arccos\chi\right)\cot\left(N\arccos\chi\right)=\\&=\left(\frac{\beta}{\beta_0}-\frac{\beta_0}{\beta}\right)\cos\alpha b\sin\beta b+\left(\frac{\alpha}{\beta_0}-\frac{\beta_0}{\alpha}\right)\sin\alpha b\cos\beta b\end{aligned} \tag{11}$$

3. The Eigen Equation of Electronic Energy in Different Quantum Dot

3.1. The Eigen Equation of the Quantum Dot When $\chi=0$

When $\chi=0$, from (4) and (5), we have, respectively

$$\tan\alpha b\tan\beta b=\frac{2\alpha\beta}{\alpha^2+\beta^2} \tag{12}$$

$$\text{and}\ \begin{cases}U_{N-1}(\chi)=0\\U_{N-2}(\chi)=1\end{cases} \tag{13}$$

Here N is **even number**. The substitution of (11) and (12) into (9) produces

$$\beta_0\cos\alpha b-\alpha\sin\alpha b+\frac{\beta_0^2}{\alpha}\sin\alpha b+\beta_0\cos\alpha b=0 \tag{14}$$

The solution of (13) is

$$\alpha b=n\pi+\arctan\left(\frac{2\alpha\beta_0}{\alpha^2-\beta_0^2}\right) \tag{15}$$

In order to demonstrates directly the relation of the energy level with the surface potential, by putting $\beta_0=\sqrt{\frac{2m}{\hbar^2}\left(U_1-E\right)}$ and $\alpha=\sqrt{\frac{2m}{\hbar^2}E}$ into (14), we have

$$\sqrt{\frac{2m}{\hbar^2}}Eb=n\pi+\arctan\frac{2\sqrt{E\left(U_1-E\right)}}{\left(2E-U_1\right)} \tag{16}$$

When N is un**even number and** $\chi=0$**,** the value of (4) is, respectively,

$$\begin{cases}U_{N-1}(\chi)=1\\U_{N-2}(\chi)=0\end{cases} \tag{17}$$

Then, the substitution of m_1, m_2 m_3, m_4 and (17) into Eq.(10) generates

$$\begin{aligned}&\beta_0\tan^3\alpha b+\frac{\left(\beta^2-\beta_0^2\right)\alpha}{\left(\alpha^2+\beta^2\right)}\tan^2\alpha b+\\&+\beta_0\tan\alpha b+\frac{\alpha\left(\beta^2-\beta_0^2\right)}{\left(\alpha^2+\beta^2\right)}=0\end{aligned} \tag{18}$$

By solving (18), we get

$$\alpha b=n\pi+\arctan\left(\frac{\alpha\left(\beta_0^2-\beta^2\right)}{\beta_0\left(\alpha^2+\beta^2\right)}\right) \tag{19}$$

Putting $\beta_0=\sqrt{\frac{2m}{\hbar^2}(U_1-E)}$, $\alpha=\sqrt{\frac{2m}{\hbar^2}E}$, $\beta=\sqrt{\frac{2m}{\hbar^2}(E-U_0)}$ into (16), we also have

$$\sqrt{\frac{2m}{\hbar^2}}Eb=n\pi+\arctan\frac{\sqrt{E}\left(U_0+U_1-2E\right)}{\sqrt{\left(U_1-E\right)}\left(2E-U_0\right)} \tag{20}$$

3.3. The Eigen Equation of the Quantum Dot with $\chi\neq0$

When the internal periodic potential is very small, Δ ($\Delta=\beta-\alpha$) is very small, Thus, Eq(6) can be simplified as

$$\begin{aligned}&\chi=\cos\left(\alpha b+\beta b\right)+\\&+\left[1-\frac{1}{2}\left(\frac{\beta}{\alpha}+\frac{\alpha}{\beta}\right)\right]\sin\alpha b\sin\beta b\approx\cos\left(\alpha b+\beta b\right)\end{aligned} \tag{21}$$

By putting $\chi\simeq\cos\left(\alpha b+\beta b\right)$ into（11）, we have

$$N\left(\alpha b+\beta b\right)=n\pi+arc\cot\left(\frac{\alpha}{\beta_0}-\frac{\beta_0}{\alpha}\right) \tag{22}$$

Now, we put $\beta_0=\sqrt{\frac{2m}{\hbar^2}\left(U_1-E\right)}$, $\alpha=\sqrt{\frac{2m}{\hbar^2}E}$, $\beta=\sqrt{\frac{2m}{\hbar^2}\left(E-U_0\right)}$ into (26) again, and have

$$\left(\sqrt{E}+\sqrt{\left(E-U_0\right)}\right)\sqrt{\frac{2m}{\hbar^2}}Nb=n\pi+arc\cot\left(\frac{\sqrt{E}}{\sqrt{\left(U_1-E\right)}}-\frac{\sqrt{\left(U_1-E\right)}}{\sqrt{E}}\right) \tag{23}$$

here *N* is the total periodic number, *n* is the quantum number.

Eq.(16), (20)and (23) are defined as the eigen equation of electronic energy in quantum dot, which can clearly describe the relationship of electronic energy with the surface potential, the internal periodic potential and structure parameters. They can more clearly describe the electronic state under different quantum number compared with that

given only when $\chi > 0$ in [17]. Especially, these relationships are simpler and clearer than the eigen equation of quantum dot in [17], which are valuable for the further study of quantum dot.

4. Conclusions

This paper demonstrates the matrix method to study the eigen equation of electronic energy in quantum dot. Using Chebyshev polynomials of the second kind, we have deduced three eigen equations, which could clearly describe the relationship of electronic energy with the surface potential, the internal periodic potential and structure parameters. The method used in this paper can also be used to investigate the effect of the surface potential, the internal periodic potential and structure parameters on the electronic energy and electronic level distribution.

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