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# The relation of the energy of electronic state with the interior periodic potential in quantum dot given by matrix method

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ABSTRACT

In this paper, we mainly investigate the effect of the interior periodic potential and the surface potential on the energy of electronic state in quantum dot. Based on Chebyshev polynomials of the second kind and matrix theory, we deduced one expression, which can clearly describe the relation of energy of electronic state with the surface and interior periodic potential. The theoretical analysis shows that the energy of electronic state in quantum dot strongly depend on surface potential and the interior periodic potential. For the same quantum dot with different surface potential, the energy of electronic state with the determined quantum number is different. For the quantum dot of same size with different interior periodic potential, the energy of electronic state with the determined quantum number is also different. The further study indicates that there are two different energy of electronic state in quantum dot for the decided quantum number.



## 1. Introduction

A quantum dot is a nanocrystal made of semiconductor materials that are small enough to exhibit quantum mechanical properties. The electronic properties of these materials are intermediate between those of bulk semiconductors and of discrete molecules, which are closely related to its size and shape. For the study of the energy of electronic state in quantum dot, there were many works on the theoretical studies about the electronic states [1–8]. In these studies, the quantum dot was considered as an infinite depth potential well. For example, on the base of the adiabatic approximation, the adiabatic approximation with averaging and full numerical solution, Yiming et al. solved the three dimensional Schrödinger equation, and gave qualitative as well as quantitative trends in electronic properties with various parameters [9]. To calculate the ground state and first excited state energy levels in quantum dot, the nonlinear three dimensional Schrödinger is solved, which shows that the principal quantum dot energy depends on various shapes [10]. By the method of integrating directly the Schrödinger equation, Xiao-Yan [11] gave the calculated energy spectra for two electrons in quantum dot, which are in excellent agreement with the results, and better than those by the WKB method and the WKB-DP method. In perturbation theory taking into account the hybridization of states for cubic, ellipsoidal, cylindrical and tetrahedral shapes. The transfer matrix method was often used for the determination of one-dimensional band structures [12–21]. For example, Hung and Wu [22] used transfer-matrix theory for calculating a few low-lying conduction sub-bands and wave functions. However, few reports consider the effect of surface and interior Periodic potential on energy band or band gap.

In this paper, we try to use Chebyshev polynomials of the second kind in matrix theory for the investigating the energy of electronic state under different potential. This paper mainly analyzes the dependence of the energy on the quantum surface's potential and interior periodic potential, which is valuable for the further study of quantum dot.

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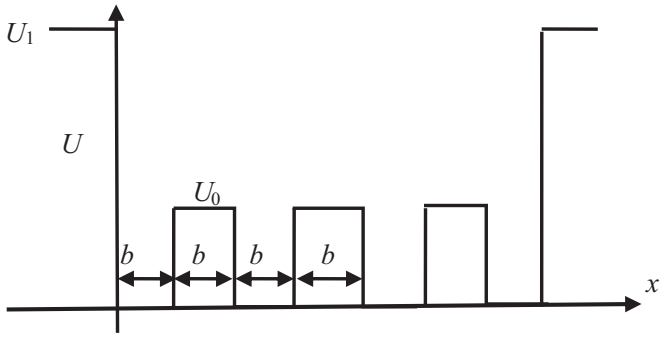


**Fig. 1.** A simplified model of periodic potential in nanocrystalline.

## 2. Theoretical derivation

For the convenience of our investigation, one simple model is presented (shown Fig. 1). In model there is the periodic potential of $U_0$ when $0 \le x \le l = Nb$ and the surface potential of $U_1$ when $x \le 0$, or $x \ge l$

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 electron energy for the corresponding electron wave function. $m$ is the electron mass, $\hbar$ is a Plank constant. By solving the one-dimensional Schrödinger equation, we can get, respectively

$$\begin{cases} \psi(x) = F_0 e^{\beta_0 x} & U = U_1 \quad x \le 0 \\ \psi(x) = A_0 e^{i\alpha x} + B_0 e^{-i\alpha x} & U = 0 \quad 0 \le x \le b \\ \psi(x) = C_0 e^{i\beta x} + D_0 e^{-i\beta x} & U = U_0 \quad b \le x \le 2b \\ \psi(x) = A_1 e^{i\alpha x} + B_1 e^{-i\alpha x} & U = 0 \quad 2b \le x \le 3b \\ \psi(x) = A_N e^{-\beta_0 (x-2Nb)} & U = U_1 \quad x \ge 2Nb \end{cases} \tag{2}$$

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

$\alpha = \sqrt{\frac{2m}{\hbar^2}E}$, $\beta = \sqrt{\frac{2m}{\hbar^2}(E - U_0)}$.

when $0 \le x \le b$, the wave function and it's derivative is expressed as

$$\begin{cases} \psi(x) = A_0 e^{i\alpha x} + B_0 e^{-i\alpha x} \\ \psi'(x) = i\alpha A_0 e^{i\alpha x} - i\alpha B_0 e^{-i\alpha x} \end{cases} \tag{3}$$

when $x = 0$, using Eq. (3), we obtained

$$\begin{cases} \psi(0) = A_0 + B_0 \\ \psi'(0) = i\alpha A_0 - i\alpha B_0 \end{cases} \tag{4}$$

It can be written in the form of matrix

$$\begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ i\alpha & -i\alpha \end{bmatrix} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} \tag{5}$$

Similarly, at $x = b$, we have also

$$\begin{cases} \psi(b) = A_0 e^{i\alpha b} + B_0 e^{-i\alpha b} \\ \psi'(b) = i\alpha A_0 e^{i\alpha b} - i\alpha B_0 e^{-i\alpha b} \end{cases} \tag{6}$$

The solutions of function group (6) are, respectively,

$$\begin{cases} A_0 = \dfrac{i\alpha\psi(b) + \psi'(b)}{2i\alpha} e^{-i\alpha b} \\ B_0 = \dfrac{i\alpha\psi(b) - \psi'(b)}{2i\alpha} e^{i\alpha b} \end{cases} \tag{7}$$

It can be written in the form of matrix