Quantum Mechanical Suppression of Classical Stochasticity in the Dynamics of Periodically Perturbed Surface-State Electrons

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The classical and the quantum mechanical descriptions of surface-state electrons which are perturbed by a periodic force $F(t)=e\epsilon\Sigma_n\delta(t-nT)$ are compared. The stochastic behavior which characterizes the classical treatment, and which is manifested by the energy diffusion and ionization rates, is suppressed by quantum effects.

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Surface-state electrons (SSE) are electrons which bind to liquid He surfaces by the induced electrostatic polarization.[1] To a good approximation, the effective binding potential depends exclusively on the vertical distance x through $V(x)=Ze^2/x$, where Ze is the induced image charge. Because of the exclusion principle, the liquid surface acts as an infinite repulsive wall.

Recently, Jensen[2] studied the effect of an rf field $E_x=\epsilon\cos wt$ on SSE. Treating the problem classically, he showed that this system displays chaotic features. It is known, however, that in similar simple systems, quantum mechanical (QM) effects suppress the classical stochasticity.[3] These observations led Jensen to propose the periodically perturbed SSE as a simple *microscopic* system where the conflicting predictions can be tested experimentally.

We present here a comparison of the classical and QM treatments of SSE perturbed by a periodic field $E_x=\epsilon\sum_n\delta(t-nT)$. The purpose of this work is to show (a) that this system also displays classical stochasticity which is manifested by the diffusive nature of the energy gain and can be probed by the rate by which SSE are removed from the surface (ionization), and (b) that *localization* rather than *diffusion* characterizes the SSE quantum dynamics, and that the ionization rate can be used to test the degree of localization of the SSE wave function. This study is motivated not only by its relevance to a realistic system. Till now, most of the available information on the quantum mechanics of classically stochastic systems came from the discussion of periodically kicked rotors.[3-6] As will be shown below, the SSE system is sufficiently different from the rotor to render the theoretical discussion of this problem interesting in its own right.

Measuring energies in units of the effective Rydberg constant, R, time in units of $\hbar/R$, and position in units of the Bohr radius a, the Hamiltonian reads

$$H(t)=H_0(\rho,\pi)+V(\rho,t);\qquad H_0=\pi^2-2/\rho,\quad V=-\beta\rho\textstyle\sum_k\delta(t-k\tau). \tag{1}$$

ρ and π are the dimensionless coordinate and momentum. τ is the time interval between successive kicks and $\beta=e\epsilon a/\hbar$. At $\rho=0$ we impose perfect elastic reflection conditions. The classical dynamics and its correspondence with the QM picture is most conveniently discussed in terms of the action-angle variables (n,θ). The canonical transformation relating the two representations is quoted in Ref. 2, and in the units used here, $H_0=-1/n^2$. In the QM treatment we set the initial state as an eigenstate $|n_0\rangle$ of H_0. Its classical analog is a phase-space distribution function $\sigma(n,\theta)=\delta(n-n_0)/2\pi$. The classical and QM descriptions will be separately discussed, omitting proofs and technical details which will be presented elsewhere.[7]

Classical treatment.— The classical equations of motion define a discrete area-preserving map of phase space onto itself. The essential features of this map are that at the kth kick, the linear momentum π_k is changed by $\Delta\pi=\beta$. The action variable n is accordingly modified since $H_0=-1/n^2$. Between kicks, n remains constant, while θ changes according to $\Delta\theta=\omega(n)\tau$, where $\omega(n)=\partial H(n)/\partial n=2/n^3$. Since θ is defined modulo 2π, the "stretching and folding"[8] mechanism which is responsible for the onset of stochasticity is provided when $\omega(n)\tau>2\pi$. This mechanism becomes less effective as more energy is pumped, and n increases. This is in contrast with the behavior of the rotor, where $\omega(n)\sim n$.

The phase-space distribution is represented by an ensemble of a few hundred phase-space trajectories $(n^{(j)},\theta^{(j)})_k$, where k denotes the conditions *just before* the kth kick. Initially, $n^{(j)}=n_0$ and the $\theta^{(j)}$ are evenly distributed on the interval

$[0, 2\pi]$.

A straightforward examination of the classical map shows that for $\beta > 0$ (the perturbing force pushes the SSE *away* from the liquid surface), the local Lyapunov exponent[8] $L_P^{(k)}$ is *positive definite* for all values of (n, θ). The following properties can be analytically derived. (i) The Sinai-Kolmogorov entropy[8] is proportional to $(6\tau\beta\langle n^{-2}\rangle)^{1/2}$, where angular brackets denote phase-space averages. (ii) The mean energy gain after N kicks is $N\beta^2$. The variance of the energy distribution scales with $\beta\langle n^{-2}\rangle^{1/2}N^{1/2}$, which clearly demonstrates the stochastic (diffusive) nature of the system. (iii) When the SSE energy becomes positive it is ionized and the corresponding trajectory is removed from the ensemble. The ionization rate per step, I_R, is defined as the mean value of $[dP_B(k)/dk]/P_B(k)$, where $P_B(k)$ is the number of trajectories which remain bound after the kth kick. The diffusive nature of the energy gain implies $I_R \simeq \beta^2/\langle n^{-2}\rangle$.

The estimates quoted above are derived by assuming that the ionization rate is much slower than the correlation time $\langle L_P\rangle^{-1}$. This condition restricts the range of the parameters β, τ, and n_0, and within this range the numerical iterations of the classical mapping reproduce accurately the above estimates.

The situation for systems with $\beta < 0$ (the perturbing force pushes the SSE *towards* the liquid surface) is quite different. Given β and τ, phase space can be divided into two regions. One corresponds to (n, θ) values for which the local Lyapunov exponent is positive and the motion is mixing. This region extends over the entire θ range for $n < (3\tau|\beta|/8)^{1/2}$. At larger n values, the stochastic region occupies strips near $\theta \sim 0, 2\pi$, which become narrower with increasing n. In the complementary region, the motion is regular, with $L_P^{(k)} = 0$. Periodic as well as stochastic trajectories are observed. Periodic trajectories never ionize and the classical probability that the SSE remain bound after many kicks is proportional to the fraction of trajectories which are trapped in periodic orbits.[9]

Quantum mechanical treatment.—The wave function $|\Psi_k\rangle$ just before the kth kick is obtained through iterating the map[6]

$$|\Psi_k\rangle = \exp(-iH_0\tau)\exp(-iV)|\Psi_{k-1}\rangle \equiv \exp(-iW)|\Psi_{k-1}\rangle. \quad (2)$$

The initial state $|\Psi_0\rangle$ is taken to be an eigenstate $|n_0\rangle$ of H_0. It is convenient to introduce the eigenvectors $|\varphi_\alpha\rangle$ of ω and the corresponding eigenvalues (quasienergies) ω_α. Then,

$$|\Psi_k\rangle = \sum_\alpha \exp(-i\omega_\alpha k)\langle\varphi_\alpha|n_0\rangle|\varphi_\alpha\rangle. \quad (3)$$

The state of the system is therefore completely determined by the expansion coefficients $\langle\varphi_\alpha|n_0\rangle$. The probabilities $p_\alpha(n_0) = |\langle\varphi_\alpha|n_0\rangle|^2$ are independent of k. Correlation functions of the type $\langle\Psi_k|\Psi_0\rangle$ are expected to be quasiperiodic, and the expectation values of observables such as the energy and its moments will be bound when the $p_\alpha(n_0)$ are well localized in α.

The pioneering QM studies of the periodically kicked rotor demonstrated the localization of the rotor wave function either numerically,[5] or by showing the formal analogy with the one-dimensional Anderson localization problem.[3,4] We shall show below that localization dominates the SSE wave function, too.

Our discussion of the SSE concentrates on situations where the perturbing-force strength β is kept sufficiently small so that the ionization rate is of the order 10^{-3}/step. We can, therefore, neglect in first approximation the continuum states of the Hamiltonian H_0, and consider only the space of bound states $|n\rangle$ with $H_0|n\rangle = e_n|n\rangle$, $e_n = -1/n^2$. The matrix $V_{nn'} = \langle n|\rho|n'\rangle$ is analytically evaluated[7] and is then exponentiated to form the propagator $\exp(-iW)$ which is numerically diagonalized in a space of 80–150 basis functions. We introduce the function

$$\Delta(n_0) = \exp\{-\textstyle\sum_\alpha p_\alpha(n_0)\ln p_\alpha(n_0)\},$$

which measures the spread of the state $|n_0\rangle$ in

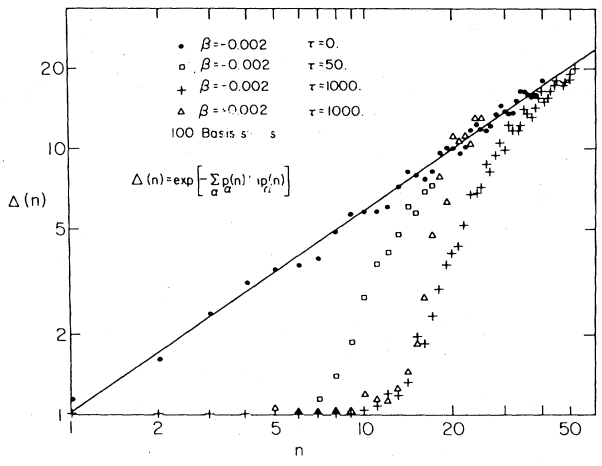

FIG. 1. The width function $\Delta(n)$ for various values of β and τ. The line through the $\tau = 0$ points is drawn to guide the eye.

the $|\varphi_\alpha\rangle$ representation. This function is displayed in Fig. 1, for a few values of the parameters β and τ. For low n_0, $\Delta(n_0)\cong 1$ which implies that $|n_0\rangle$ is localized on a single eigenstate of W. An abrupt change occurs at $n_0 = n_{crit}$, where $\Delta(n_0)$ increases and approaches the envelope $\Delta_{\tau=0}(n_0)$. At $\tau = 0$, $W = V$, and $\Delta_{\tau=0}(n_0)$ is the maximal width which V can induce. Iterating the QM map we calculated the variance of the n distribution as a function of the kick number. In all cases the variance remains bound, in contrast with the classical result. The variance increases appreciably when n_0 scans across n_{crit}, in a manner similar to $\Delta(n_0)$.

In order to get a better insight into the numerical results, we expand W[10] to first order in V, but to all orders of H_0:

$$W_{nm} = \begin{cases} V_{nm}\, i(e_n - e_m)\tau/\{1-\exp[-i(e_n-e_m)\tau]\}, & n \neq m, \\ \tau e_n + V_{nn}, & n = m. \end{cases} \tag{4}$$

An eigenstate $|\varphi_\alpha\rangle$ will have a large overlap with a single state $|n\rangle$ if $|\tau(e_n - e_m)| > |V_{nm}|$ for all $m \neq n$. Here, for $|m| \ll n$ we find numerically that $V_{n,n+m} \simeq C\beta n^2/|m|^{1.6}$ and $|\tau(e_n - e_{n+m})| \simeq 2\tau|m|/n^3$, so that the above condition will be satisfied whenever $n < n_{crit} = (2\tau/C\beta)^{1/5}$. This estimate for n_{crit} was verified in all our numerical checks.

Resonance mixing of states can occur when $\tau(e_n - e_m) \mathrm{mod} 2\pi \cong 0$, and $V_{nm} \neq 0$. Such resonances may affect strongly the value of some observables, as will be shown below.

Comparing the present system with the periodically kicked rotor, we observe the following important differences. (1) In the rotor case, $e_n \cong n^2$ and $V_{nn'} = \mathrm{const}$. Hence, as n_0 increases, localization becomes more effective, in contrast with the partial delocalization observed for SSE. (2) For the rotor, $e_n - e_{n-1} \sim n$ so that resonance conditions can be expressed in terms of one frequency and its harmonics. In the SSE system resonance mixing between some states cannot be avoided.

The effects of the continuum are approximately introduced by projecting the exact propagator $\exp(-iW)$ on the subspace of bound states $|n\rangle$. In this subspace, $\exp(-iW)$ is not unitary, and the probability to remain bound, $\langle\Psi_k|\Psi_k\rangle$, decreases with k. The ionization rate is defined as in the classical case.

The ionization rate from a pure state $|n\rangle$ is given by

$$I_R(n) = \int_0^\infty d\chi\, |\langle n|\exp(-i\beta\rho)|\chi\rangle|^2,$$

where $|\chi\rangle$ are properly normalized continuum eigenstates of H_0. $I_R(n)$ is independent of τ and is proportional to $\beta^2 n^{5/3}$. A system with a localized wave function should ionize with a rate which follows $I_R(n)$, and the strong dependence of $I_R(n)$ on n can be used to assess the value of n. In Fig. 2 we plot $I_R(n=10)$ together with the ionization rates calculated from the iteration of the map, for various values of τ, as a function of β ($n_0 = 10$ for all cases). Using our estimate for $n_{crit}(\beta,\tau)$, we expect that in all cases plotted here, Ψ_k should be well localized on $n_0 = 10$. This is indeed observed for the systems with $\tau = 500$, $\tau = 1000$ ($\beta < 0$), and $\tau = 1000$ ($0 < \beta < 1.5\times10^{-3}$). The resonance structure at $\beta = 1.7\times10^{-3}$ and the steep rise at $\beta = 2\times10^{-3}$ can be explained in the following way. A semiclassical approximation for W in Eq. (2) is obtained by neglecting the commutators in the Hausdorf-Baker expansion for W. Thus, $W^{sc} = H_0\tau + V$. The effective potential is $-2\tau/\rho - \beta\rho$, which for $\beta > 0$ reaches a maximum $V_{max}^{eff} = -(8\tau\beta)^{1/2}$ at $\rho = (2\tau/\beta)^{1/2}$. Hence,

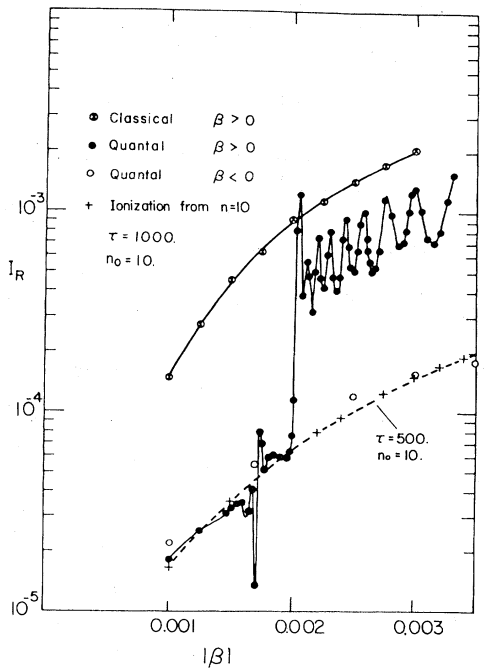

FIG. 2. Ionization rates calculated in various approaches. In all cases $n_0 = 10$. The dashed line corresponds to $\tau = 500$; all the other cases were calculated with $\tau = 1000$.

the continuous part of the spectrum of W^{sc} extends to negative energies, and at lower energies resonance states with energies $e_n \cong -\tau/n^2$ dominate the spectrum. It is therefore expected that the ionization rates will be strongly affected by the threshold and resonances mentioned above, if $|\Psi_k\rangle$ appreciably overlaps with a state $|n\rangle$ whose energy exceeds V^{eff} or overlaps with a resonance near threshold. For $n_0 = 10$ ($\tau = 1000$), $e_n = V_{max}{}^{eff}$ at $\beta = 12.5 \times 10^{-3}$ which is beyond the range of β discussed here. The state with $n = 16$, however, is resonantly mixed with the $n = 10$ state, and $e_{n=16} = V_{max}$ at $\beta = 1.9 \times 10^{-3}$. $e_{n=16}$ overlaps with the first bound resonance when $\beta = 1.71 \times 10^{-3}$. These values correspond quite accurately to the observed structures. For $\beta < 0$ W^{sc} has only a discrete spectrum so that resonance and threshold effects are not expected. When $\tau = 500$, $\beta > 0$ no structure is expected since no state resonates with the $n_0 = 10$ state. This analysis illustrates the sensitivity of the ionization rate as a probe testing the finer details in the wave function.

The ionization rates calculated classically depend quadratically on β and are displayed in Fig. 2. This dependence follows directly from the assumption that the energy gain is a diffusive process. The large difference between the classical and QM predictions, especially for low values, demonstrates again the QM suppression of the classical stochasticity.

The approximate quantum mechanical treatment described above is based on the assumption that once an electron ionizes, it will never return to the subspace of bound states. To check the accuracy of this approximation, we modified the QM mapping to include higher-order continuum effects.[7] The resulting n-state distribution and ionization rates are altered by a few percent at most.

Conclusions.—(a) Quantal effects suppress the stochastic features predicted by classical mechanics, in spite of the fact that in the SSE system a sudden spreading of the wave function over quasienergy eigenstates can occur. (b) The QM ionization rates confirm the localized nature of the SSE wave function, and display pure quantum mechanical effects which can be qualitatively understood without invoking any assumptions concerning stochasticity. (c) In spite of the essential differences between the rotor and the SSE systems, their behavior is almost completely determined by the same feature—localization of the wave function in the quasienergy representation. Whether this is a general feature of periodically perturbed simple systems and under which conditions delocalization may occur are interesting questions which deserve further study.

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