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Modelling of electron states in quantum-wire systems - influence of stochastic effects on the confining potential

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***Abstract*—**In this work, we address theoretically the influence of red and white Gaussian noise for electronic energies and eigenstates of cylindrically shaped quantum dots. The stochastic effect can be imagined as resulting from crystal-growth statistical fluctuations in the quantum-dot material composition. In particular we obtain analytical expressions for the eigenvalue shifts and electronic envelope functions in the $\vec{k}\cdot\vec{p}$ formalism due to stochastic variations in the confining band-edge potential. It is shown that white noise in the band-edge potential leaves electronic properties almost unaffected while red noise may lead to changes in state energies and envelope-function amplitudes of several percentages. In the latter case, the ensemble-averaged envelope function decays as a function of distance. It is also shown that, in a stochastic system, constant ensemble-averaged envelope functions are the only bounded solutions for the infinite quantum-wire problem and the energy spectrum is completely discrete. In other words, the infinite stochastic quantum wire behaves, ensemble-averaged, as an atom.

***Keywords*—**cylindrical quantum dots, electronic eigenenergies, red and white Gaussian noise, ensemble averaging effects.

I. Introduction

QUantum structures of practically any shape and size down to nanometer size can be made with recent advances in crystal-growth technology allowing for tailoring of optical and electronic properties [1], [2], [3], [4], [5], [6], [7]. However, as such structures are heterogeneous, quantum-dot structures are affected by statistic fluctuations in material composition, disorder, and size and shape variations. Hence, it is important to assess the influence of such stochastic mechanisms for the properties of the quantum structures. We employ here a Bourret integral formalism [8], [9] to analyze analytically the effect of stochastic fluctuations on a system of first-order differential equations. The procedure, for a cylindrical quantum dot, is here applied to the axial equation of the separated Schrödinger equation written as a system of two linear equations in the axial coordinate z. The formalism is proposed for electrons obeying, in the $\vec{k}\cdot\vec{p}$ theory, a one-band model for their envelope-function parts accounting for magnetic-field effects (neglecting electron-spin effects).

II. Theory and Numerical Results

In this section, the theory of electronic eigenstates in a one-band $\vec{k}\cdot\vec{p}$ formalism accounting for stochastic variations in the band-edge potential is presented. Case examples of the influence of noise characteristics for energy eigenvalues and eigenstates are also given.

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A. Theory

Electrons in cylindrical quantum-dots in the presence of a constant axial magnetic field B and a DC electric field $\mathcal{E}$ (neglecting spin-magnetic effects) can be described by a one-band differential equation in the envelope-function approximation [10]:

$$\vec{\nabla}\cdot\left(\frac{1}{m(z)}\vec{\nabla}\right)+\frac{2}{\hbar^2}\left[E-V(\vec{r})+e\mathcal{E}z\right.$$
$$\left.+\frac{1}{2m(z)}\left(\frac{ieB\hbar}{2c}\frac{\partial}{\partial\theta}-\frac{e^2r^2}{4c^2}B^2\right)\right]\psi=0, \quad (1)$$

where ψ, m, $\hbar$, e, c, E, V, r, θ, and z are the electron envelope function, the z-dependent electron effective mass, Planck's constant divided by 2π, the electron charge, the speed of light in vacuum, the electron energy, the band-edge potential, and the three cylindrical coordinates, respectively.

We seek to determine the influence of stochastic variations in the band-edge potential V on electronic states and energies. For simplicity, we shall next assume that the effective mass is independent of position. Further, we point out that the analysis presented in the following applies equally well to one-dimensional quantum-well- and two-dimensional quantum-wire-problems.

Equation (1) can be solved by the separation-of-variables method:

$$\psi(r,\theta,z)=\psi_1(r)\psi_2(z)e^{ik\theta}, \quad (2)$$

where $k\in\mathbb{Z}$. Assuming stochastic variations along the quantum-wire z axis only, ψ_1 is a deterministic function while ψ_2 is stochastic.

Substituting (2) into Equation (1), we obtain:

$$-\frac{\hbar^2}{2m}\left(\frac{\frac{d^2\psi_1}{dr^2}}{\psi_1}+\frac{1}{r}\frac{\frac{d\psi_1}{dr}}{\psi_1}-\frac{k^2}{r^2}\right)\psi_2-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dz^2}+$$
$$+\frac{1}{2m}\left(\frac{\hbar eBk}{2c}+\frac{e^2r^2B^2}{4c^2}\right)\psi_2+(V+e\mathcal{E}z)\,\psi_2=E\psi_2. \quad (3)$$

Since ψ_2 is a function of z only, the function $\psi_1(r)$ must satisfy the following equation:

$$h^2\left(\frac{d^2\psi_1}{dr^2}+\frac{1}{r}\frac{d\psi_1}{dr}-\frac{k^2}{r^2}\psi_1\right)$$
$$-\left(\frac{\hbar eBk}{2c}+\frac{e^2r^2B^2}{4c^2}\right)\psi_1=\Lambda_R\psi_1, \quad (4)$$

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where the constant Λ_R is determined by the Dirichlet condition $\psi_1(R) = 0$ and R is the quantum-dot radius corresponding to complete confinement within the quantum-dot region.

Equation (4) is the Bessel wave equation, and the solution can be found as a power series in r [11]. For a specific example on the solution of the Bessel wave equation for lens-shaped quantum dots refer to, e.g., Ref. [12]. In the following analysis, we shall for simplicity disregard the DC electric-field effect with the remark that this effect can be handled in a similar way.

The envelope-function component ψ_1 then satisfies:

$$\frac{d^2\psi_2}{dz^2} + \left(\frac{2m}{\hbar^2}(E - V) + \frac{\Lambda_R}{\hbar^2}\right)\psi_2 = 0, \tag{5}$$

as follows immediately from Equations (3) and (4). Writing for the band-edge potential:

$$V(z) = \langle V\rangle + \tilde{V}, \tag{6}$$

where $\langle V\rangle$ and $\tilde{V}$ are the average band-edge potential and the Gaussian red-noise part, respectively, we may recast Equation (5):

$$\frac{d^2\psi_2}{d\tilde{z}^2} + \left(1 - \frac{\frac{2m}{\hbar^2}\tilde{V}}{\frac{2m}{\hbar^2}\left(E - \langle V\rangle\right) + \frac{\Lambda_R}{\hbar^2}}\right)\psi_2 \equiv$$
$$\frac{d^2\psi_2}{d\tilde{z}^2} + (1 + \epsilon\eta)\,\psi_2 = 0, \tag{7}$$

where

$$\tilde{z} = \sqrt{\frac{2m}{\hbar^2}\left(E_q - \langle V\rangle\right) + \frac{\Lambda_R}{\hbar^2}}\,z. \tag{8}$$

Let us consider the influence of stochastic variations in the band-edge potential representing, e.g., a stochastic composition of material layers along the z direction. This can be imagined as a result of a small (and stochastic) mixture of barrier-material atoms within the quantum-dot material. To simplify the analysis, we shall disregard stochastic variations in the effective mass in the following. We remind that for a stochastic system of linear equations:

$$\frac{d\mathbf{x}}{dz} = [\mathbf{A}_0 + \epsilon\eta(z)\mathbf{A}_1]\mathbf{x}, \tag{9}$$

where $\mathbf{A}_0$ and $\mathbf{A}_1$ are constant matrices, ϵ is a small parameter, and $\eta(z)$ represents Gaussian noise, the Bourret approximation for the stochastically averaged variables reads [8], [9]:

$$\frac{d\langle\mathbf{x}\rangle}{dz} = \left[\mathbf{A}_0 + \epsilon^2\int_0^\infty \langle\eta(z)\eta(z-\tau)\rangle\mathbf{A}_1 e^{\mathbf{A}_0\tau}\mathbf{A}_1 e^{-\mathbf{A}_0\tau}d\tau\right]\langle\mathbf{x}\rangle, \tag{10}$$

where $\langle\cdot\rangle$ denotes statistically averaging (or ensemble averaging). We assume that η obeys the following equations corresponding to red Gaussian noise:

$$\langle\eta(z)\rangle = 0,$$
$$\langle\eta(z)\eta(z-\tau)\rangle = \alpha\exp\left(-|\tau|/\tau_c\right), \tag{11}$$

where τ_c is the correlation distance for the noise and α is the variance. We can recover the white noise limit by letting τ_c approach zero while keeping the product $\alpha\tau_c$ constant.

The wave equation [Equation (7)] can be written as two first-order linear differential equations in $x_1 = \psi_2$ and x_2:

$$\frac{dx_1}{d\tilde{z}} = x_2,$$
$$\frac{dx_2}{d\tilde{z}} = -\left(1 + \epsilon\eta\right)x_1. \tag{12}$$

The Bourreq approximation [Equation (10)] applied to the system: Equation (12) then gives for the stochastic average envelope function:

$$\frac{d^2\langle\psi_2\rangle}{d\tilde{z}^2} + \left(\frac{2\epsilon^2\alpha\tau_c^3}{1 + 4\tau_c^2}\right)\frac{d\langle\psi_2\rangle}{d\tilde{z}} + \left(1 - \frac{\epsilon^2\alpha\tau_c^2}{1 + 4\tau_c^2}\right)\langle\psi_2\rangle = 0. \tag{13}$$

Notice that formally, Equation (13) is not inversion-symmetric with respect to $\tilde{z}$: the "damping" term:

$$\left(\frac{2\epsilon^2\alpha\tau_c^3}{1 + 4\tau_c^2}\right)\frac{d\langle\psi_2\rangle}{d\tilde{z}},$$

changes sign under the transformation $\tilde{z} \to -\tilde{z}$. The whole system, however, is inversion-symmetric: the transformation $\tilde{z} \to -\tilde{z}$ must be done *before* the ensamble averaging and this leads to the *same* Equation (13) since Equations (11)-(12) are both inversion-symmetric.

III. General solution and discussions

The above differential equation represents electronic states damped in space:

$$\langle\psi_{2,q}\rangle = \exp\left(-\frac{\epsilon^2\alpha\tau_c^3}{1 + 4\tau_c^2}\sqrt{\frac{2m}{\hbar^2}\left(E_q - \langle V\rangle\right) + \frac{\Lambda_R}{\hbar^2}}\,z\right)\times$$
$$\sin\left(\left(1 - \frac{1}{2}\frac{\epsilon^2\alpha\tau_c^2}{1 + 4\tau_c^2}\right)\sqrt{\frac{2m}{\hbar^2}\left(E_q - \langle V\rangle\right) + \frac{\Lambda_R}{\hbar^2}}\,z\right), \tag{14}$$

$$E_q = \langle V\rangle + \frac{\hbar^2}{2mL^2}\left(\frac{\pi^2 q^2}{1 - \frac{\epsilon^2\alpha\tau_c^2}{1+4\tau_c^2}}\right) - \frac{\Lambda_R}{2m}, \tag{15}$$

where $q \in \mathbb{Z}$. The result that the stochastically averaged wavefunction decays in space is true but must be interpreted with care. Evidently, it does not mean that a single quantum dot wavefunction decays in space since this would imply absorption takes place in the quantum dot and this is not the case (our Hamiltonian does not reflect absorption channels). Rather it means that the averaging procedure over, e.g., an ensemble of quantum dots corresponds to averaging over slightly different wavefunctions (with slightly different phases) which, in effect, is described by a damping term. It should also be pointed out that Λ_R is quantized and characterized by two indices: k and another one resulting from imposing the radial boundary condition on Equation (4), thus a general wavefunction $\langle\psi_2\rangle$ is specified by a quantum index for each spatial coordinate r, θ, z.

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The spectrum of a stochastic semi-infinite quantum wire with red-noise perturbations, i.e., when $z \in [z_0, +\infty)$, is continuous similar to the system without noise. However, the spectrum of a stochastic red-noise quantum wire, infinite in both directions ($z \in (-\infty, +\infty)$), is purely *discrete* unlike the case without noise. Indeed, Equation (13) has a bounded non-zero solution for $z \in (-\infty, +\infty)$ only if the "damping" term is zero. This is possible whenever:

$$2m\left(E - \langle V \rangle\right) + \Lambda_R = 0,$$

[one has to make the inverse transformation $\tilde{z} \rightarrow z$ in Equation (13)], thus the allowed energy values of an infinite quantum wire form a discrete spectrum determined by the discrete set of Λ_R values. The corresponding solutions are constants, which, as above, can be interpreted as the result of ensemble averaging wavefunctions with different phases.

Let us consider quantum dot electron eigenstates in the absence of a magnetic field ($B = 0$). The solution for the radial part of the envelope function is:

$$\psi_1(r) = J_k\left(\frac{j_{kn}}{R} r\right), \tag{16}$$

$$\Lambda_{R,kn} = -\left(\frac{j_{kn}\hbar}{R}\right)^2, \tag{17}$$

where j_{kn} is the n'th zero point of the Bessel function J_k.

Assume now that the stochastic variation in quantum-dot potential corresponds to parameters: $\alpha = 20$, $\tau_c = 1$, and $\epsilon = 0.01$. The length of the quantum dot is taken to be $L = 5$ nm and the radius $R = 5$ nm. The zero point for the potential energy is chosen to be $\langle V \rangle = 0$. In Figure 1 (upper plot), the associated envelope function is plotted versus the quantum-dot axial coordinate z. There is apparently only a minor influence of stochastic averaging on energy eigenvalues and envelope functions. In Figure 1 (lower plot), the envelope function is plotted versus z for the parameters $\alpha = 20$, $\tau_c = 1$, $\epsilon = 0.1$, $L = 5$ nm, and $R = 5$ nm. It is now evident with the increase in ϵ from 0.01 to 0.1 that the stochastically-averaged envelope function is damped pronouncedly and energies strongly affected.

IV. Conclusions

Electron eigenstates in quantum-dot structures are found accounting for stochastic variations in the band-edge potential. The model takes into account magnetic effects (albeit neglecting the electron spin character) within the one-band $\vec{k} \cdot \vec{p}$ formalism for electrons applying to, e.g., GaAs/AlGaAs quantum-dot heterostructures. Emphasis is given to the red or white noise character governing the stochastic variations for electronic eigenstates and energy eigenvalues. Finally, case examples are provided indicating that white-noise fluctuations are of little importance for electronic properties, however, red-noise fluctuations may lead to considerable changes in the energies and envelope functions. As a corollary, in a stochastic infinite quantum-wire system, bounded ensemble-averaged envelope functions are constant in space and the energy spectrum is completely discrete. In other words, the infinite stochastic quantum wire behaves, ensemble-averaged, as an atom.

TABLE I
The first three energy eigenvalues for a quantum dot with parameters (Case 1) $\epsilon = 0$, $L = 5$ nm, $R = 5$ nm, $k = 0$, and $n = 1$; (Case 2) $\alpha = 20$, $\tau_c = 1$, $\epsilon = 0.01$, $L = 5$ nm, $R = 5$ nm, $k = 0$, and $n = 1$; (Case 3) $\alpha = 20$, $\tau_c = 1$, $\epsilon = 0.1$, $L = 5$ nm, and $R = 5$ nm, $k = 0$, and $n = 1$.

	Case 1 [eV]	Case 2 [eV]	Case 3 [eV]
$E_q, q = 1$	0.2245	0.2246	0.2338
$E_q, q = 2$	0.8979	0.8983	0.9353
$E_q, q = 3$	2.020	2.021	2.104

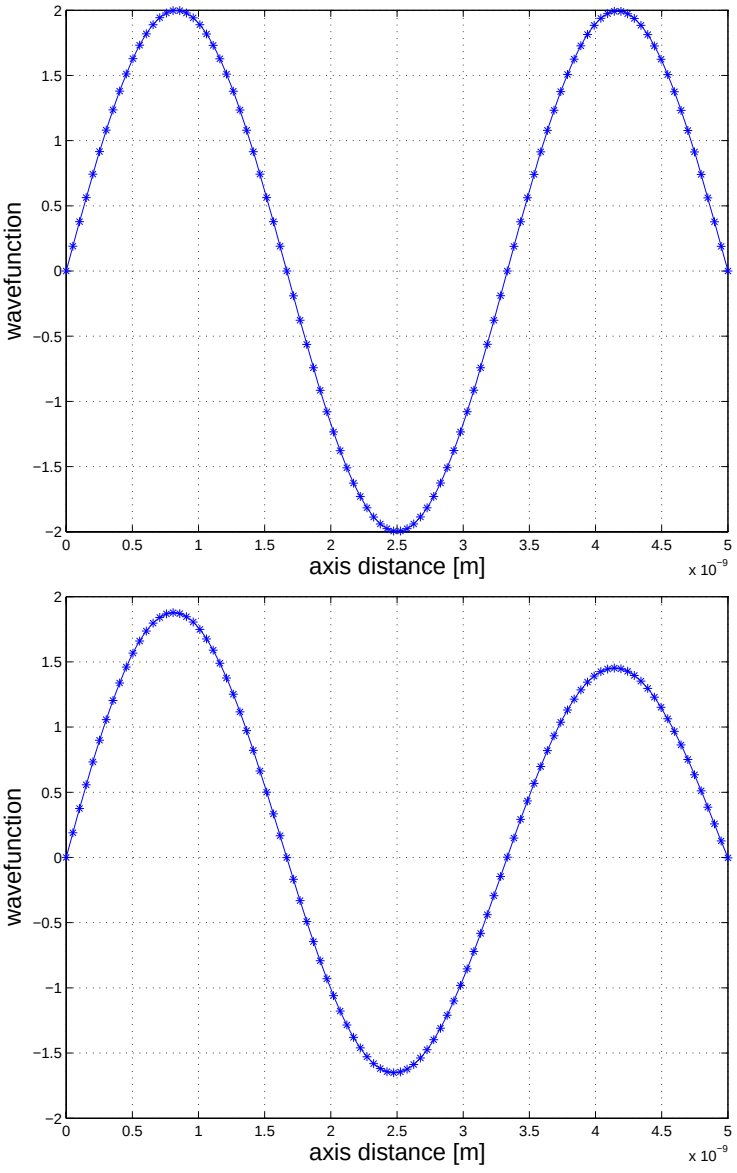


Fig. 1. (Upper plot) $\langle \psi_2 \rangle$ as a function of the axial quantum-dot coordinate z. Parameters are $\alpha = 20$, $\tau_c = 1$, $\epsilon = 0.01$, $L = 5$ nm, and $R = 5$ nm; (lower plot) $\langle \psi_2 \rangle$ as a function of the axial quantum-dot coordinate z. Parameters are $\alpha = 20$, $\tau_c = 1$, $\epsilon = 0.1$, $L = 5$ nm, and $R = 5$ nm.

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