Chaotic Quantum Phenomena without Classical Counterpart

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(Received 27 January 1992)

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.

PACS numbers: 05.45.+b, 03.65.−w, 73.40.Gk

Heterostructures, besides offering very interesting new technological perspectives, represent a unique opportunity to study fundamental questions of quantum mechanics [1,2]. In a previous paper [3] we pointed out the possibility of effective nonlinearities due to many-body interactions in electron transport through resonant tunneling heterostructures. It is a natural question to ask whether such nonlinearities can give rise under appropriate conditions to chaotic behavior.

The situation studied in Ref. [3] 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 (see Fig. 1). In other words we deal now with a cloud of electrons moving in a three-well heterostructure. In a mean-field approximation the corresponding Hartree-like equation describing the motion of the cloud represents a confined nondissipative 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. Indeed we find chaotic behavior in a variable, the electric charge trapped in a well, which is in principle experimentally observable [4].

It is important to realize that in the phenomenon we consider, the phase of the wave function is a relevant dynamical variable. Resonant tunneling is possible only if the electrons remember their phase which, of course, may be different from electron to electron. Our case belongs to mesoscopic physics which deals with systems that are macroscopic but retain essential quantum features [2]. It has novel features which enrich the wealth of chaotic quantum phenomena already considered in the literature [5].

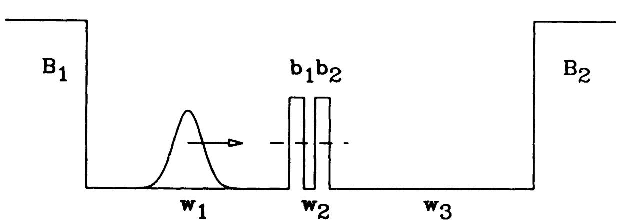

FIG. 1. Energy diagram of the three-well, two-barrier heterostructure considered in the present paper. The barriers b_1 and b_2 separated by the well w_2 produce a resonance in the currents between wells w_1 and w_3 at the energy indicated by the dashed line. An electron cloud is initially localized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

The heterostructure envisaged is described in Fig. 1. 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 b_1-b_2. Assuming, as discussed in Ref. [3], a factorization of the wave function of the electron cloud with respect to longitudinal and transversal degrees of freedom, we may reduce ourselves to one-dimensional propagation along the longitudinal direction, i.e., the direction x orthogonal to the junction planes of the heterostructure. This description, as shown in [3], is compatible with the Pauli principle. We represent the state of the electrons with a one-particle wave function obeying a nonlinear Hartree equation [3]. 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 [6]. When a fraction of the charge penetrates inside the double barrier, the resonance is shifted and the nonlinear charge oscillations described in Ref. [3] 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. 1, is assumed to be a step function (no electric field is applied):

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

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. [3] 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 enormously simplifies the numerical calculation. On the other hand, we have verified that a more precise calculation using a screened Coulomb potential does not modify any important feature of the dynamics of the system. The nonlinear Schrödinger equation describing the evolution of the electron cloud wave function is therefore

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

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

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

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 one-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 $\hbar k_0$:

$$\psi(x,0) = \frac{1}{(\sigma\sqrt{\pi})^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2 + ik_0 x\right]. \quad (4)$$

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. [3]. Their values correspond to a situation in which nonlinear oscillations in the transient regime are enhanced. We consider $|w_1| = |w_3| = 1100a_0$, $|w_2| = 15a_0$, $|b_1| = |b_2| = 20a_0$, $\sigma = 110a_0$ ($a_0 \simeq 0.529$ Å, being the Bohr radius), and $V_0 = 0.3$ 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 $|B_1| = |B_2| = 440a_0$ 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. [7].

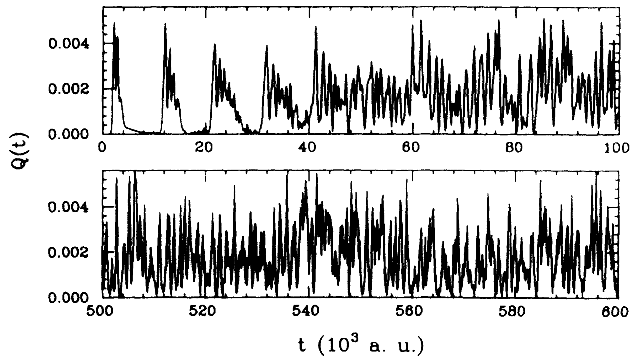

FIG. 2. Time development of the charge $Q(t)$ in the case $\alpha = 3$ Ry. An atomic unit of time corresponds to 4.83×10^{-17} s.

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. 2 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 10 (everywhere we use as the time unit 10^3 atomic units of time, $\simeq 4.83 \times 10^{-17}$ s), reproduces exactly the transient behavior explored in Ref. [3]. Between $t=10$ and 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 is evident from the behavior of $Q(t)$ between $t=500$ and 600. This suggests an approach to a stationary state as also evidenced in Fig. 3, where the

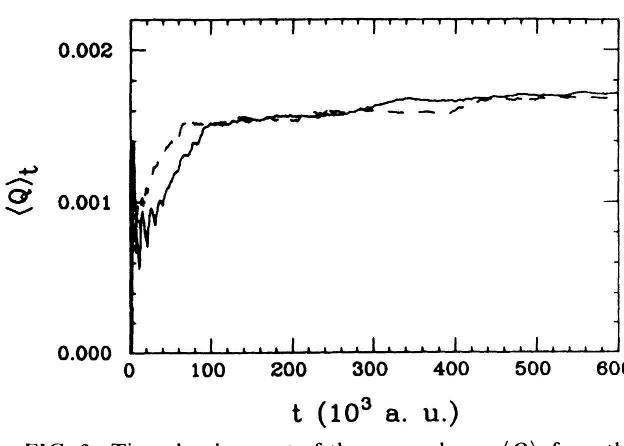

FIG. 3. Time development of the mean charge $\langle Q \rangle_t$ from the data of Fig. 2 (solid line). The dashed line represents the case where the starting single electron cloud of Fig. 1 is replaced by two equal half-density electron clouds moving from the wells w_1 and w_3.

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 quasiequilibrium.

Concerning the attainment of quasiequilibrium a crucial question is what happens if the initial conditions are varied. In the case of an energetically equivalent initial condition the same quasiequilibrium state is reached. An example is shown in Fig. 3 where the dashed curve refers to an initial condition in which the single electron cloud of Fig. 1 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 [8].

We examine first the autocorrelation function

$$C(t)\equiv \int_T q(t')q(t'+t)dt' \Big/ \int_T q(t')q(t')dt'$$

of the zero-mean charge

$$q(t)\equiv Q(t)-|T|^{-1}\int_T Q(t')dt' .$$

In Fig. 4 we give for comparison the autocorrelation function calculated in the time interval $T=[100,600]$ for the linear and the 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 they 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 the 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 [3] 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 $P(\omega)$ not reported here. Going from T_1 to T_2, in fact, we observe a corresponding 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 quasiequilibrium measure associated with the evolution of our system during the intervals T_1 and T_2. We have used the Grassberger-Procaccia algorithm [9]. As expected from the results of

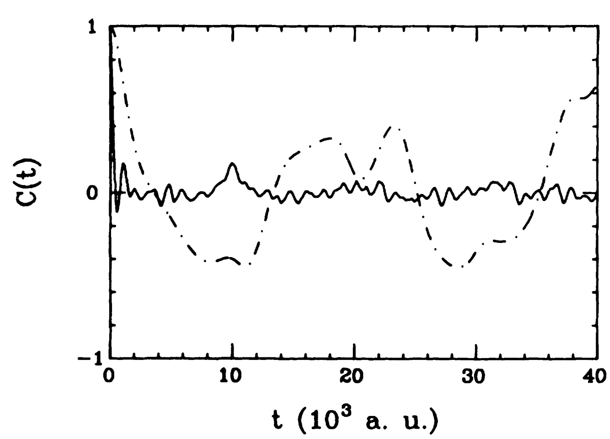

FIG. 4. Normalized time autocorrelation function $C(t)$ of the zero-mean charge from the data of Fig. 2 (solid line). The dot-dashed line represents the corresponding linear case $\alpha=0$.

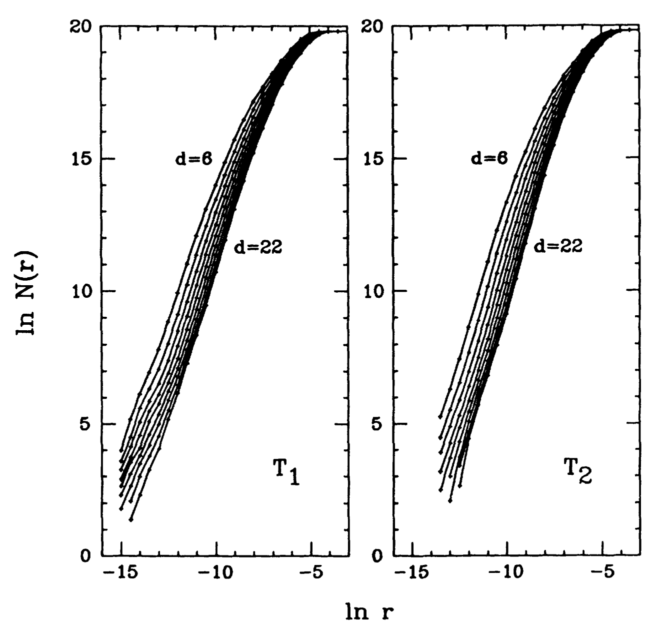

FIG. 5. Information dimension $\dim_H(\rho)$ calculated by the slope of the straight-line portion of the curves $\ln N(r)$ vs $\ln r$ in the two intervals $T_1=[180,260]$ and $T_2=[480,560]$. $N(r)$ is the number of pairs of points $(Q(t),Q(t+\Delta t),\ldots,Q(t+[d-1]\Delta t))$ with distance less than r in a d-dimensional embedding space with $d=6,8,10,\ldots,22$ (see Ref. [9]).

Ref. [10], $\dim_H \rho$, i.e., the slope of the straight lines in Fig. 5, has a noninteger 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 $\ln N(r)$ vs $\ln(r)$ is absent in the linear case. From the same data of Fig. 5 we can compute the order-2 Renyi entropy $K_2(\rho)$, a lower bound for the Kolmogorov-Sinai entropy, by an extrapolation process to the infinite embedding dimension d [9]. For both time intervals we obtain a positive value for $K_2(\rho)$. We have also made an independent calculation of the first Lyapunov exponent which turns out to be strictly positive.

We conclude with some general observations. In the mean-field model the mathematical origin of chaos resides in the nonlinearity of the Hartree equation. This nonlinearity provides an approximate description which captures to a certain extent for some time interval the very complicated evolution of the true many-body system. The question then arises: Does this chaotic behavior persist in time? One must always remember that quantum systems evolve according to a linear equation and this is an important feature which makes them different from classical systems. Confined quantum systems with a finite number of degrees of freedom, e.g., consisting of a finite number of particles, are quasiperiodic. This means that persistent chaotic behavior in the evolution of the observables is not possible [5]. We think that this limitation does not apply to an infinitely extended system with infinitely many particles. In particular it does not apply to our heterostructure which can be considered infinite in the plane orthogonal to the direction of the junctions. We can conceive of persistent motions of an extended electronic fluid which are chaotic in space and time. We hope to come back to this question in a future publication.

It is a pleasure to thank G. C. Benettin, J. Palis, Ya. G. Sinai, and S. Tenenbaum for very useful discussions. We are also grateful to C. Di Castro and P. Hohenberg for discussions on the many-body aspects of the problem and to B. V. Chirikov for critical remarks on an earlier version of this paper.

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