CHAOS IN MANY BODY QUANTUM SYSTEMS

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Abstract

A many body quantum system undergoing multiple resonant tunneling in a double barrier heterostructure is studied within a mean field approximation. The resulting nonlinear Schrödinger equation shows genuine chaos with a positive maximum Lyapunov exponent. A simplified model of the same system suggests that chaos develops only if the interaction among the particles is nonuniform in space.

1. Introduction

The quantum mechanical behavior of systems with a finite number of degrees of freedom whose classical dynamics is chaotic has attracted a considerable interest in recent years[1]. Due to the linearity of Schrödinger equation the classical properties of such systems, e.g. local exponential instability of motion, are lost at quantum level[2]. Nevertheless the Wigner distribution for random matrices[3] is believed to characterize the energy level spacing distribution of these systems while the Poisson distribution is typical of classically nonchaotic systems[4,5].

Recently we have suggested the possibility of observing true chaotic behavior, not necessarily present at the classical level, in a many body quantum system, that is a quantum system with infinitely many degrees of freedom[6]. The system is a cloud of electrons (in principle infinitely extended at least in one direction) moving in a resonant tunneling heterostructure[7]. The electron-electron interaction is taken into account by a mean field approximation. Within this approximation the Schrödinger

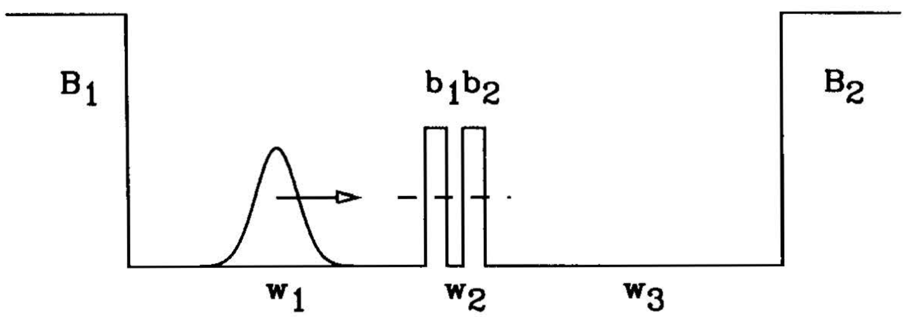

Figure 1: Energy diagram of a three-well two-barrier heterostructure. The barriers b_1 and b_2 separated by the well w_2 produce a resonance in the currents between wells w_1 and w_3 at the energy indicated by the dashed line. An electron cloud is initially localized in the well w_1 and moves toward the well w_3 with a mean kinetic energy close to the resonance.

equation describing the system, still being norm and energy conserving, becomes nonlinear[8]. In this case the evolution is characterized by positive Lyapunov exponents.

The analysed resonant tunneling system, which we will call the quantum capacitor hereafter, needs a considerable computational effort. A relevant simplification is achieved in a few-site hopping model which mimics the chaotic properties of the quantum capacitor. The analysis of this simplified model indicates that a chaotic behavior is established only when the nonlinear interaction term is nonuniform in the sites.

The plan of the paper is the following. The quantum capacitor is described in section 2 while its simplified version is introduced in section 3. This section covers unpublished results obtained in the spring 1992. Simplified models of a many body system similar to our quantum capacitor were later investigated by Berkovits from the standpoint of spectral properties[9]. This aspect is briefly recalled in section 4.

2. The quantum capacitor

Interaction among the electrons can play a crucial role in electrical transport properties of mesoscopic systems[10]. We have suggested as an example electrons moving in a double barrier heterostructure in which the well region confined between two potential barriers acts like a capacitor whose energy changes according to the electron charge trapped in it[11]. We emphasize that the localization of the interaction is justified only due the existence of a resonance state which permits a long sojourn time inside the double barrier and therefore an accumulation of charge. A slightly modified system, namely a closed three-well two-barrier heterostructure like that sketched in Fig. 1, is suitable to study the chaotic properties of a cloud of interacting electrons. Initially the electrons are localized in one of the large wells and move toward the internal double barrier giving rise to reflected and transmitted currents which reenter this sort of billiard after total reflection by the external large barriers.

The exact time evolution of the depicted system can be written in terms of the anticommuting field operator associated to the electron cloud

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(x) + \int \frac{e^2}{\varepsilon|\vec{r}-\vec{r}\,'|}\hat{\Psi}^\dagger(\vec{r}\,',t)\hat{\Psi}(\vec{r}\,',t)\, d\vec{r}\,'\right]\hat{\Psi}(\vec{r},t) \quad (1)$$

where the external potential $V(x)$ shown in Fig. 1 depends only on the coordinate x orthogonal to the interfaces. As argued in Ref. 11 we can assume a decoupling between the degrees of freedom parallel and orthogonal to the interfaces and set up an approximate description in terms of a Hartree equation for a one particle wave function which depends only on the orthogonal coordinate. More precisely we factorize the single particle mean field in the following way

$$\Psi(\vec{r},t) \equiv \langle\hat{\Psi}(\vec{r},t)\rangle/\sqrt{N} \simeq \psi(x,t)\phi(y,z)e^{-\frac{i}{\hbar}E_{\|}t} \ . \quad (2)$$

where $\langle\ldots\rangle$ means expectation in the many body state at time t; N is the number of electrons in the cloud; $\phi(y,z)$ is a normalized solution of the free particle Schrödinger equation in the plane parallel to the interfaces. We consider the interaction term effective only inside the well w_2 and we approximate it by the expression

$$\int \frac{e^2}{\varepsilon|\vec{r}-\vec{r}\,'|}N|\psi(x',t)|^2|\phi(y',z')|^2\, d\vec{r}\,' \simeq \alpha\chi_{w_2}(x)Q(t) \quad (3)$$

where $\chi_S(x)$ is the characteristic function of the set S, i.e. $\chi_S(x) = 1$ if $x \in S$, 0 otherwise. The constant α is Ne^2/C where C summarizes the result of the integration on the plane yz and an averaging of the potential over the width of the well w_2. Dimensionally C is a length and defines the capacitance of the double barrier;

$$Q(t) = \int_{w_2} |\psi(x,t)|^2\, dx \quad (4)$$

is the adimensional charge trapped in the well w_2 at time t. Within the above approximations we get the following one-dimensional nonlinear Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + \alpha\chi_{w_2}(x)Q(t)\right]\psi(x,t) \quad (5)$$

which describes the dynamics of our quantum capacitor. Equation (5) has two conserved quantity, namely the norm

$$\int \psi(x,t)^*\psi(x,t)\, dx \quad (6)$$

and the energy

$$\int \psi(x,t)^*\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t)\, dx + \frac{1}{2}\alpha Q(t)^2 \ . \quad (7)$$

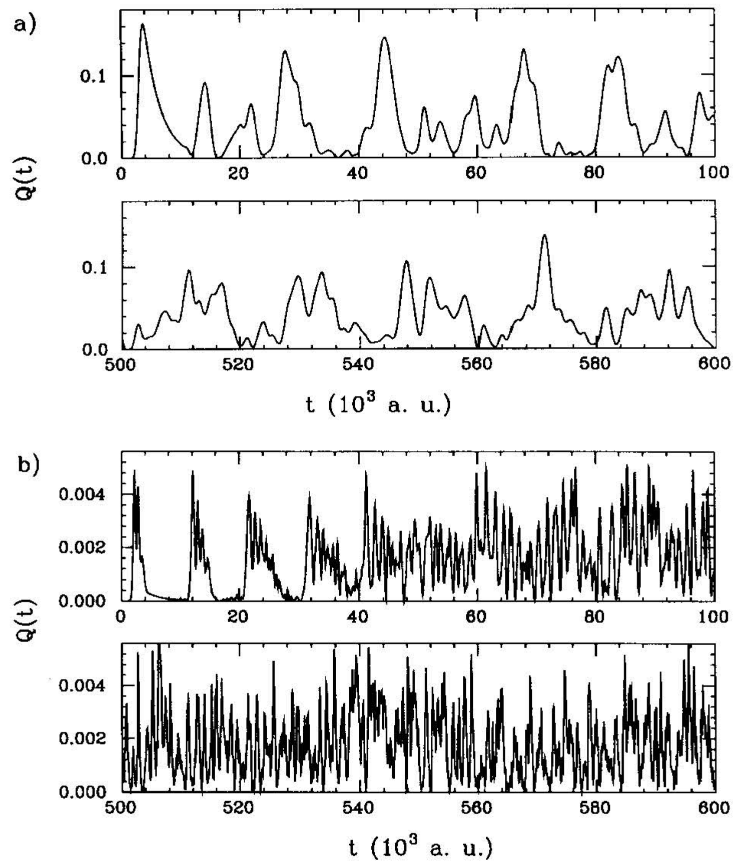

Figure 2: Time evolution of the charge $Q(t)$ for $\alpha = 0$ (a) and $\alpha = 3$ Ry (b). An atomic unit of time corresponds to 4.83×10^{-17} s.

We analyze the behavior of the charge $Q(t)$ for different choices of α. As an example we show in Fig. 2 the results obtained by numerically integrating Eq. (5) for $\alpha = 0$ and $\alpha = 3$ Ry. (for a more detailed description see Ref. 6). Due to the infinite number of eigenvalues of the associated stationary Schrödinger equation, in the linear case $\alpha = 0$ the charge $Q(t)$ has a complicated quasiperiodic behavior. In the interacting case $\alpha = 3$ we have a qualitatively different behavior. Already at small times, corresponding to the first few passages of the electron cloud through the device, we observe a series of rapid oscillations (10^{-13} s). The origin of these oscillations is discussed in detail elsewhere[11,12]. The number of oscillations increases progressively in time until an apparently irregular motion sets in.

Characterization of the different behaviors observed in Fig. 2 can be obtained by analyzing the local exponential instability. Let us consider two different initial

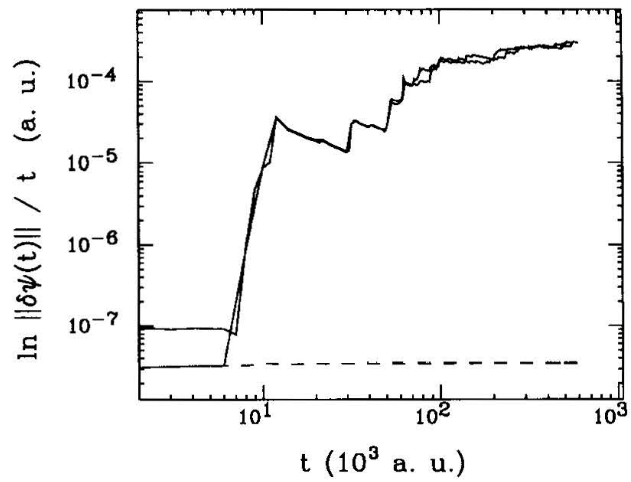

Figure 3: Behavior of $\ln\|\delta\psi(t)\|/t$ as a function of time for $\alpha = 0$ (dashed line) and for $\alpha = 3$ Ry (two solid lines corresponding to different initial conditions).

wave functions $\psi(x,0)$ and $\psi(x,0)+\varepsilon\delta\psi(x,0)$ with ε small. We define the maximum Lyapunov exponent λ in the usual manner

$$\lambda = \lim_{t\to\infty}\frac{1}{t}\ln\frac{\|\delta\psi(t)\|}{\|\delta\psi(0)\|} \tag{8}$$

so that if $\lambda > 0$ we have an exponential growth of the difference $\|\delta\psi(t)\|$ between the two initially chosen wave functions. An equation of motion for $\delta\psi(x,t)$ is obtained by varying Eq. (5) with respect to ψ and its complex conjugate ψ^*

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\delta\psi(x,t) &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)+\alpha\chi_{w_2}(x)Q(t)\right]\delta\psi(x,t)+\alpha\chi_{w_2}(x)\psi(x,t)\times \\ & \left[\int_{w_2}\psi(x',t)^*\delta\psi(x',t)\,dx'+\int_{w_2}\delta\psi(x',t)^*\psi(x',t)\,dx'\right] . \end{aligned} \tag{9}$$

Note that if $\alpha = 0$ this equation reduces to the usual Schrödinger equation and the norm of $\delta\psi$ is conserved. In the linear case the maximum Lyapunov exponent vanishes. On the other hand when $\alpha > 0$ the norm of $\delta\psi$ is not conserved and a positive Lyapunov exponent can eventually be found.

The results obtained by numerically integrating both Eq. (5) and Eq. (9) are shown in Fig. 3; $\delta\psi(x,0)$ is normalized to unity and orthogonal to $\psi(x,0)$. As predicted, in the linear case the Lyapunov exponent vanishes within the numerical accuracy. In the nonlinear case two very different initial conditions, namely $\delta\psi(x,0)$ localized in the well w_2 or w_3, show similar long time behavior. A true asymptotic regime is not reached within the maximum time investigated, however, a developing chaos with marked exponential instability is well established. The value of the maximum Lyapunov exponent readable from Fig. 3 compares to the inverse decorrelation time observed for the charge $Q(t)$[6].

3. A minimal model

The numerical solution of Eq. (5) is obtained by a finite difference method in which each well or barrier region is represented by a large number of points adequate to reproduce the continuum limit. We now describe simple models which preserve some of the features of Eq. (5), in particular the chaotic behavior. The idea is to introduce one site for each region of constant potential. This leaves us with a system of five complex functions of time. However a minimal model of three sites with the nonlinearity concentrated only in one of them is sufficient. Two methods can be used to close the system. The three sites are thought to lie inside an infinitely deep well or periodic boundary conditions are imposed and a ring geometry is realized. In the first case the quantum capacitor is represented by the following system of ordinary differential equations

$$\begin{aligned} i\hbar\frac{d}{dt}\psi_1(t) &= -\frac{\hbar^2}{2m\Delta x^2}\left(2\psi_1-\psi_2\right) \\ i\hbar\frac{d}{dt}\psi_2(t) &= -\frac{\hbar^2}{2m\Delta x^2}\left(2\psi_2-\psi_1-\psi_3\right)+V_2\psi_2 \\ i\hbar\frac{d}{dt}\psi_3(t) &= -\frac{\hbar^2}{2m\Delta x^2}\left(2\psi_3-\psi_2\right)+\alpha|\psi_3|^2\psi_3 \end{aligned} \tag{10}$$

where ψ_n, $n=1,2,3$, are the wave functions in the three sites and $|\psi_3|^2$ is the charge trapped in the interacting site. V_2 can be interpreted as a potential barrier separating the sites 1 and 3.

By the transformation $\psi_n=(q_n+ip_n)/\sqrt{2}$ Eq. (10) is mapped into a classical system with generalized coordinates q_n and momenta p_n. This system has three degrees of freedom and two integrals of motion corresponding to conservation of norm and energy as in the continuum limit. Therefore the model represented by Eq. (10) is minimal in the sense that no chaotic features could appear for a two-site system.

The chaotic properties of the minimal model of Eq. (10) are studied by evaluating the maximum Lyapunov exponent analogously to the continuum system. The equation of motion for the difference $\delta\psi_n$ is obtained by linearizing the system of Eq. (10)

$$\begin{aligned} i\hbar\frac{d}{dt}\delta\psi_1(t) &= -\frac{\hbar^2}{2m\Delta x^2}\left(2\delta\psi_1-\delta\psi_2\right) \\ i\hbar\frac{d}{dt}\delta\psi_2(t) &= -\frac{\hbar^2}{2m\Delta x^2}\left(2\delta\psi_2-\delta\psi_1-\delta\psi_3\right)+V_2\psi_2 \end{aligned} \tag{11}$$

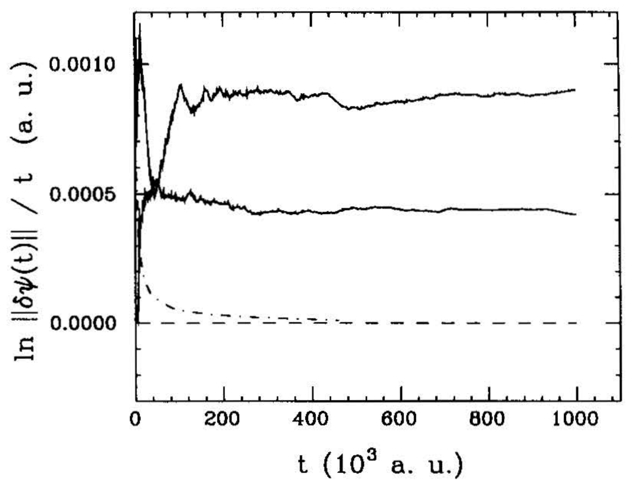

Figure 4: Behavior of $\ln\|\delta\psi(t)\|/t$ as a function of time for the three site system. The dashed line is the non interacting case $\alpha = 0$ while for the other curves an interaction with $\alpha = 3$ Ry has been taken into account in all the sites (dot-dashed line) or only in one site with (upper solid line) or without (lower solid line) a barrier potential.

$$i\hbar\frac{d}{dt}\delta\psi_3(t) = -\frac{\hbar^2}{2m\Delta x^2}\left(2\delta\psi_3 - \delta\psi_2\right) + \alpha|\psi_3|^2\delta\psi_3 + \alpha\psi_3(\delta\psi_3\psi_3^* + \psi_3\delta\psi_3^*) \ .$$

The results of the numerical integration of Eq. (10) and Eq. (11) are shown in Fig. 4. The maximum Lyapunov exponent vanishes in the noninteracting case while it is strictly positive when the interaction is concentrated in one site. From a mathematical point of view the presence of the barrier is not relevant for observing chaos. In fact when $V_2 = 0$ the maximum Lyapunov exponent decreases with respect to the case $V_2 > 0$ but it is still positive. However, from a physical point of view only the presence of a barrier region allows to consider space regions with different interaction properties and a spatial nonuniform interaction seems to be crucial for observing chaos. In fact spatial uniformity is restored by considering a non linear interaction term of the type $\alpha|\psi_n|^2\psi_n$ at each site n. In this case, with or without an added external potential V_n, we observe a behavior like that shown by the dot-dashed line in Fig. 4. After an initial positive transient the function defining the maximum Lyapunov exponent asymptotically vanishes. This behavior is confirmed also by studying the correlation functions of the charge in one site. Strong decorrelation appears in the case of a spatial nonuniform interaction while correlation is retained when interaction is effective in all the sites.

4. Concluding remarks

The main theme of this paper is the conjecture that a quantum system with infinitely many degrees of freedom can evolve chaotically. In this perspective it would be very interesting to show, by solving exactly the motion of a large but finite system, that complex behavior increases when the number of degrees of freedom increases, as suggested by the mean field approximation.

Recently Berkovits has investigated a hopping Hamiltonian describing a 10 site ring with 5 spinless electrons[9]. He studied the same three distinct cases we have discussed with our minimal model. Electrons are noninteracting; they interact everywhere in the ring through a Coulomb-like potential; the interaction is restricted to a couple of sites representing a well region between two potential barriers. In each case the quasi-particle energy spectrum of the many body system was evaluated numerically without any approximation. The resulting energy level spacing distribution shows interesting features. In the noninteracting case as well as in the interacting case with spatial uniform interaction the distribution is compatible with the Poisson distribution. In the interacting case with interaction restricted to the well region the distribution is more Wigner-like (GOE).

Our conjecture and mean field results combined with Berkovits' findings suggest a possible connection between the spectral properties of a quantum system and its tendency to show chaotic behavior when the number of degrees of freedom increases.

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