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Damping in Schrödinger's equation for macroscopic variables

A. Davidson
IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598
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A simple damping term is proposed, to be added to the Hamiltonian in Schrödinger's equation. It is shown that this term removes energy without altering the wave-function normalization. It is also demonstrated that the dynamics of the damped wave function are in reasonable agreement with (in one dimension): classical motion in a harmonic potential; tunneling in a cubic potential in a Caldeira-Leggett oscillator bath; and spreading in a flat potential, also in the oscillator-bath model. The use of this new damping term should allow direct simulation in the time domain of several problems, including the dynamic behavior of nanometer scale Josephson junctions.

Over the past decade or so, two fields in mechanics have been revolutionized by progress in two different directions. The orderly behavior of Newtonian mechanics has unfolded into fractals and chaos, using new mathematical concepts and intense numerical simulation;[1] and the conservative structure of microscopic quantum mechanics has moved into the dissipative macroscopic domain,[2-4] using ingenious analysis, and virtually no simulation.

The study of chaotic Newtonian mechanics requires simulation. Although the motion is typically governed by a handful of ordinary differential equations, there are few general analytical results, and progress has come from either analog or digital simulation. Dissipative quantum mechanics, on the other hand, defies simulation. The rigorous treatment of dissipation in the quantum domain requires consideration of a large number of degrees of freedom, each of which is governed by a partial differential equation. Hence the largest and fastest computers would be required to compute even the simplest problem. Yet we want to know what happens to a chaotic, lossy, Newtonian system as it approaches the quantum limit. Hence there is a need to find some practical way to simulate a lossy quantum system.

Let us be clear about the type of lossy quantum system that we wish to simulate. We are not dealing with the quantum mechanics of a microscopic particle in a macroscopic potential, like the solid-state Aharonov-Bohm[5] problem. Rather, we are dealing with the quantum behavior of a macroscopic variable, like that for the phase difference across a Josephson tunnel junction. For the present purposes, we will ignore fluctuations, and take only the zero-temperature case. We suppose that in the absence of dissipation, the variable would be described by the time-dependent Schrödinger equation. To the Hamiltonian of this Schrödinger equation we seek to add a term that will remove energy.

Some years ago, Kostin[6,7] showed that such terms exist. He showed that it is possible to remove energy from the system, consistent with the classical limit, without changing the wave-function normalization, provided that the term is Hermitian, that it commutes with the position operator, and that it satisfies the following equation:

$$\frac{d}{dt}\langle E\rangle = -\int_{-\infty}^{\infty} JS_x dx \leq 0 , \tag{1}$$

$\langle E\rangle$ is the expectation value of the energy, J is the probability current density, and S is the new term in the Hamiltonian. S_x is the partial derivative of S with respect to the position coordinate x. If there is an S such that the integral in Eq. (1) is always positive for any wave function, and this S is Hermitian and commutes with x, then that S is a candidate damping term.

Kostin proposed a term consistent with these conditions,[6] and subsequently[7] showed that there is a broad class of consistent terms. Kostin's term is $S \propto (1/i\hbar) \times \ln(\psi/\psi^*)$. Unfortunately, he had no quantum results to compare to the effects of his term.

We propose a new term consistent with Kostin's conditions, and we compare it to two quantum results.

(1) The new term should exponentially inhibit tunneling, as Caldeira and Leggett[2] have shown.

(2) The new term should cause the wave function to spread approximately as the logarithm of time, as derived by Hakim and Ambegaokar[3] for a flat potential.

Schrödinger's equation, with the new damping term, would be written

$$\begin{aligned} &(H_0+S)\psi = i\hbar\frac{\partial}{\partial t}\psi , \\ &S = \eta'\xi^2\frac{\partial}{\partial t}\ln(\psi^*\psi) , \end{aligned} \tag{2}$$

where H_0 is the usual Hamiltonian, involving terms for the kinetic and potential energies, and S is the new term that provides damping. η' is a damping coefficient with the units of viscosity, which we will relate to the classical viscosity. $\xi = (\langle x^2\rangle - \langle x\rangle^2)^{1/2}$ is the width of the wave packet, and x is the position coordinate. The physical condition for the validity of this damping term is that the wave function should have a single well-defined packet. Difficulties occur for pure momentum eigenstates, or for problems with multiple bumps in the wave function. In the first case there would be no damping since $(\psi^*\psi)$ would have no time dependence. In the second case, damping would still occur provided the singularity in the logarithm is eliminated, but the normalization in Eq. (1) would make no sense because the width ξ is poorly defined for multiple bumps. It is interesting to note that Kostin's damping term depends only on the phase of the wave function, while S in Eq. (2) depends only on the wave

function's amplitude and width.

S in Eq. (2) meets all of Kostin's requirements. It is Hermitian and commutes with the position operator x. S from Eq. (2) will have no effect on the ground state, since the condition $(\partial/\partial t)(\psi^*\psi)=0$ is necessary for all stationary states, including the ground state. S will remove energy from any nonstationary state, however, since it shifts the potential energy up or down so as to oppose any change in the wave packet. This may be shown by evaluating Kostin's integral in Eq. (1). If we integrate Eq. (1) by parts, and take $\psi(\pm\infty)=0$, we get

$$\frac{d}{dt}\langle E\rangle=\int_{-\infty}^{\infty}J_x S\,dx=\left\langle\frac{J_x S}{\rho}\right\rangle. \tag{3}$$

Recall that $J_x=-\dot{\rho}$, where $\rho=\psi^*\psi$, and note that S in Eqs. (2) and (3) may be written as $S\sim\xi^2\dot{\rho}/\rho$. These may be substituted in Eq. (3), yielding $d/dt\langle E\rangle\propto-\langle(\xi\dot{\rho}/\rho)^2\rangle\leq 0$, and the removal of energy is proven.

The ξ^2 factor is in S to cancel the width dependence due to the time derivative. That is, the time derivative of a moving wave packet will have a ξ^{-2} factor in its amplitude. Since we do not want a width dependence in the effective viscosity, we must write the damping as in Eq. (2). Similarly, the logarithm serves to renormalize the derivative, removing all dependence on the local amplitude of the wave function.

The effects of the proposed damping were tested by the direct numerical simulation of Eq. (2) in the time domain, using standard techniques and three different potentials: quadratic, cubic, and flat. The time integration was by a fourth-order Runge-Kutta algorithm, and the spatial derivative was computed by simple finite differences. Figure 1 shows the results for a one-dimensional quadratic potential (simple harmonic oscillator), where the minimum wave packet was displaced from zero and released. The Schrödinger equation was normalized as follows in the simulation: Time was put in units of the reciprocal of the natural angular frequency ω_0 and length was normalized to $\lambda=(\hbar/m\omega_0)^{1/2}$. The resulting partial differential equation was

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi+\tfrac{1}{2}x^2\psi+\alpha'\xi'^2\left(\frac{\partial}{\partial t}\ln(\psi^*\psi)\right)\psi=i\frac{\partial}{\partial t}\psi, \tag{4}$$

where $\alpha'=\eta'/m\omega_0$ is a dimensionless damping parameter, related to the reciprocal of the Q of a classical oscillator, and $\xi'=\xi/\lambda$. The variables x and t in Eq. (2) are understood to have been normalized. We note that the classical equation with equivalent normalization is

$$\ddot{x}+\alpha\dot{x}+x=0 \tag{5}$$

and we seek a relationship between α in Eq. (5), and α' in Eq. (4).

The damped harmonic motion[8] is evident as the wave passes back and forth in Fig. 1. The time dependence of the energy of the oscillator is shown in Fig. 2, with the zero-point energy subtracted. This plot demonstrates the classical behavior of the damping term, and also fixes the effective Q such that $\alpha\sim\alpha'$. The ratio of unity was found to be constant for α' between 0 and at least 1.25. This result is expected, since it can be shown that for a Gaussian wave packet moving with velocity v, $-\partial S/\partial x=\eta' v$, the classical damping force.

To test the effect of S on tunneling, a Gaussian wave packet was placed in the metastable minimum of a cubic potential, according to the prescription of Caldeira and Leggett,[2] and the rate at which the probability increased in the classically forbidden area was measured from simulations. The potential used was

$$V=\tfrac{1}{2}x^2-0.0833x^3+0.00024e^x. \tag{6}$$

The coefficients on the right-hand side were chosen to get as close as possible to the semiclassical regime, where the analysis of Caldeira and Leggett should be most accurate, without using excessive computer time. This potential has a nearly stationary wave function approximately equal to the ground-state wave function for the harmonic oscillator of Eq. (4), but the x^3 term creates a falloff for large positive x, making this state metastable. The exponential term in Eq. (6) was put in to prevent the falloff from becoming too rapid, which would require a finer spatial grid in the simulation. The spatial variable x was bound-

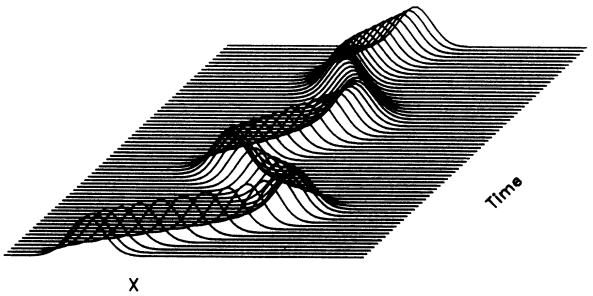

FIG. 1. Perspective view of an oscillating wave packet in a harmonic potential with damping. Position × is plotted horizontally, and $\psi^*\psi$ is vertical. The plot is displaced upward and to the right for equal time intervals, showing that the wave packet behaves like a classical damped harmonic oscillator.

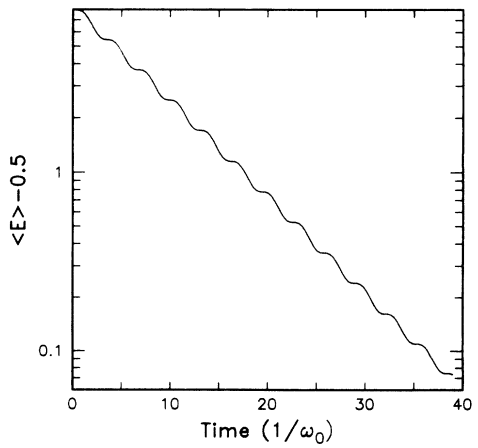

FIG. 2. Normalized energy vs time for the motion of Fig. 1. The ground-state energy of 0.5 has been subtracted, and the exponentially decaying energy is plotted on a logarithmic scale. This confirms the classical nature of the motion, and fixes an effective damping coefficient.

ed between -3.5 and 11.5. The gradient of the wave function was set equal to zero at the boundaries.

A region at the exit point of the barrier, in the classically forbidden area, was chosen in which to measure the tunneling rate, since it would allow the longest time before reflections from the edge of the potential would begin to contaminate the rate. The rate was observed to build up over time, reach a broad maximum, and then decline. We have used the rate at the maximum as a measure of the steady-state tunneling rate. The results are shown in Fig. 3, which plots the rate of probability increase against the damping factor α, as determined from the behavior of the harmonic oscillator.

According to Caldeira and Leggett,[2] the tunneling rate for a cubic potential in the presence of damping should be

$$\tau^{-1}=\sqrt{60b/2\pi}e^{-b}, \qquad b=\Delta V-A(\Delta x)^2\alpha . \tag{7}$$

All units have been normalized as in Eq. (2). Note that energy is normalized to $\hbar\omega_0$. ΔV is the barrier height, taken from the top of the barrier down to the ground-state energy of the initial wave packet. ω_0 corresponds to the classical frequency of the metastable well. Δx is the distance under the barrier that the trapped particle must tunnel. α is the damping constant of the classical oscillator as in Eq. (5) and A is a constant. For this problem, with the assumption of many levels in the well and no backscattering, Caldeira and Leggett have shown A to be 0.464. The lower line in Fig. 3 is the result of Caldeira and Leggett, with no adjustments. The slope of the line could be adjusted to match that found by simulation if A is changed to 0.255, as shown by the upper solid line in Fig. 3.

Hence, the S term in the Hamiltonian suppresses tunneling with the expected exponential form, and comes within a factor of 2 of the predicted coefficient in the exponent. It should be emphasized that this was accomplished with the exact same term that provided classical damping for the displaced harmonic oscillator, with the same effective viscosity.

Figure 4 shows the result of setting the potential energy in H_0 to zero everywhere and starting the simulation with a narrow wave packet. Hakim and Ambegaokar[3] have shown that with enough damping, the square of the wave-packet width should grow more or less logarithmically in time

$$\xi^2\sim\xi_0^2+\frac{4}{\pi}\alpha^{-1}\ln(\alpha t), \tag{8}$$

where ξ_0 is the initial width. This is in marked contrast to the frictionless case, where the square of the width is known to grow as the square of the time. Figure 4 plots the square of the width ξ^2 against time, along with Hakim and Ambegaokar's prediction. Note that to fit the data we changed Hakim and Ambegaokar's prefactor of $4/\pi$ to ~ 1. It is seen that damping from S is in approximate agreement with the predictions. We have found that damping from S agrees with Eq. (8) (with the reduced prefactor) within $\approx 20\%$ over a decade in time. Again, we point out that this behavior was obtained only by changing the potential in H_0. The damping term S was kept the same as for the simple harmonic oscillator and for the cubic tunneling problem.

We have shown that S in Eq. (2) reasonably satisfies a stringent set of constraints, and so should be useful in simulations of damped macroscopic quantum variables. We note here that we have also simulated Kostin's term $S\propto\ln(\psi/\psi^*)$. This damping term produced similar results in the case of the harmonic oscillator and tunneling in a cubic potential, but showed too strong a time dependence for the spreading wave function in a flat potential.[9] We also note that Kostin's term is essentially the phase of the wave function, and as such it has difficulties with gauge invariance. Even so, our choice of S is probably not unique. The time derivative of any monotonic function of $\psi^*\psi$ would remove energy without changing the normali-

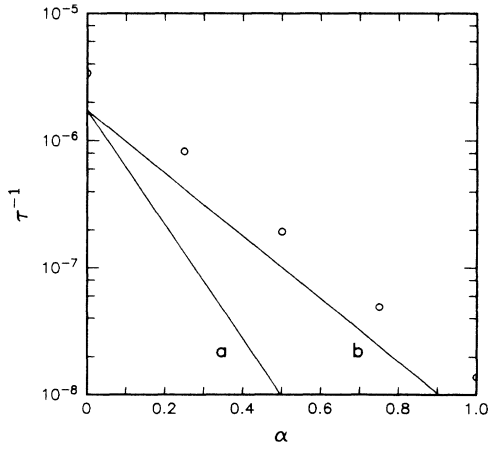

FIG. 3. Normalized tunneling rate vs damping for a wave packet in the metastable minimum of a cubic potential. The circles are the result of simulations. The line marked a is the unadjusted result of Caldeira and Leggett, $A=0.464$ (see Ref. 2). Line b would be the Caldeira and Leggett result if their parameter A were adjusted to 0.255.

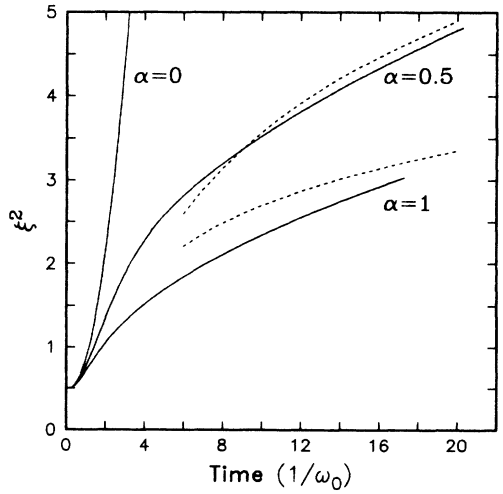

FIG. 4. Square of the width of a wave packet as a function of time for a flat potential. The solid lines are from simulation. The dotted lines are from Ref. 3, scaled down by 25%.

zation. The claim for Eq. (2) is that its results satisfy Kostin's requirements, and are in reasonable agreement with the available microscopic analysis. It should therefore allow meaningful simulation on modest computers of Schrödinger's equations for a macroscopic variable in a lossy environment.

In summary, a term has been proposed and tested for putting damping directly into Schrödinger's equation. We find that for the case of a single wave packet it is possible to reasonably reproduce the known results for tunneling from a one-dimensional cubic potential, for the spreading of a wave packet in a flat potential, and for classical damping of a packet in a harmonic well, all with the identical term S in Eq. (2). It is to be understood that the use of this term to describe losses in macroscopic quantum systems is phenomenological, nonunique, and apparently limited to quasiclassical wave-packet solutions. Nonetheless, it seems to be well suited for the study of small area Josephson tunnel junctions,[10-13] and dissipative chaotic systems in the quantum limit.

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