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Quantum Chaos Without Classical Counterpart

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Abstract

We describe a quantum many-body system undergoing multiple resonant tunneling which exhibits chaotic behavior in numerical simulations of a mean field approximation. This phenomenon, which has no counterpart in the classical limit, is due to effective nonlinearities in the tunneling process and can be observed in principle within a heterostructure.

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In current studies the problem of quantum chaos is usually posed in the following terms. We are given a system which exhibits chaotic behavior classically: does this property survive quantization? Typically one studies the spectrum of the quantum mechanical Hamiltonian operator. However spectral differences at the quantum level between classically integrable and chaotic systems do not seem to imply dramatic differences in the time evolution of the quantum mechanical observables. Relics of classical chaos exist in low dimensional systems in short wavelength or large quantum numbers limits where the discrete quantum spectrum approximates a continuous spectrum. Persistent chaotic behavior in the evolution of the observables however does not seem possible [1].

In this paper we propose to explore the opposite road by asking the following question: is it possible to have quantum chaos, transient or persistent, independently of what happens in the classical limit? To tackle this question we observe that another way of approximating a continuous spectrum is by increasing the number of degrees of freedom of the system, that is by considering a many body system. It is well known that under appropriate conditions a many body system can be approximately described in terms of a single particle wave function obeying a nonlinear and nonlocal Schrödinger equation (Hartree or Hartree-Fock equations). The importance of effective nonlinearities due to the particle interaction in concrete cases has been emphasized in our previous paper [2] where we showed that nonlinear quantum oscillations can be present in resonant tunneling of electrons through a double barrier heterostructure [3]. The situation studied in Ref. [2] represented a transient phenomenon because we dealt with an open system. In the present paper we consider the same system enclosed between two potential barriers. In other words we deal now with a cloud of electrons moving in a three well heterostructure (see later). In this way our Hartree-like equation describing the motion of the cloud represents a confined non dissipative system which may be ergodic or even mixing at least in some regions of its phase space and which therefore may exhibit irregular behavior during its evolution. Two points should be emphasized: *i)* chaos is found numerically in a mesoscopic variable, the electric charge in a well, which is in principle experimentally observable [4], *ii)* the phenomenon we describe has no classical analogue being based on resonant tunneling.

As in our previous work we consider the quantum transport of electrons through a double barrier via resonant tunneling. However in the present case the heterostructure is shaped in such a way that the system is closed. The situation is described in Fig. . An electron cloud is initially created in one of the large wells with a kinetic energy peaked around the resonance energy of the double barrier. As discussed in Ref. [2] we may reduce ourselves to one dimensional propagation along the x axis orthogonal to the heterostructure junction planes. We describe the state of the electrons with a one particle wave function obeying a nonlinear Hartree equation [2]. The effect of the nonlinearity depends strongly on the materials in the heterostructure regions. We assume that the wells w_1 and w_3 consist of a heavily doped semiconductor so that in these regions the nonlinearity can be neglected during the time evolution of the system, while the barriers b_1 and b_2 and the well w_2 are undoped semiconductors [5]. When a fraction of the charge penetrates inside the double barrier, the resonance is shifted and the nonlinear charge oscillations described in Ref. [2] appear. The reflected and transmitted charges in regions w_1 and w_3 after some time will return to the double barrier and a fraction of them will penetrate inside the well w_2 depending on the height of the resonance at that moment. We expect that after a few cycles the charge in w_2

will show a very complicated time dependence losing memory of how the process initiated.

Let us now turn to the mathematical model of the system. The external potential, as depicted in Fig. , is assumed to be a step function (no electric field is applied):

$$V(x) = V_0\Big[\chi_{b_1}(x) + \chi_{b_2}(x)\Big] + V_1\Big[\chi_{B_1}(x) + \chi_{B_2}(x)\Big] \tag{1}$$

where V_0 and V_1 are positive constants (*i.e.* the height of the barriers b_1, b_2 and B_1, B_2 respectively) with $V_1 > V_0$ and χ_S is the characteristic function of the set S (*i.e.* $\chi_S(x) = 1$ if $x \in S$, 0 otherwise).

As in Ref. [2] we simplify the shape of the nonlinear term by considering a rigid displacement of the well w_2. This looks legitimate because the essential effect of the nonlinearity is the displacement of the resonance energy and in addition this choice simplifies enormously the numerical calculation. On the other hand we have verified that a more precise calculation using a screened Coulomb potential does not modify in any important feature the dynamics of the system. The nonlinear Schrödinger equation describing the evolution of the electron cloud wave function is therefore:

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

where $Q(t)$ is the charge inside the well w_2 at time t

$$Q(t) \equiv \int_{w_2} |\psi(x,t)|^2\, dx \tag{3}$$

In these notations $\psi(x,t)$ is normalized to 1, $Q(t)$ is dimensionless and α has the dimension of an energy and measures the strength of the mean field acting on each electron. The parameter α is proportional to the transversal areal density of the electrons and depends on the electric capacitance of the double barrier.

The 1-particle state which is the initial condition in the mean field equation has been chosen to be a gaussian shaped superposition of plane waves with mean momentum $\hbar k_0$:

$$\psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}}\exp\left[-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2 + ik_0x\right] \tag{4}$$

x_0 is chosen to coincide with the middle point of the well w_1 which has a width so large with respect to σ that at the initial time no appreciable charge sits in w_2, i.e. $Q(0) \simeq 0$.

The choice of the various parameters has been made on the basis of the results obtained in Ref. [2]. Their values correspond to a situation in which nonlinear oscillations in the transient regime are enhanced. We consider $|w_1| = |w_3| = 1100\ a_0$, $|w_2| = 15\ a_0$, $|b_1| = |b_2| = 20\ a_0$, $\sigma = 110\ a_0$ ($a_0 \simeq 0.529$ Å, being the Bohr radius), $V_0 = 0.3\ eV$. The mean kinetic energy of the initial state is equal to the resonance energy ($E_R \simeq 0.15\ eV$) of the double barrier b_1-b_2. The width of the two external barriers $|B_1| = |B_2| = 440\ a_0$ and their height $V_1 = 0.9\ eV$ assure the complete confinement of the electron cloud between them.

The solution of the differential equation (2) with the initial condition (4) has been achieved by a numerical integration on a suitable two-dimensional lattice, taking into account the remarks of Ref. [6].

Now we report the results of the numerical simulations and we provide an analysis which shows that in our system a chaotic behavior develops during its evolution. We concentrate on the charge $Q(t)$ and we treat it as if it were an experimental signal. A mathematical study of the system is deferred to another publication.

In Fig. we show the behavior of $Q(t)$ as a function of time in two different widely separated time intervals. The first structure appearing between $t = 0$ and $t = 10$ (everywhere we use as time unit 10^3 atomic units of time $\simeq 4.83\ 10^{-14}$ s), reproduces exactly the transient behavior explored in Ref. [2]. Between $t = 10$ and $t = 40$ we observe a qualitative repetition of almost the same structure due to the multiple reflections of the wave packet inside the large wells w_1 and w_3. The number of oscillations per structure increases progressively until, after $t = 40$ the isolated structures tend to disappear and an apparently irregular motion sets in. The irregularity increases with time as it is evident from the behavior of $Q(t)$ between $t = 500$ and $t = 600$. This suggests an approach to a stationary state as also evidenced in Fig. where the evolution of the mean charge $\langle Q \rangle_t \equiv t^{-1} \int_0^t Q(t')\ dt'$ is reported. It is clear that a true stationary state is not yet reached at $t = 600$ but the approach at this stage is already very slow so that one can safely speak of quasi equilibrium.

Concerning the attainment of quasi equilibrium a crucial question is what happens if the initial conditions are varied. In the case of an energetically equivalent initial condition the same quasi equilibrium state is reached. An example is shown in Fig. where the dashed curve refers to an initial condition in which the single electron cloud of Fig. is replaced by two equal half-density electron clouds moving from the wells w_1 and w_3. When the initial conditions are energetically nonequivalent the asymptotic behavior changes. For instance, we have examined the case of an initial cloud with mean energy below the resonance energy. In this case the mean charge $\langle Q \rangle_t$ tends to a lower asymptotic limit and the irregular variation of the charge $Q(t)$ in the time interval considered is less pronounced. This is due to a reduced charge accumulation in the well w_2 and therefore to a weakening of the nonlinearity. A more systematic study of the dependence of the phenomenon on the initial conditions will be presented in a forthcoming paper.

We now show that the irregular behavior we have found has all the features of chaotic behavior by estimating commonly used indicators like correlation functions, power spectra, information dimension and entropy [7].

We examine first the autocorrelation function $C(t) \equiv \int_T q(t')q(t'+t)\ dt' \ / \int_T q(t')q(t')\ dt'$ of the zero-mean charge $q(t) \equiv Q(t) - |T|^{-1} \int_T Q(t')\ dt'$. In Fig. we give for comparison the autocorrelation function calculated in the time interval $T = [100, 600]$ for the linear and nonlinear case respectively. The difference is striking. In the nonlinear case we have a short correlation time followed by small oscillations around zero. The interpretation of these oscillations is not immediate. In part they reflect the complicated dynamics of the system and in part are a noise effect which tends to disappear when the interval T is enlarged. Furthermore a preliminary analysis shows that when the parameter α measuring the strength of the nonlinearity decreases these oscillations increase in amplitude and their characteristic times become comparable to those of linear case. A rather sharp transition seems to take place in the region of values of α in which the transient oscillations observed in our previous work [2] disappear.

In order to study the approach of the system to the true equilibrium state we chose to calculate the chaotic indicators in two different time intervals $T_1 = [180, 260]$ and $T_2 =$

$[480, 560]$ where $\langle Q \rangle_t$ is almost constant and has a slightly different value. Between these two intervals we observe a reduction of the correlation time τ. We have $\tau = 0.28$ in T_1 and $\tau = 0.25$ in T_2. This fact is also reflected in the behavior of the power spectrum $P(\omega)$ reported in Fig. . Going from T_1 to T_2, in fact we see an evident increase of the spectrum flatness.

We have next calculated the information dimension $\dim_H \rho(T_{1,2})$ where $\rho(T_{1,2})$ is the quasi equilibrium measure associated with the evolution of our system during the intervals T_1 and T_2. We have used the Grassberger-Procaccia algorithm [8]. As expected from the results of Ref. [9] $\dim_H \rho$, *i.e.* the slope of the straight lines in Fig. , has a non integer value increasing slowly with time from 2.20 ± 0.05 in the first interval to 2.50 ± 0.05 in the second interval. The straight line behavior of $\log N(r)$ versus $\log(r)$ is absent in the linear case. ¿From the same data of Fig. we can compute the order-2 Renyi entropy $K_2(\rho)$, a lower bound for the Kolmogorov-Sinai entropy, by an extrapolation process to infinite embedding dimension d [8]. For both time intervals we obtain for $K_2(\rho)$ a positive value of the order of magnitude of the inverse correlation time τ^{-1} in agreement with the remarks of Ref. [10].

The example we have discussed raises several problems. The relationship of the one dimensional Hartree approximation to an exact treatment of the three dimensional many electron system was briefly discussed in our previous paper [2], but has to be analysed further. This is crucial for the following reasons. Let us assume that the chaotic behavior found numerically is persistent in time and is a feature of our nonlinear Schrödinger equation that can be proved rigorously. In general this does not imply that the many body system of which the nonlinear Schrödinger equation (2) is an approximate description exhibits persistent chaos. In fact, if we view the equation (2) as an approximation to a one dimensional many body system, the latter will have discrete spectrum due to the fact that the number of particles must remain finite (the system is confined) in order to have a finite density. According to the accepted wisdom this is compatible with transient chaos, possibly persisting over a long time interval. However, our real heterostructure system is *three dimensional* and can be considered infinite in the transversal directions. This means that the physical system should be characterized in this limit by a continuous spectrum due to the electron-electron interaction which couples the longitudinal and transversal variables. In these conditions persistent chaos is not forbidden.

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FIGURES

Energy diagram of the three-well two-barrier heterostructure considered in the present paper. 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.

Time development of the charge $Q(t)$ in the case $\alpha = 3$ Ryd. An atomic unit of time corresponds to $4.83\ 10^{-17}$ s.

Time development of the mean charge $\langle Q \rangle_t$ from the data of Fig. (solid line). The dashed line represents the case where the starting single electron cloud of Fig. is replaced by two equal half-density electron clouds moving from the wells w_1 and w_3.

Normalized time autocorrelation function $C(t)$ of the zero-mean charge from the data of Fig. (solid line). The dot-dashed line represents the corresponding linear case $\alpha = 0$.

Power spectrum $P(\omega)$ of the zero-mean charge from the data of Fig. in the two intervals $T_1 = [180, 260]$ and $T_2 = [480, 560]$.

Information dimension $\dim_H(\rho)$ in the two intervals T_1 and T_2 calculated by the slope of the straight line portion of the curves $\ln N(r)$ versus $\ln r$. $N(r)$ is the number of pairs of points $(Q(t), Q(t + \Delta t), ..., Q(t + (d - 1)\Delta t))$ with distance less than r in a d-dimensional embedding space with $d = 6, 8, 10, ..., 22$ (see Ref. [8]).