Anomalous Collective Diffusion

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A new region characterized by Lévy diffusion exists in collective motion between the adiabatic and diabatic limits. Repeated chaotic scattering off of level crossings, whose repulsive or attractive nature changes dynamically, can result in localization of the collective motion for arbitrarily periods of time, and anomalous diffusion.

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Complex systems, from nuclei, atomic clusters, and deformable cavities to various mesoscopic systems, have characteristic to them degrees of freedom which one can identify as low frequency/slow and fast/intrinsic. While in some systems there is a natural separation of these degrees of freedom, in strongly interacting many-body systems such as nuclei, there is no *a priori* obvious separation of collective degrees of freedom. Experimentally, however, there are striking experimental signatures of large amplitude collective motion which can be well described by a few collective variables. Over the past decade, there have been many advances concerning the nature of the collective manifold and how it can be realized from an interacting fermionic theory [1]. In particular, it has been shown that one can perform an approximate separation of a general many-body Hamiltonian into a collective piece $H_c(Q,P)$, whose dynamics evolves on a collective submanifold of the full theory, and the remaining noncollective component [2].

With such constructions of the collective manifold, one can in principle consider families of collective surfaces describing the *total energy states* of the system, or perhaps the interaction of two nearby mean-field configurations. The relevant physics now concerns how one hops between surfaces when two manifolds are close, which is frequent when the density of (total energy) states is generally high. The interplay of the collective and intrinsic degrees of freedom plays a central role in the microscopic understanding of macroscopic phenomena from dissipation, energy transfer, and the nature of collective diffusion. Common approaches (for the case of nuclei) are to assume either an adiabatic dynamics [for instance, applying adiabatic time dependent Hartree-Fock (ATDHF) approximation] or diabatic Landau-Zener (LZ) dynamics (such as dissipative diabatic dynamics [3]) near this "avoided level crossing," motivated by the pioneering study of Hill and Wheeler as well as many more recent investigations [1,3–5]. The limit is arbitrarily selected by the value of the LZ probability P, with $P \gtrsim \frac{1}{2}$ ($P \lesssim \frac{1}{2}$) indicating that diabatic (adiabatic) methods are best. I show here that this transition region is "chaotic," and cannot be simply characterized by a smooth passing from adiabatic to diabatic pictures, and even simple corrections to the adiabatic picture are often not sufficient. The smallest departure from the adiabatic dynamics can be nontrivial and result in very surprising phenomena. In particular, one can have repeated chaotic scatterings of the collective variables off of these avoided level crossings, resulting in a new regime of anomalous collective diffusion, and that identical level crossings can have completely opposite effects on the collective dynamics, acting as sources of either repulsive or attractive forces, and that even this can change in time (dynamically). In conventional diabatic treatments as well as stochastic formulations of collective diffusion, one consistently obtains as the time scale for irreversible behavior $\tau \sim 10^{-22}$ s [6]. Stochastic models which include random noise with this time scale provide an external source for irreversible effects which is directly responsible for diffusive behavior and the introduction of dissipation. In this same time scale, the collective motion already interacts with a number of avoided level crossings [3–6]. I will show that a diffusion process exists which is dynamical and reversible and hence does not require the stochastic influence of an external agent, and that avoided level crossings are responsible.

In order to clearly understand the underlying physical mechanisms, I introduce here a tractable Hamiltonian in the spirit of the LZ model, which while idealized, still embodies the basic physical ingredients: It includes schematic residual interactions (e.g., pairing, multipole deformation, etc.) coupled to collective motion, allows for both adiabatic and diabatic limits, and has many avoided level crossings:

$$h=\frac{P^2}{2}+V, \quad V=\kappa\begin{pmatrix}\sin Q & \Delta \\ \Delta & -\sin Q\end{pmatrix}. \qquad (1)$$

I have assumed that h is known in the vicinity of several level crossings, and (1) contains the essential interaction information. Here Q,P are collective variables, and $2\kappa\Delta$ is the energy gap at the avoided crossings (the periodicity is not relevant for our results.) Since many similar models have been used, from studies of LZ hopping between collective surfaces to extensions of the time dependent Hartree-Fock method to include residual interactions [1,3–5,7,8] it should come as a surprise that there is still much more physics hidden in (1). The energies of the interaction V are $E_\pm = \pm\kappa\sqrt{\Delta^2+\sin^2 Q}$, which has avoided level crossings at $Q=n\pi, n=0,\pm 1,\ldots$; see Fig. 1 (top). The quantum time evolution of the intrinsic states can be described in terms of its density matrix, parametrized as

$$\rho=\frac{1}{2}\begin{pmatrix}1+z & x-iy\\ x+iy & 1-z\end{pmatrix}=\frac{1}{2}(1+\boldsymbol{\sigma}\cdot\mathbf{r})\,, \tag{2}$$

where $\mathbf{r}=(x,y,z)$. A pure state $\rho^2=\rho$ has $r=1$, and a mixed state $\rho^2\neq\rho$ has $r<1$. The resulting dynamics are

$$\dot{Q}=P,\quad \dot{P}=-\kappa z\cos Q,\quad \dot{\mathbf{r}}=2\kappa\mathbf{a}\times\mathbf{r}\,, \tag{3}$$

where $\mathbf{a}=(\Delta,0,\sin Q)$, and the last equation is $i\dot{\rho}=[h,\rho]$, and is fully quantum. The density matrix evolves self-consistently with the collective trajectory. These equations have two integrals of motion, $r=$const and $E=P^2/2+\kappa\mathbf{a}\cdot\mathbf{r}$, and can be derived from the Lagrangian

$$\mathcal{L}=P\dot{Q}+\mathbf{A}_D\cdot\dot{\mathbf{r}}-\left(\frac{P^2}{2}+\kappa\mathbf{a}\cdot\mathbf{r}\right),\qquad \mathbf{A}_D=\frac{z(y,-x,0)}{2r(r^2-z^2)}\,, \tag{4}$$

where $A_D(r)$ is a Dirac gauge potential [9–11]. While this model consists of the fewest possible number of degrees of freedom, it is already chaotic; certainly less idealized systems will be even more so.

The completely integrable limits of h correspond to different types of adiabatic collective dynamics. If one takes $\kappa=0$, the intrinsic and collective spaces decouple, and $[h,\rho]=0$. The equations of motion become $\mathbf{r},P,\dot{Q}$ $=$const, so the collective coordinate moves at uniform velocity ($Q\propto t$), while ρ is static. The second integrable

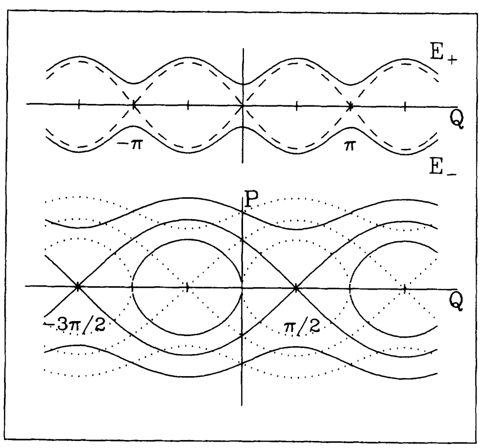

FIG. 1. Top: Eigenstates $E_\pm$ of the interaction V between collective and intrinsic states (solid). Adiabatic surfaces of h (dashes; $\Delta=0$). Bottom: Phase space of the (adiabatic) collective dynamics, for fixed $\tilde{z}>0$ (solid) [$\tilde{z}<0$ is shifted by π (dots)]. The quasibound states have $E<\tilde{z}$, and the unbound states $E>\tilde{z}$ are separated by the separatrix $E=\tilde{z}$.

limit occurs in the absence of "residual interactions," $\Delta=0$, giving real level crossings. The equations in this case are $z=$const, $\dot{x}=-y(\sin Q)$, $\dot{y}=x\sin Q$, and $\ddot{Q}+\kappa z\cos Q=0$. Although $[h,\rho]\neq 0$ here, by changing to a rotating frame, this limit satisfies the equivalent ATDHF (or cranked Hartree-Fock) adiabaticity condition, since $Q(t)$ obeys the dynamics of a pendulum. Since $z=\rho_{11}-\rho_{22}$ measures the intrinsic population difference, this regular limit also has no transitions. The collective phase space is shown in Fig. 1 (bottom) for $z>0$ (solid) and $z<0$ (dots). One sees surprisingly that the collective dynamics evolves on one of two intertwined noninteracting adiabatic surfaces (dashed lines in Fig. 1 top, and bottom of Fig. 1) with a periodicity different (by a factor of 2) from the level crossings of V (solid lines in Fig. 1, top).

Now consider the full dynamics (3). The slightest departure from the adiabatic dynamics results in motion which is nonintegrable, the collective dynamics obeying a variation of the equation of motion of the pendulum,

$$\ddot{Q}+\kappa(\rho_{11}-\rho_{22})\cos Q=0\,, \tag{5}$$

where $\tilde{z}\equiv\kappa(\rho_{11}-\rho_{22})=\kappa z$ is a dynamical variable with range $-\kappa r\leq\tilde{z}\leq\kappa r$ (one can choose $\kappa\geq 0$ without loss of generality). The pendulum phase space is shown in the bottom of Fig. 1, for two fixed values of $\tilde{z}$: $\tilde{z}>0$ (solid) and $\tilde{z}<0$ (dots). A manifestation of the difference in periodicity of the exact versus the adiabatic dynamics (compare Fig. 1 top and bottom) is that neighboring level crossings have opposite forces associated with them: Attractive points $Q=2n\pi$ are surrounded by repulsive points $Q=(2n+1)\pi$. Further, the attractive or repulsive nature changes in time according to the sign of z, the population difference. Hence seemingly identical avoided level crossings ($Q=n\pi$) have different forces associated with them in the full dynamics (3), which vary in time due to nonadiabatic transitions. This is in stark contrast to the LZ scheme which has the same prediction for such identical level crossings.

This nonintuitive behavior also gives rise to dynamical localization and diffusion phenomena. Assume $E<\tilde{z}=\kappa z$. If there are infrequent nonadiabatic transitions (collective energies $\lesssim$ residual interactions), z will remain fairly constant, and the collective motion will remain bound behind the sepatrix [Fig. 1 bottom (solid)]. (Strictly speaking, the separatrix only rigorously separates localized and free states for $z=$const. But for collective trajectories not near the separatrix and $\dot{z}\sim 0$ it can still be used to interpret the dynamics.) When a nonadiabatic transition occurs, the population shifts, and z will change sign, passing through zero, at which point the separatrix ($E=\tilde{z}$) in Fig. 1 will vanish, and reappear shifted along the Q axis by π [Fig. 1 bottom (dots)]. As a result, motion which had been (quasi) trapped in the well can now become free: The collective trajectory can appear on the other side of the separatrix, corresponding

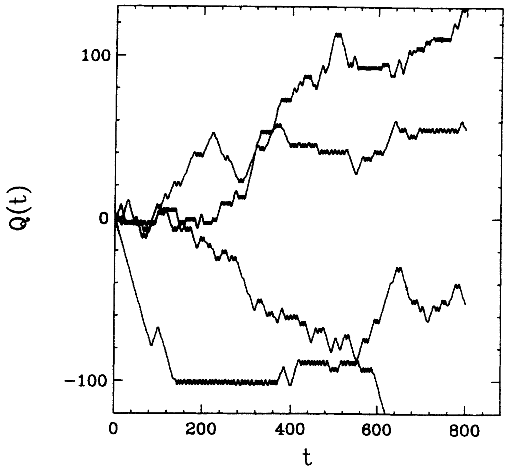

FIG. 2. Diffusing collective trajectories $Q(t)$ displaying temporary localization in phase space as a result of a nonadiabatic transition. As $\Delta \to 0$, the localization times become infinite (or zero), and the dynamics adiabatic. The two distinct elements of trapping within repulsive level crossings, and the large scale (adiabatic or diabatic) motion through many level crossings, are characteristic of Lévy flights. The spacing between level crossings is π.

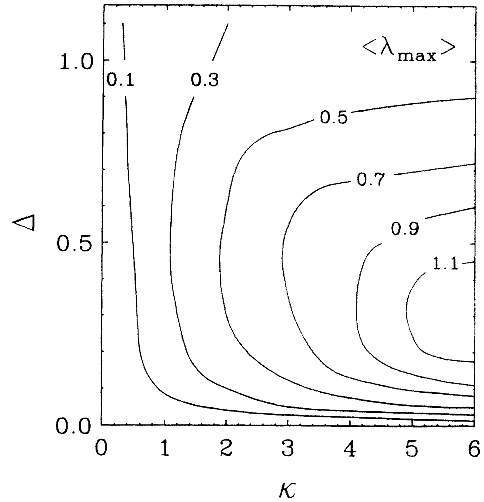

FIG. 3. Maximum Lyapunov exponent of h, averaged over phase and Hilbert space as a function of Δ and κ. The system is generally quite chaotic, but also completely (adiabatic) integrable for $\Delta=0$ as well as for $\kappa=0$.

to free motion. Subsequent shifts in the population will result in the collective trajectory becoming trapped again. The converse also holds for $E > \tilde{z}$. Such collective trajectories $Q(t)$ are shown in Fig. 2. One can see as $Q(t)$ evolves that it becomes trapped by level crossings (the repulsive crossings force a temporary localization), due to chaotic scattering off the (repulsive) level crossing, losing to internal excitation, and cannot escape until there is sufficient energy exchange. This can be quite long —there are trajectories which are trapped for arbitrary lengths of time; in other words, the collective scattering is *fractal.* When it can escape, there is generally sufficient energy for it to pass through many avoided level crossings before becoming trapped once again. This has the characteristic behavior of anomalous diffusion processes known as Lévy flights: diffusion on short times (trapped situation) together with large steps of arbitrary size (motion through many level crossings adiabatically or diabatically), characterized by the non-Brownian property $\langle Q^2(t)\rangle \propto t^\alpha$, $0<\alpha\le 2$ [12]. As $\Delta\to 0$, the level crossings become real, the motion adiabatic (integrable), and the localization times become infinite (or zero depending on what side of the separatrix the collective trajectory is on). This is precisely analogous to the stochastic modeling of anomalous diffusion, where one typically has a random potential which alone admits either free motion or localized states, and thermal noise, which can move a localized state from one local minimum of the random potential to another [12]. In the present case the collective/intrinsic interaction plays the role of the random potential, and the nonadiabatic transitions act as the random noise. Hence one can achieve *dynamically* the diffusive behavior of collective motion one puts in by hand in other models of collective motion.

The modification to the simple adiabatic/diabatic classification is explored in Fig. 3, where I consider the range of collective energies and residual interaction strengths used in the past to address LZ behavior in nuclear collective motion [7,8] (e.g., collective energies of similar order of magnitude as residual interactions). Here, the maximum Lyapunov exponent $\langle\lambda_{max}\rangle$, averaged over phase space *and Hilbert space*, is plotted as a function of Δ and κ. (I use $|P|\lesssim 2$; for large $|P|$ one is in the diabatic limit and feels the finiteness of the two level Hilbert space, requiring more levels to study such situations further.) In spite of the excessive regularity of our model system, it is important to observe that the slightest departure from adiabaticity (the Δ and κ axes) can result in chaos, and that chaos implicitly means that the collective trajectory will "bounce off" or scatter from the level crossings. Hence the localization and anomalous diffusive phenomena are ubiquitous to the dynamics beyond the adiabatic approximation. it is not hard to see that this novel mechanism is generic and will persist to less idealized and inherently more chaotic systems.

The diffusion constant $D(t)$ induced by repeated chaotic scattering from the (repulsive) avoided crossings can be computed using the Green-Kubo theory. By defining the ensemble as a uniform quantum population and a Gaussian distribution (of width 2) in momentum at $Q=0$, one obtains $D(t)$, where $\langle Q^2(t)\rangle = D(t)t$, as shown in Fig. 4. For short times, the motion is ballistic, with $D(t)\sim t$. On longer time scales, the memory effects due to bouncing off of sequential level crossings result in an

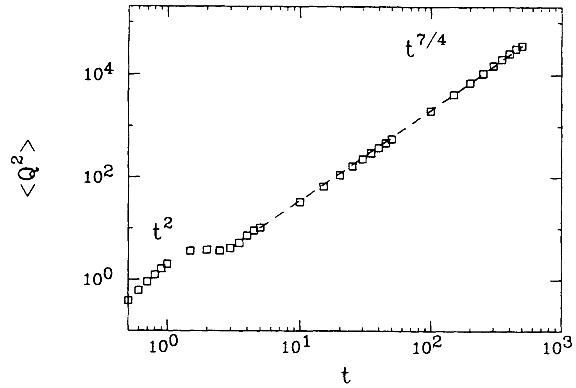

FIG. 4. Diffusive behavior of the collective coordinate $\langle Q^2 \rangle = D(t)t$, as induced by level crossings. For small times, the motion is restricted to a single potential well, and diffusion is ballistic, $Q \propto t$. On longer time scales, the interaction induces an approximate behavior of $\langle Q^2 \rangle \propto t^{7/4}$, which indicates persistent fractional Brownian-type behavior.

anomalous diffusion of $D(t) \propto t^{\alpha-1}$ with $\alpha \sim \frac{7}{4}$. Possible effects of anomalous diffusion will be on time dependent quantities such as response functions, fission time distributions, and so forth. Thus, the adiabatic-diabatic scheme, motivated by even a simpler model than (1), must be modified to include a quantitatively new regime of anomalous diffusion. When the two energies in Fig. 1 are well separated ($\kappa\Delta$ large) due to strong residual interactions, and conditions seem favorable for application of ATDHF, Fig. 3 shows that the slightest departure from the adiabatic approximation yields chaos, regardless of the strength of $\kappa\Delta$. Further, even identical level crossings can have opposite dynamical effects on the collective dynamics, in complete contradiction to the two state adiabatic/diabatic wisdom. As a consequence, I find a new dynamical mechanism for collective diffusion: chaotic scattering off level crossings. As a result, the LZ mechanism, which occurs on long time scales, is modified locally at the level crossing by chaos. Finally, it should also be emphasized that this separation of slow classical and fast quantum modes is not restricted to nuclei, and the results here should apply to other many body systems which exhibit large amplitude collective motion such as atomic clusters, deformable cavities, finite Fermi systems, and so forth.

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