ΦΥΣΙΚΗ.— **Charge and current density fluctuations in a double quantum well,** by *G. J. Papadopoulos**, διὰ τοῦ Ἀκαδημαϊκοῦ κ. Καίσαρος Ἀλεξοπούλου.

ABSTRACT

According to classical mechanics a particle momentarily situated at a potential minimum with zero momentum will remain motionless for ever. The nearest state in quantum mechanics approaching the above initial conditions is given by a wavefunction providing zero current density, probability of finding the particle symmetrically locating the particle about the position of the potential minimum and a least possible energy. In contrast to classical mechanics the evolution of motion as time proceeds leads to spatial and temporal charge and current density fluctuations. In the present study such fluctuations are obtained for an electron in a double potential well with an initial state of the sort that corresponds to a classical state from which no motion follows. The fluctuations in question provide a rough estimate for noise to be expected in quantum semiconductor devices in the submicron region.

1. Introduction

According to classical mechanics a particle that is momentarily situated at a potential minimum with zero momentum will remain motionless for ever. It is of interest to examine the quantum mechanical counterpart of the above state of affairs in the case of a double quantum well. As is well known double quantum wells can nowadays be realized in epitaxially grown semiconductors and form the simplest form of superlattices. Superlattices are destined to play an important role in the minuturization of semiconductor devices, where quantum effects will constitute the dominant driving mechanism. Contrary to classical mechanics, where a state of complete rest exists the quantum regime imposes continual movement, a situation that superposes an intrinsic noise. With the above in mind we subsequently proceed to present calculations pertaining to current and charge density fluctuations starting from a quantal state intimately related to the classical initial state leading to continuation of tranquility.

The quartic potential problem has been treated by a number of authors, but mostly within time independent frameworks [1]. There have been treated aspects like the spectrum and tunnelling [2]. As far as we are aware the case of low energy fluctuations has not been dealt with. In what follows we proceed in a time dependent fashion which enables treatment of both temporal and spatial fluctuations.

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2. Evolution of the wavefunction

We begin by considering the one dimensional double well expressed by

$$U = \frac{m\omega^2}{2}\left(x^2 - \frac{x^3}{a} + \frac{x^4}{4a^2}\right) \tag{2.1}$$

which represents, as shown in Fig.1, joined wells with minima located at x=0 and x=2α. These wells in the vicinity of their bottoms can be approximated by oscillator potentials associated with natural frequency ω. This situation allows use of the lowest energy eigenfunction as an initial state in the present investigation for such a wavefunction leads to zero current density on one hand and on the other provides a probability density locating the particle at the bottom of the well. We choose for our evaluations the l.h.s. well, and we have

$$\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{2.2}$$

With (2.2) as initial state the required wavefunction $\Psi(x,t)$ is governed by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\Psi(x,t) \tag{2.3}$$

To facilitate both the ensuing symbolic and numerical evaluations we switch at this stage to dimensionless quantities. The pertaining units of time, length and energy are respectively ω^{-1}, $\ell=(\hbar/m\omega)^{1/2}$ and $\hbar\omega$. We now introduce the corresponding dimensionless quantities for time and lengths as

$$\tau=\omega t \quad , \quad A=a/\ell \quad , \quad y=x/\ell$$

Denoting the intitial and evolving wavefunctions in terms of the dimensionless time and the spatial coordinate y by $Y_o(y)$ and $Y(y,\tau)$ we express the wavefucntion as

$$Y(y,\tau) = Y_o(y)\, P(y,\tau), \qquad Y_o=(\pi\ell^2)^{-1/4} \exp(-y^2/2) \tag{2.4}$$

Introducing (2.4) into (2.3) with the appropriate changes in variables ($t\longrightarrow\tau$, $x\longrightarrow y$) we obtain the equation of motion for P as

$$i\frac{\partial P}{\partial \tau}+\left(\frac{1}{2}\frac{\partial^2}{\partial y^2}-y\frac{\partial}{\partial y}\right)P=u(y)P \tag{2.5}$$

where

$$u=-\frac{y^3}{2A}+\frac{y^4}{8A^2} \tag{2.5a}$$

For obtaining the required wavefunction (2,4), (2.5) must be solved under the initial condition $P(y,0)=1$. It is now clear that the solution for P takes the form of a power series in y with time dependent coefficients. Furthermore we can carry out an iterative solution of (2.5) analytically.

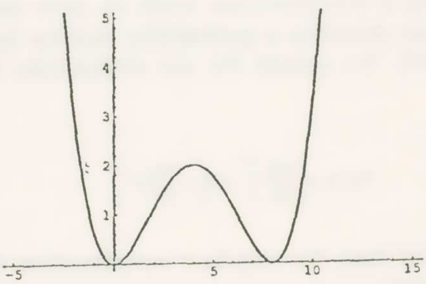

Figure 1. Symmetric double well. Minima at 0 and 8ℓ. Horizontal axis in units ℓ. Vertical axis in units $\hbar\omega$.

The iteration starts with $P_0=1$ on the r.h.s. of (2.5) and produces $P_1(y,\tau)$ under the initial condition $P_1=(y,0)=0$. The procedure is repeated in the usual manner using P_j on the r.h.s. and obtaining the next iterant P_{j+1}. In this way the required solution can be approximately obtained as

$$P(y,\tau)=1+P_1(y,\tau)+P_2(y,\tau)+.... \tag{2.6}$$

As we go higher in the hierarchy the further we extend the length of time over which the solution is valid.

For obtaining the various terms $P_j(y,\tau)$ we have devised a program in the Mathematica System utilizing symbolic computation. These terms are polynomials in y with coefficients expressed as terminating Fourier series. The first couple of terms P_j are of limited length, but the size and complexity increase considerably for larger j and we see no point in writing down explicit expressions. In the computations which follow in the next Section we have used the first 5 terms in (2.6) and tested the validity of the approximation by considering the deviation of the approximate probability of finding the particle everywhere from unity.

3. Charge and current densities

Having at hand an expression for the evolving wavefunction we can, utilizing standard procedures, write down the formulae for the charge and current densitiew which in the present case take the form

$$\rho(y,\tau) = \left(\frac{e}{\ell}\right)|P(y,\tau)|^2 \pi^{-1/2} \exp(-y^2) \tag{3.1}$$

$$j(y,\tau) = (e\omega)\,\mathrm{Re}\left[-iP^*\left(\frac{\partial P}{\partial y} - y\right)\right]\pi^{-1/2} \exp(-y^2) \tag{3.2}$$

(e/ℓ) is the unit for charge density and $(e\omega)$ the unit for current density.

The above formulae enable us to provide a few diagrammes giving the evolution of the charge and current densities at certain locations as they vary with time as well as frames of the corresponding spatial distributions at different times, as depicted in Fig 2,3,4,5 and 6.

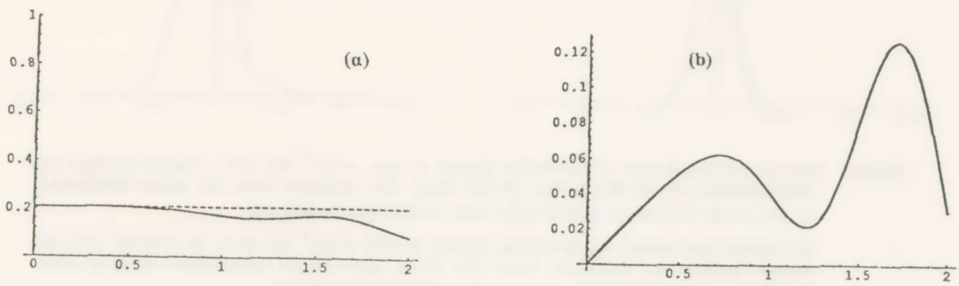

Figure 2. (a) Variation of the charge density (continuous line) with time at position x=-ℓ for a=4ℓ (A=4) about the corresponding initial value (dashed line). Horizontal axis in units of time $1/\omega$ and vertical axis in units e/ℓ.

(b) Evolution of the current density at position x=-ℓ for A=4. The current density rises signifiantly from its initial value zero and fluctuates. Horizontal axis in units $1/\omega$ and vertical axis in units $e\omega$.

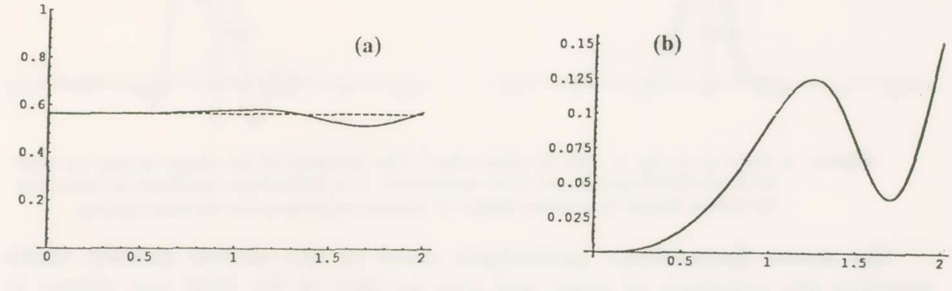

Figure 3. Same as in Fig. 2, but for location x=0

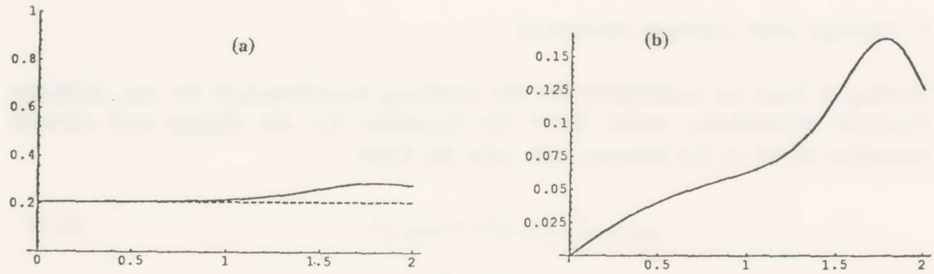

Figure 4. Same as in Fig. 2, but for location x=ℓ.

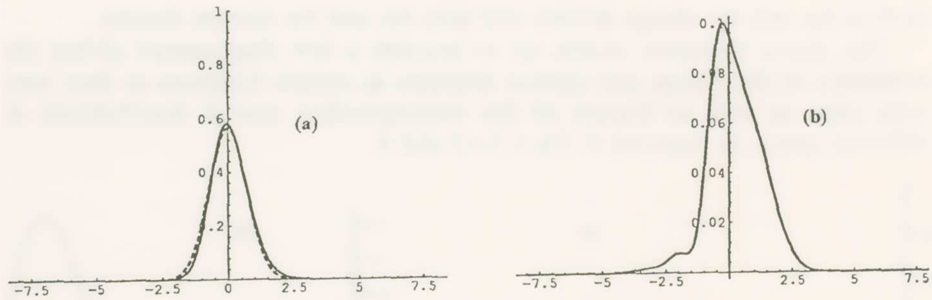

Figure 5.(a) Spatial distribution of the current density at time $t=1\omega^{-1}$ for A=4 (continuous line) and corresponding initial distribution (dashed line). The deviation from the initial distribution is very small. Horizontal axis in units ℓ and vertical axis in units e/ℓ.

(b) Spatial distribution of the current density at time $t=1\omega^{-1}$ for A=4. In contrast with the charge density the deviation from the initial distribution (everwhere zero) is now significant. Horizontal axis in units ℓ and vertical axis in units $e\omega$.

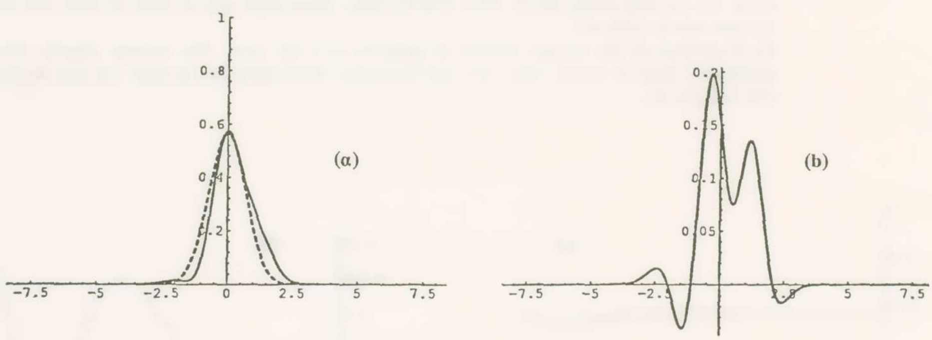

Figure 6. Same as in Fig. 5, but for time $t=2\omega^{-1}$. The deviation of the charge density (a) from its initial distribution is now more pronounced. It is furthermore significant to notice that the current density (b) exhibits regions of opposite movements for the same electron.

The above fluctuations, particularly these of the current density, make manifest the existence of noise and give an idea of the what can expect in quantum semiconductor devices (submicron region) emanating from the dynamics exploited for their operation.

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2. Dekker H., Phys. Rev. A **35**, 1825, 1987.

ΠΕΡΙΛΗΨΗ

Διακυμάνσεις πυκνότητας φορτίου καὶ ρεύματος σὲ διπλὴ κβαντικὴ κοιλάδα.

Σύμφωνα μὲ τὴν κλασσικὴ μηχανική, σωματίδιο ποὺ βρίσκεται στιγμιαῖα μὲ μηδενικὴ ὁρμὴ σὲ ἐλάχιστο δυναμικοῦ θὰ παραμείνει ἀκίνητο γιὰ πάντα. Ἡ ἐγγύτερη κατάσταση στὴν κβαντικὴ μηχανικὴ πρὸς τὶς πιὸ πάνω ἀρχικὲς συνθῆκες δίνεται ἀπὸ μιὰ κυματικὴ συνάρτηση ποὺ παρέχει μηδενικὴ πυκνότητα ρεύματος, πιθανότητα εὑρέσεως τοῦ σωματιδίου ἐπικεντρωμένη συμμετρικὰ περὶ τὴ θέση ἐλαχίστου δυναμικοῦ καὶ κατὰ τὸ δυνατὸ ἐλάχιστη ἐνέργεια. Σὲ ἀντίθεση μὲ τὴν κλασσικὴ μηχανικὴ ἡ ἐξέλιξη τῆς κινήσεως μὲ τὴν πάροδο τοῦ χρόνου ὁδηγεῖ σὲ χωρικὲς καὶ χρονικὲς διακυμάνσεις τῶν πυκνοτήτων πιθανότητας καὶ ρεύματος. Στὴν προκείμενη μελέτη ὑπολογίζονται τέτοιες διακυμάνσεις γιὰ ἕνα ἠλεκτρόνιο σὲ διπλὴ κοιλάδα δυναμικοῦ ὅταν ἡ ἀρχικὴ κβαντικὴ κατάσταση προσιδιάζει πρὸς τὴν ἀντίστοιχη κλασσικὴ κατὰ τὴν ὁποίαν ἡ ἠρεμία ἐπακολουθεῖ. Οἱ ἐν λόγῳ διακυμάνσεις παρέχουν μία ἁδρομερὴ ἐκτίμηση τοῦ θορύβου ποὺ μπορεῖ νὰ ἀναμένεται σὲ ἡμιαγωγικὲς διατάξεις κβαντικῆς λειτουργίας στὴν κάτω τοῦ μικροῦ περιοχή.