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Finite difference method for the arbitrary potential in two dimensions: Application to double/triple quantum dots

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ABSTRACT

A finite difference method (FDM) applicable to a two dimensional (2D) quantum dot was developed as a non-conventional approach to the theoretical understandings of quantum devices. This method can be applied to a realistic potential with an arbitrary shape. Using this method, the Hamiltonian in a tri-diagonal matrix could be obtained from any 2D potential, and the Hamiltonian could be diagonalized numerically for the eigenvalues. The legitimacy of this method was first checked by comparing the results with a finite round well with the analytic solutions. Two truncated harmonic wells were examined as a realistic model potential for lateral double quantum dots (DQDs) and for triple quantum dots (TQDs). The successful applications of the 2D FDM were observed with the entanglements in the DQDs. The level-splitting and anti-crossing behaviors of the DQDs could be obtained by varying the distance between the dots and by introducing asymmetry in the well-depths. The 2D FDM results for linear/triangular TQDs were compared with the tight binding approximations.

1. Introduction

The recent developments in quantum phenomena in mesoscopic systems predict many future applications of quantum devices, such as quantum information, quantum computing, next-generation logic. A quantum dot with a submicron feature-size is considered as an artificial atom with a unique shell structure [1] that can be engineered artificially by manipulating a highly-mobile two-dimen-

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sional electron gas (2DEG) formed at the interface of a semiconductor heterostructure (GaAs/AlGaAs). The lateral confinement of a 2DEG is accomplished by shaping the local potential wells using gate electrodes. When two quantum dots are moved close enough to each other, they are considered as an artificial molecule that might be a candidate for a solid state quantum bit in a quantum computation [2–4].

The theoretical understanding on the quantized bound states and the transport properties of QDs is based on the methods of quantum mechanics developed to date, such as perturbation theory with the tight-binding Anderson model [5–7], variational calculations [8–10], the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian method within the envelope-function approximation [11–13], density-functional theory [14], mode space approach [15], filter-diagonalization method [16], transmitting boundary method [17,18], numerical coupled-channel method [19], and direct diagonalization techniques in finite difference scheme [20–23].

Regarding the *realistic* potentials, theoretical modeling has a weakness. For example, the experimental data [24] revealed the breaking of Kohn's theorem [25]. In particular, when it comes to closely-coupled shallow QDs, it is more challenging to employ the *ideal* parabolic confining potential rigorously to describe each QD: a harmonic potential requires an infinite range and height. Most theoretical methods assume an ideal and symmetric model potential and often recur to the expansions or approximations using the analytic basis functions [26,27]. Numerical methods are feasible alternatives and the finite difference method (FDM) can be one of the most powerful techniques for solving real quantum systems being considered recently [28–39]. This paper reports the capability of 2D FDM by examining double QDs (DQDs) and triple QDs (TQDs) with a model potential composed of truncated parabolic potential wells. This study first reviewed the 2D FDM with a single QD with round well, and examined the level-splittings and anti-crossing behaviors of DQDs. The 2D FDM and the tight binding approach are compared quantitatively in the linear TQDs and in the triangular TQDs.

2. Theoretical model and validation

2.1. The FDM in 2D

In the effective-mass approximation for a arbitrary N-electron quantum dot, the single-particle Schrödinger equation can be given as

$$\left\{-\frac{\hbar^2\vec{\nabla}}{2}\cdot\left[\frac{\vec{\nabla}}{m^*(\vec{r})}\right]-e\left(V^{ee}+V^b\right)+E^{xc}\right\}\psi(\vec{r})=E\psi(\vec{r}), \tag{1}$$

where $m^*(\vec{r})$ is the electron effective mass, V^{ee} is the electrostatic potential between electrons, V^b is the confining barrier potential, and E^{xc} is the exchange-correlation energy. Eq. (1) can be solved self-consistently by solving the Poisson eq. for V^{ee} and by applying the Hartree or the local density approximation for E^{xc} [40]. When a single electron is trapped within a quantum dot with a diameter of several tens of nanometers, the carrier density is very low, $\sim 10^{12}$–$10^{13}/\mathrm{cm}^2$, and the contributions from the V^{ee} and E^{xc} can be neglected.

By applying a FDM to 2D regularly-spaced grid points with a grid-spacing, Δ, Eq. (1) can be approximated with a set of coupled finite difference equations,

$$\gamma\left(4\psi_{j,k}-\psi_{j+1,k}-\psi_{j,k+1}-\psi_{j-1,k}-\psi_{j,k-1}\right)-eV^b_{j,k}\psi_{j,k}=E\psi_{j,k}, \tag{2}$$

where $\gamma=\hbar^2/2m^*\Delta^2$, $\psi_{j,k}=\psi(x_j,y_k)$, and $V^b_{j,k}=V^b(x_j,y_k)$. By aligning the grid points with indices, j and k (=1, …, N), into an one-dimensional sequence with an index $i\equiv(j-1)N+k$ (=1, …, N^2) [41], a large but sparse Hamiltonian matrix, H, with non-zero elements $H_{i,i}=4\gamma-eV^b_i$ and $H_{i+N,i}=H_{i,i+N}=H_{i+1,i}=H_{i,i+1}=-\gamma$ can be obtained. In addition, the homogeneous domain is assumed to be surrounded by an impenetrable barrier, such that wavefunction vanishes outside, and $H_{nN+1,nN}=H_{nN,nN+1}=0$ for integer n. The Hamiltonian is a block tridiagonal matrix that can be diagonalized iteratively with the Krylov subspace method [42] realized using MATLAB code. The effective mass, $m^*=0.067m_e$, was used for an electron in GaAs. A $300\times300\ \mathrm{nm}^2$-area with a spatial-resolution $\Delta=1$ nm required $\sim 9\times10^4$ grid-points.