Exact solution of the wave dynamics of a particle bouncing chaotically on a periodically oscillating wall

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(Received 27 September 1993; revised manuscript received 28 June 1994)

An exact solution to the Schrödinger equation corresponding to the problem of a particle falling under gravitational acceleration and bouncing on a harmonically oscillating surface is derived. Stationary phase approximations to the transition amplitudes from an initial state to eigenfunctions of the problem with a fixed surface are worked out and illustrated.

PACS number(s): 03.40.Kf, 03.65.−w

I. INTRODUCTION

We consider the following version of the Fermi-Ulam cosmic ray acceleration problem. A particle falls under gravitational acceleration g and bounces off a surface that is oscillating with frequency ω, $x_\omega(t)=h_0(1+\cos\omega t)$. It is known that particle trajectories accelerate indefinitely [1] and that they exhibit technical chaos [2].

Less well known is the fact that the quantum mechanical formulation of the above problem is mathematically identical to a problem in underwater acoustics. This is the problem of acoustic propagation under the influence of a restoring velocity profile with a periodic reflecting wall in the "parabolic approximation" to the full wave equation [3]. Here the "time" variable of the quantum problem is replaced by the "range," or distance in the direction of propagation. The wall is static but varies with range. Thus solutions to the wave equation are interesting both from the point of view of quantum systems which exhibit chaos in the classical limit [4], and for underwater acoustics in situations where the rays are chaotic.

The purpose of this paper is to supply an analytic solution to the wave equation

$$i\partial_t\Phi=-\tfrac{1}{2}\partial_z^2\Phi+gz\Phi\equiv H_0\Phi \ , \tag{1}$$

subject to the boundary condition

$$\Phi(z=x_\omega(t),t)=0 \ . \tag{2}$$

Those eigenstates of H_0 for which the spatial wave functions vanish at $z=0$ are well known to be Airy functions, and the eigenvalues are quantized. It is the boundary condition (2) that renders the problem nonseparable and nontrivial, although an implicit solution is possible in terms of an integral equation [5].

The mathematical problem of solving Eq. (1) subject to Eq. (2) is sufficiently difficult that a frontal assault on the problem is not the most efficient way to proceed. In Sec. II, an operator representation of Eq. (1) will be introduced. Then a solution motivated by the structure of the Hamiltonian path integral representation will be postulated. In Sec. III, subtle questions regarding the suitability of the operator representation will be addressed, resulting in verification of the solution in Sec. IV.

The solution so obtained is a superposition of the Airy functions mentioned above, with modal projection amplitudes as coefficients. Thus it is necessary to compute the latter in order to exhibit the spatial wave functions. The calculations are not trivial. Section V contains a discussion of a stationary phase estimate of these amplitudes; full details of the derivation of the approximation are reserved for the Appendix.

II. HEURISTIC SOLUTION OF THE DYNAMICAL EQUATION

Step 1 is to change variables to $x=z-x_\omega(t)$. After the replacement $\phi(x,t)=\Phi(x,t)\exp[(igh_0)(t+\sin\omega t/\omega)]$ we obtain

$$i\partial_t\phi=-\tfrac{1}{2}\partial_x^2\phi+gx\phi-if(t)\partial_x\phi \tag{3}$$

subject to $\phi(x=0,t)=0$, and with $f(t)=h_0\omega\sin\omega t$. This form seems well suited for ordinary Dirac time-dependent perturbation theory, which proceeds through the introduction of time-dependent coefficients through the representation $\phi(x,t)=\sum_n\phi_n(x)e^{-iE_nt}a_n(t)$. Here the $\phi_n e^{-iE_nt}$ are eigensolutions to Eq. (3) with $f(t)=0$. However [6], a nonperturbative solution will be sought, and we dispense with the $a_n(t)$ notation in what follows.

We denote the inner product in the coordinate representation $\int_0^\infty dx\ A^*(x)B(x)=(A,B)$, so that $\phi(x,t)=\sum_n\phi_n(x)(\phi_n,\phi)$. For the remainder of this section, we will be concerned with the projections (ϕ_n,ϕ), which are functions of t. From Eq. (3), it is easily seen that these satisfy

$$i\partial_t(\phi_n,\phi)=E_n(\phi_n,\phi)-if(t)(\phi_n,\partial_x\phi) \ . \tag{4}$$

To motivate the proposed form of the solution to Eq. (4), we rewrite Eq. (3) abstractly as

$$\begin{aligned} i\partial_t|\phi(t)\rangle &= [\tfrac{1}{2}\hat{p}^2+g\hat{x}+f(t)\hat{p}]|\phi(t)\rangle \\ &= [\hat{H}_0+f(t)\hat{p}]|\phi(t)\rangle \ . \end{aligned} \tag{5}$$

Now, because $[\hat{H}_0,\hat{p}]=ig\hat{1}$, *for this special problem* the usual machinery of building a Hamiltonian path integral solution [7] to Eq. (5) can be short circuited through repeated use of the Baker-Campbell-Haussdorf identity $e^{A}e^{B}=e^{A+B}e^{[A,B]/2}$, valid when $[A,B]$ is a c number. It should be reasonably clear that this procedure will lead to

$$|\phi(t)\rangle=e^{-i\xi(t)}e^{-i\hat{H}_0 t}e^{-ih(t)\hat{p}}|\phi(0)\rangle \ , \tag{6}$$

where $h(t)=\int_0^t dt' f(t')$, while $\xi(t)$ remains to be determined [8].

Thus we aim for a solution of the form

$$(\phi_n,\phi)=e^{-i\xi(t)}e^{-iE_n t}\int_0^\infty dx\ \phi_n(x)\Psi_0(x-h(t)) \ . \tag{7}$$

In passing from Eq. (6) to Eq. (7), we have used $\langle\phi_n|\hat{H}_0=\langle\phi_n|E_n$, $(\phi_n,\phi)=\langle\phi_n|\phi(t)\rangle$, $\Psi_0(x)=\langle x|\phi(0)\rangle=\phi(x,0)$; and we have used the property that $\hat{p}$ generates translations, $\langle x|e^{-ih(t)\hat{p}}|\phi(0)\rangle=\Psi_0(x-h(t))$.

We now verify this solution heuristically and obtain in the process an explicit expression for $\xi(t)$. Since $\partial_t\psi_0(x-h(t))=-f(t)\partial_x\Psi_0(x-h(t))$, it follows that

$$i\partial_t(\phi_n,\phi)=(\partial_t\xi+E_n)(\phi_n,\phi)-if(t)e^{-i\xi(t)}e^{-iE_n t}\times\int_0^\infty dx\ \phi_n(x)\partial_x\Psi_0(x-h(t)) \ .$$

The second term on the right-hand side (RHS) may be rewritten as $f(t)e^{-i\xi(t)}\langle\phi_n|e^{-i\hat{H}_0 t}\hat{p}e^{-ih(t)\hat{p}}|\phi(0)\rangle$. Under the assumption that the commutation relation $[e^{-i\hat{H}_0 t},\hat{p}]=gte^{-i\hat{H}_0 t}$ holds (following from $[\hat{H}_0,\hat{p}]=ig\hat{1}$), Eq. (4) collapses to

$$\partial_t\xi\langle\phi_n|\phi\rangle=-gtf(t)\langle\phi_n|\phi\rangle \ ,$$

so we conclude that $\xi(t)=-g\int_0^t dt' t' f(t')$.

Equation (7) is the principal result of this paper. It is equivalent to solving Eq. (1) subject to Eq. (2). We turn to proving that Eq. (7) is a correct solution, although the commutation relations we used are more subtle than it seems at first sight. Thus we will not recover Eq. (7) until the end of the calculation.

III. RESTRICTION OF THE PROBLEM TO THE HALF-SPACE

A. Remarks on why caution is required in a half-space

Care has been exercised to deem the preceding derivations "heuristic" because the conventional manipulations that have been exhibited are open to question when the problem is formulated in a half-space. Following von Neumann [9], one way to exhibit the complications introduced by restriction to a half-space is to examine simple Fourier transforms.

Consider an admissible function $f(x)=\int_{-\infty}^{\infty}dk\,\not{f}(k)e^{ikx}$, with the inverse transform

$$\not{f}(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dx\ f(x)e^{-ikx} \ .$$

Now constrain $f(x)$ to vanish for negative x, $f(x)\rightarrow f(x)\theta(x)$, and insert into the formula for the inverse:

$$\not{f}(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dx\ \theta(x)e^{-ikx}\int_{-\infty}^{\infty}dk'\not{f}(k')e^{ik'x} \ .$$

Consistency requires

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}dx\ \theta(x)e^{-i(k-k')x}=\delta(k-k') \ ,$$

which is false. Consequently, the transform of the restricted function is different from the transform of the original function unless $f(x)$ "happens" to vanish for negative x without the intervention of $\theta(x)$.

This unremarkable and seemingly innocuous observation presages worse things to come. Formalize by introducing eigenstates of the momentum operator $|k\rangle$ and of the position operator $|x\rangle$, and assume that these are orthonormal and complete (with δ function normalization). Now sandwich the commutation relation $[\hat{x},\hat{p}]=i$ between momentum eigenstates:

$$\langle k|[\hat{x},\hat{p}]|k'\rangle=(k'-k)\langle k|\hat{x}|k'\rangle=i\delta(k-k') \ .$$

A consistent solution to this equation as a distribution in k space is $\langle k|\hat{x}|k'\rangle=i\partial_k\delta(k-k')$. [An additional contribution proportional to $\delta(k-k')$ is not precluded but can be shown to be trivial for all manipulations which follow, i.e., the coefficient is safely set equal to 0.]

Next, to compute the transition coefficients $\langle x|k\rangle$ we use the assumed completeness of the $|k\rangle$ states to write

$$x\langle x|k\rangle=\int_{-\infty}^{\infty}dk'\langle x|k'\rangle\langle k'|\hat{x}|k\rangle=-i\partial_k\langle x|k\rangle \ .$$

It follows (with the standard normalization) that $\langle x|k\rangle=(1/\sqrt{2\pi})e^{ikx}$. If we now apply completeness of the coordinate eigenstates *restricted to the half-space,*

$$\langle k|k'\rangle=\int_{-\infty}^{\infty}dx\ \theta(x)\langle k|x\rangle\langle x|k'\rangle \ ,$$

it is clear that $\langle k|k'\rangle=\delta(k-k')$ *fails.*

One way of summarizing this result is that the hypothesis that there exist complete orthonormal eigenstates of both the position and momentum operators is inconsistent with the canonical commutation relation between $\hat{x}$ and $\hat{p}$, when the $|x\rangle$ are restricted to support functions on the half-space. In Sec. III B, this formal statement is elaborated through the example of the free particle.

B. The free particle in a half-space

Consider the operator equation $\frac{1}{2}\hat{p}^2|n\rangle=E_n|n\rangle$. Assume the existence of momentum eigenstates, and so obtain the equation $\frac{1}{2}k^2\langle k|n\rangle=E_n\langle k|n\rangle$. Assume further that these states are complete and orthonormal, and so introduce a separate basis,

$$|x\rangle=\int_{-\infty}^{\infty}dk|k\rangle\langle k|x\rangle=\int_{-\infty}^{\infty}dk|k\rangle\frac{1}{\sqrt{2\pi}}e^{-ikx} \ . \tag{8}$$

It is readily verified that, with the specified choice of the basis coefficients $\langle k|x\rangle$, the $|x\rangle$ are indeed eigenstates of the position operator. It is also true that $\langle x'|x\rangle=\delta(x-x')$. However, we have seen that it may not be assumed that the $|x\rangle$ are complete.

Introduce now the notation

$$\psi_n(x)=\langle x|n\rangle=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\, e^{ikx}\langle k|n\rangle \ .$$

Clearly, $\psi_n(x)$ is meant to represent the ordinary configuration space wave function, and for the problem at hand it must vanish at the origin. This leads to the condition $\langle k|n\rangle+\langle -k|n\rangle=0$, so up to an overall normalization, $\psi_n(x)\propto\int_0^\infty dk\,\sin kx\langle k|n\rangle$. From the equation satisfied by the $\langle k|n\rangle$, it follows at once that the ordinary free particle equation, $-\frac{1}{2}\partial^2\psi_n(x)=E_n\psi_n(x)$, is satisfied. The coefficients $\langle k|n\rangle$ themselves may consistently be chosen to be proportional to $[\delta(k-n)-\delta(k+n)]$.

So, starting from the operator equation, we have successfully constructed an ordinary function of x that satisfies the differential equation and the boundary condition. Although no explicit condition that $\psi_n(x)$ vanishes for $x<0$ has been introduced, one many proceed to normalize the wave functions, integrating over the non-negative half-space without changing the form we have derived.

However, consider next the operator statement $[\hat{p}^2,\hat{p}]=0$. Under the stated assumptions this may be elaborated in the form

$$\int_{-\infty}^{\infty}dk\langle n|\hat{p}^2|k\rangle\langle k|\hat{p}|m\rangle=\int_{-\infty}^{\infty}dk\langle n|\hat{p}|k\rangle\langle k|\hat{p}^2|m\rangle .$$

Under the further assumption that $\hat{p}^2$ is Hermitian, this reads

$$E_n\int_{-\infty}^{\infty}dk\langle n|k\rangle k\langle k|m\rangle=E_m\int_{-\infty}^{\infty}dk\langle n|k\rangle k\langle k|m\rangle \ .$$

Inserting the aforementioned expression for $\langle k|m\rangle$, we obtain $0=0$.

Now suppose we proceed differently. Take one derivative on the left and right sides of the differential equation $-\frac{1}{2}\partial^2\psi_n(x)=E_n\psi_n(x)$; multiply by $\psi_m(x)$; and integrate over non-negative x. Keep careful track of the surface terms in two integrations by parts to obtain

$$(E_m-E_n)(\psi_m,\psi_n')=\tfrac{1}{2}\psi_m'(0)\psi_n'(0) \ . \quad (9)$$

With the conventional notation $\langle x|n\rangle=\psi_n(x)$ and $\langle x|\hat{p}|y\rangle=i\partial_y\delta(x-y)$, this true equation (it can be checked using explicit expressions) would appear to contradict the statement $[\hat{p}^2,\hat{p}]\neq 0$. From a physicist's point of view, the question arises whether this apparent contradiction constitutes a deep inconsistency in the quantum mechanical formulation of the problem, or merely an inconvenience that can be resolved through a more careful specification of the coordinate representation.

We opt for the latter interpretation. First, to disentangle the physics, note that the formal statement $\frac{1}{2}\hat{p}^2|n\rangle=E_n|n\rangle$ is an incomplete depiction of the problem of a free particle in a half-space. One way to improve the formulation is to introduce a potential $V(\hat{x})$, which expels the particle from the left half-space, say $V\theta(-x)$, as V approaches infinity.

With such a potential in place (at finite though very large V), both the $|k\rangle$ states and the $|x\rangle$ states are complete and the formal manipulations are entirely correct. The Hamiltonian operator is Hermitian, the kinetic energy commutes with the momentum, and the analog of Eq. (9) reads

$$\begin{aligned}E_n\int_{-\infty}^{\infty}dx\,\psi_m(x)\partial\psi_n(x)&=\int_{-\infty}^{\infty}dx\,\psi_m(x)\partial[-\tfrac{1}{2}\partial^2\psi_n(x)+V\theta(-x)\psi_n(x)]\\&=\int_{-\infty}^{\infty}dx\,\partial\psi_m(x)\tfrac{1}{2}\partial^2\psi_n(x)+V\int_{-\infty}^{\infty}dx\,\psi_m(x)[-\delta(x)\psi_n(x)+\theta(-x)\partial\psi_n(x)]\\&=E_m\int_{-\infty}^{\infty}dx\,\psi_m(x)\partial\psi_n(x)-V\psi_m(0)\psi_n(0) \ ,\end{aligned}$$

since $\psi_m(x)$ also satisfies the differential equation.

The term proportional to V does not vanish in the limit $V\to\infty$. Textbook calculations reveal that (neglecting normalization factors, which in any case cancel from both sides of the equation) $\psi_n(0)\to C_n/\sqrt{V}$ and $\psi_n'(0)\to -C_n\sqrt{2}$. Thus $V\psi_m(0)\psi_n(0)\to\frac{1}{2}\psi_m'(0)\psi_n'(0)$, in complete accord with Eq. (9). This verifies that the explicit introduction of the "excluding" potential $V\theta(-x)$, $V\to\infty$, is mathematically as well as physically equivalent to restriction to the half-space. It also indicates that Eq. (9) makes sense physically.

But then what is the source of the "paradox" regarding the commutation relation $[\hat{p}^2,\hat{p}]$? Note that no V term was present in that discussion. It must be viewed as a consequence of our inability to use "completeness" of the coordinate representation $\hat{p}^2\hat{p}\neq\int_0^\infty dx\,\hat{p}^2|x\rangle\langle x|\hat{p}$, and so forth, in establishing the equivalence of Eq. (9) with the commutation relation in question. Stated differently, the coordinate space representative of $\hat{p}^2$ is not self-adjoint in the half-space when this differential operator acts on functions that do not vanish at the origin (such as $\cos nx$). It would thus seem that a consistent prescription, when in doubt, is to fall back on the extended Hamiltonian formulation, introducing $V\theta(-x)$.

On the other hand, the half-space problem can be represented in yet another way. Introduce the function $\Phi(x)=\phi(x)\theta(x)$, where $\phi(x)$ is a solution to the differential equation $-\frac{1}{2}\partial^2\phi(x)=E_n\phi(x)$, and with $\phi(0)=0$. Thus $\Phi(x)$ is the restriction of function ϕ to the non-negative half-space. We record

$$\Phi_n'(x)=\phi_n'(x)\theta(x) \ ,$$

$$\Phi_n''(x)=\phi_n''(x)\theta(x)+\phi_n'(0)\delta(x) \ ,$$

$$\Phi_n'''(x)=\phi_n'''(x)\theta(x)+\phi_n''(0)\delta(x)+\phi_n'(0)\delta'(x) \ .$$

Multiply the last line by $\phi_m(x)$ and integrate over all x. Making explicit use of the θ function, the RHS ($\mathcal{R}$) of the last line becomes

$$\mathcal{R}=\int_0^\infty dx\,\phi_m(x)\phi_n'''(x)+\phi_n'(0)\int_{-\infty}^\infty dx\,\phi_m(x)\delta'(x)\ .$$

Use the equation satisfied by ϕ_n and integrate the second term to obtain the RHS,

$$\mathcal{R}=-2E_n\int_0^\infty dx\,\phi_m\phi_n'-\phi_m'(0)\phi_n'(0)\ .$$

But if we integrate the first term by parts twice, we obtain

$$\mathcal{R}=-2E_m\int_0^\infty dx\,\phi_m\phi_n'\ .$$

The surface term in the second integration by parts cancels the explicit $\phi_m'(0)\phi_n'(0)$ term. Thus again Eq. (9) is recovered.

This time the lesson is that we can first solve a full-space problem to obtain $\phi(x)$, subject to $\phi(0)=0$. There is no problem with the canonical commutation relations, completeness, etc. We then restrict the solution to the half-space via $\Phi(x)=\phi(x)\theta(x)$. For our purposes in this paper, it is sufficient to show, as we have done, that the surface term consistent with Eq. (9) is produced.

C. Summary of a prescription for calculations

Physically, the problem of the free particle in a half-space may be formulated in terms of a full-space problem subject to expulsion from the left half-space by a large potential. When this is done, the Hamiltonian does not commute with the momentum operator, although the kinetic energy (of course) does.

In the limit, as the barrier height goes to infinity, the effect of this lack of commutation manifests itself as a surface term in evaluating the inner product (ϕ_m,ϕ_n'''), which one would ordinarily interpret as being proportional to the matrix element $\langle m|\hat{p}^3|n\rangle$. However, this identification is incorrect because, in the limit, resolution of the identity by coordinate eigenstates $|x\rangle$ is flawed. Nonetheless, one may recover the correct surface term by restricting the solution to the half-space through multiplication by $\theta(x)$ at the end of the calculation.

Alternatively, one may dodge the issues stemming from the problems with the states $|x\rangle$ by working in the momentum representation, recovering the coordinate representative of the wave function at the end of the calculation using Eq. (8). The resulting wave function is then multiplied by $\theta(x)$ as before. This is the prescription to be employed in what follows. It must be kept in mind that the problem of constraining the particle to the half-space is no different in the full problem than in the case of the free particle. It is for this reason that the "recipe" can be trusted: *The surface term contains no physics beyond taking the "naive" solution sin(nx), which vanishes at the origin, and restricting it to the half-space.*

IV. VERIFICATION OF THE SOLUTION

A. Is the operator formulation equivalent to the differential equation?

Recall that the objective is to solve Eq. (3) together with the boundary condition. Ordinarily, passage from the operator form Eq. (5) to the differential equation may be accomplished using the completeness of the coordinate eigenstates. But, as was seen in the preceding section, this is neither legal nor necessary. For example, using Eq. (8) and the completeness of the momentum eigenstates,

$$\begin{aligned}\langle x|\hat{p}^2|\phi(t)\rangle&=\int_{-\infty}^\infty dk\,k^2\langle x|k\rangle\langle k|\phi(t)\rangle\\&=-\partial^2\int_{-\infty}^\infty dk\,\langle x|k\rangle\langle k|\phi(t)\rangle\\&=-\partial^2\langle x|\phi(t)\rangle\ .\end{aligned}$$

Thus, with the prescription discussed above, the differential equation may be "recovered" from the operator equation using legal operations. Further detail is contained in the following.

B. Operator representation of the eigenvalue equation for the $\phi_n(x)$

In Sec. I, we introduced the eigenstates of the "unperturbed" Hamiltonian according to

$$\hat{H}_0|\phi_n\rangle=(\tfrac{1}{2}\hat{p}^2+g\hat{x})|\phi_n\rangle=E_n|\phi_n\rangle\ . \tag{10}$$

Introduce momentum eigenstates $|k\rangle$ and denote $\langle k|\phi_n\rangle=\phi_n(k)$. As we have seen, the representative of the position operator in the momentum representation is $\langle k|\hat{x}|k'\rangle=-\partial_k\delta(k-k')$. It follows that

$$ig\partial_k\phi_n(k)=[E_n-\tfrac{1}{2}k^2]\phi_n(k)\ , \tag{11}$$

which has solutions

$$\phi_n(k)=\mathcal{N}\exp\left[i\left[\frac{k^3}{6g}-k\frac{E_n}{g}\right]\right]\ . \tag{12}$$

Introduce $\phi_n(x)=\langle x|\phi_n\rangle$ through the intermediary of the $\phi_n(k)$:

$$\phi_n(x)=\mathcal{N}\int_{-\infty}^\infty dk\,\exp\left[i\left[\frac{k^3}{6g}-k\frac{E_n}{g}\right]\right]e^{ikx}\ . \tag{13}$$

[A factor $1/\sqrt{2\pi}$ has been absorbed into the normalization constant $\mathcal{N}$ in passing from Eq. (12) to Eq. (13).] Equation (13) is a standard representation for the Airy function, which satisfies the equation

$$E_n\phi_n(x)=[-\tfrac{1}{2}\partial_x^2+gx]\phi_n(x)\ . \tag{14}$$

In addition, the condition that

$$\phi_n(0)=0 \Longrightarrow \int_0^\infty dk\,\cos\left[\frac{k^3}{6g}-k\frac{E_n}{g}\right]=0\ ,$$

the well-known condition that quantizes the eigenvalues E_n. One can say equally well that the $\phi_n(k)$ "satisfy the boundary condition" provided the eigenvalues E_n take the required values. Absolutely no unconventional steps have been employed.

C. Projection of the solution of the full problem onto the $|\phi_n\rangle$

Our aim is now to solve the projection of Eq. (5) onto the states $|\phi_n\rangle$. Explicitly,

$$i\partial_t\langle\phi_n|\phi(t)\rangle=E_n\langle\phi_n|\phi(t)\rangle+f(t)\langle\phi_n|\hat{p}|\phi(t)\rangle\ . \tag{15}$$

The ansatz provided by Eq. (6) reads

$$\langle\phi_n|\phi(t)\rangle=e^{-i\xi(t)}e^{-iE_nt}\int_{-\infty}^{\infty}dk\,\phi_n^*(k)e^{-ih(t)k}\langle k|\phi(t=0)\rangle. \tag{16}$$

[In what follows, $|\phi(t=0)\rangle$ will be denoted more succinctly as $|\phi(0)\rangle$.] As in Sec. I, application of the time derivative leads to

$$i\partial_t\langle\phi_n|\phi\rangle=(\partial_t\xi+E_n)\langle\phi_n|\phi\rangle+f(t)e^{-i\xi(t)}e^{-iE_nt}\int_{-\infty}^{\infty}dk\,k\phi_n^*(k)e^{-ih(t)k}\langle k|\phi(0)\rangle\ . \tag{17}$$

On the other hand, if we insert Eq. (6) into the rightmost member of Eq. (15), we obtain

$$\begin{aligned}\langle\phi_n|\hat{p}|\phi(t)\rangle&=\int_{-\infty}^{\infty}dk\,\phi_n^*(k)\langle k|\hat{p}|\phi(t)\rangle\\&=\int_{-\infty}^{\infty}dk\int_{-\infty}^{\infty}dk'\phi_n^*(k)e^{-i\xi(t)}\langle k|\hat{p}e^{-i\hat{H}_0t}|k'\rangle e^{-ih(t)k'}\langle k'|\phi(0)\rangle\ .\end{aligned} \tag{18}$$

We need to relate this expression to the RHS of Eq. (17). To do so, we first *assume* the validity of the following commutation relation and then return to verify that it is true:

$$\langle k|\hat{p}e^{-i\hat{H}_0t}|k'\rangle=\langle k|e^{-i\hat{H}_0t}\hat{p}|k'\rangle-gt\langle k|e^{-i\hat{H}_0t}|k'\rangle\ . \tag{19}$$

Inserting Eq. (19) into Eq. (18), we find

$$\langle\phi_n|\hat{p}|\phi(t)\rangle=e^{-i\xi(t)}e^{-iE_nt}\int_{-\infty}^{\infty}dk\,k\phi_n^*(k)e^{-ih(t)k}\langle k|\phi(0)\rangle-gt\langle\phi_n|\phi(t)\rangle\ . \tag{20}$$

It follows that the proposed solution is verified, provided $\xi(t)$ is that of Sec. I.

Equation (19) is an "obvious" result if one believes that (a) the exp of the operator is defined by its power series expansion, and (b) the commutator $[\hat{H}_0,\hat{p}]$ has been evaluated correctly. We will not demonstrate these points in general, discussing only (b) within the eigenstates of the momentum operator. Our discussion mirrors the discussion for the free particle—through use of the momentum representation, results valid in the half-space excluding the origin are obtained. At the end of the day, our configuration space answer must be multiplied by $\theta(x)$.

D. The commutator $[\hat{H}_0,\hat{p}]$

We aim to evaluate $\langle k|[\hat{H}_0,\hat{p}]|k'\rangle$. To this end, we develop $\langle k|[\hat{H}_0,\hat{p}]|k'\rangle=(k'-k)\langle k|\hat{H}_0|k'\rangle$. From the remarks preceding Eq. (11), we have $\langle k|\hat{H}_0|k'\rangle=ig\partial_k\delta(k-k')+\frac{1}{2}k^2\delta(k-k')$. On test functions, $(k'-k)\partial_k\delta(k-k')=\delta(k-k')$, so that

$$\langle k|[\hat{H}_0,\hat{p}]|k'\rangle=ig\langle k|k'\rangle\ , \tag{21}$$

as was required in the preceding section.

A brief remark on the exponentiated Hamiltonian is in order. Expanding the operator in a power series, we really are confronted with the commutator $\langle k|[\hat{H}_0^n,\hat{p}]|k'\rangle$. Equation (19) is obtained by carefully "peeling" one power of $\hat{H}_0$ off at a time, inserting complete sets of momentum eigenstates, using Eq. (21) for that term, and then removing extraneous complete sets. If this is done in a consistent fashion, Eq. (19) emerges without surprises. (If one attempts a representation for $\hat{H}_0^n$ directly, a rat's nest of overlapping integrals ensues.)

E. Discussion

The previous sections demonstrate that there exists a basis within which the formal manipulation of operators, which motivated the "heuristic" derivation of Sec. I, is demonstrably correct. We found in Sec. II that in the simplest possible case, the free particle, these same formal manipulations may be likewise justified. They yield solutions to the differential equation that satisfy the boundary condition—but they fail to impose the requirement that the wave function vanish in the entire left half-space.

Intuitively this is unsettling. A hard wall reverses the sense of momentum and thus acts as an impulsive force. Nonetheless, we saw that the physics is entirely reproduced in its mathematical consequences (for those matrix elements we need) through the *a posteriori* restriction of the wave function to the half-space through the introduction of $\theta(x)$.

Thus it appears that if we solve the problem the way it is usually posed—satisfying the equation and the boundary condition—the solution that has been obtained is valid in the entire half-space, with an innocuous mathematical embarrassment precisely at the origin. Yet another way of describing the source of this embarrassment is to say that since the first derivative is discontinuous at the wall, the second derivative does not properly exist. We conclude that the mathematical problem of the boundary term is inherent in the restriction of the coordinate eigenstates, but that it has no physical significance.

F. Solution in coordinate representation

Ultimately, one is interested in a coordinate representation of the solution. Again, the ordinary procedure would be to insert complete sets of coordinate eigenstates, a procedure which is not valid for the problem at hand. Consequently, a careful construction based on valid operations is required. To this end our starting point is Eq. (6). Assume that the operator $e^{-i\hat{H}_0 t}$ has an inverse, so that Eq. (6) may be rewritten

$$e^{i\hat{H}_0 t}|\phi(t)\rangle = e^{-i\xi(t)}e^{-ih(t)\hat{p}}|\phi(0)\rangle \ . \tag{22}$$

On the left-hand side (LHS) we insert a complete set of eigenstates of the unperturbed problem and project with $\langle x|$; on the RHS, simply project

$$\sum_n e^{iE_n t}\phi_n(x)\langle\phi_n|\phi(t)\rangle = e^{-i\xi(t)}\langle x|e^{-ih(t)\hat{p}}|\phi(0)\rangle \ . \tag{23}$$

Inserting a complete set of momentum eigenstates, the matrix element on the RHS of Eq. (23) becomes

$$\langle x|e^{-ih(t)\hat{p}}|\phi(0)\rangle = \int_{-\infty}^{\infty} dk\,\langle x|k\rangle e^{-ih(t)k}\langle k|\phi(0)\rangle \equiv \Psi_0(x-h(t)) \ .$$

If we now multiply both sides of Eq. (23) by $\phi_m(x)$ and integrate over non-negative x, we obtain precisely Eq. (7) in the form $\langle\phi_n|\phi(t)\rangle = (\phi_n,\phi(t))$, "as though" insertion of a complete set of coordinate eigenstates had been introduced. The coordinate representation of the wave function is then constructed through

$$\phi(x,t) = \langle x|\phi(t)\rangle = \sum_n \phi_n(x)(\phi_n,\phi(t)). \tag{24}$$

This method of derivation may seem somewhat circuitous, but it is necessary in order to avoid an invalid introduction of complete sets of coordinate eigenstates. As we will see below, the quantities $(\phi_n,\phi(t))$ are nonsingular. Thus the representation Eq. (24) assures that the full solution $\phi(x,t)$ satisfies the boundary condition because the $\phi_n(x)$ do. But if we had opted to reintroduce the extended Hamiltonian formulation, introducing $V\theta(-x)$, we might have been tempted to perform a certain x integration extending from $-\infty$ to $+\infty$, and so extract a singular contribution $\delta(x_n - x_m - h(t))$. [Here the x_j are the classical turning points, and we have in mind the case that the initial state is the unperturbed eigenstate $\phi_m(x)$.] Since $h(t)$ is a continuous function, this condition would force the eigenvalue $E_n = gx_n$ off the value for which vanishing of the wave function $\phi_n(x)$ is assured. The procedure we have implemented avoids this possible pitfall.

V. APPROXIMATE EVALUATION OF THE QUANTITIES (ϕ_n,ϕ)

We have proved that

$$\phi(x,t) = e^{-i\xi(t)}\sum_n \phi_n(x)e^{-iE_n t} \times \int_0^{\infty} dx'\phi_n(x')\Psi_0(x'-h(t)) \ , \tag{25}$$

where $\xi(t) = -g\int_0^t dt' t' f(t')$ is a solution of Eq. (3) subject to the boundary condition $\phi(0,t)=0$. Again, $\Psi_0(x) = \phi(x,t=0)$, the initial condition.

For the remainder of this paper we will examine approximations to the integral

$$T_{nm}(t) = \int_{h(t)}^{\infty} dx\,\phi_n(x)\phi_m(x-h(t)) \ . \tag{26}$$

This corresponds to the initial condition that the system is definitely in state m of the unperturbed problem $\phi(x,0) = \phi_m(x)$. The lower limit of this integral is set equal to $h(t)$ because the eigenfunctions to the unperturbed problem vanish not only at the boundary but at all points on the negative axis. In the interest of concise presentation, all details of the development that follow are deferred to the Appendix.

Recall the (unnormalized) representation

$$\phi_n(x) = \int_{-\infty}^{\infty} dk \exp\left[i\left[\frac{k^3}{6g} + k(x-x_n)\right]\right] \ ,$$

where $x_n = E_n/g$ is the classical turning point. Then, T_{nm} is a triple integral that eventually can be expressed as a single remaining integral (Appendix, Sec. 1):

$$T_{nm}(t) = -\Sigma^{-1/4}\,\mathrm{Im}\int_0^{\infty}\frac{dv}{\sqrt{v}}\exp\{i[\pi/4+\chi(v)]\} \ . \tag{27}$$

Here, $\chi(v) = \Sigma^{3/2}[1/24gv^3 - 1/v - 2g\rho^2 v]$, $\Sigma = [x_n + x_m - h(t)]/2, \Delta = [x_n - x_m - h(t)]/2$, and $\rho = \Delta/\Sigma$. No approximations have been made to this point, although $\Sigma > 0$ has been assumed with a view to the semiclassical limit.

From the form of T it is natural to attempt a stationary phase estimate to the integral for $\Sigma \gg 1$. The stationary points of the phase occur at

$$v_{\pm} = \{[1 \pm (1-\rho^2)^{1/2}]/4g\rho^2\}^{1/2} \ . \tag{28}$$

By definition, $1 \geq |\rho|$, but if we further assume that ρ is small, we have one root at large v and the other at $v^2 \approx (8g)^{-1}$. Since, in principle, g can be large, some care is needed in estimating the integral at this second root due to the presence of $\sqrt{v}$ in the denominator of the integrand [10] (Appendix, Sec. 2). Similarly, care must be exercised in estimating the normalization integrals (Appendix, Sec. 3). The result for large E_n is

$$(\phi_n,\phi_n) \approx 4\pi\sqrt{2E_n} \ , \tag{29}$$

and we also record here (Appendix, Sec. 4)

$$E_n^{3/2} \approx (3\pi g/2^{3/2})(n-\tfrac{1}{4}) \quad \text{for } n = \text{large integer} \ . \tag{30}$$

Omitting the normalization factors, the stationary phase estimate is

$$T_{nm}(t) \approx (2\pi/\Delta)\sin(2\Delta\sqrt{2g\Sigma}) - (\pi\sqrt{2}/2\Sigma)[\sin\{\tfrac{2}{3}(2g\Sigma^3)^{1/2}\} + \sqrt{2}\cos\{\tfrac{4}{3}(2g\Sigma^3)^{1/2}\}]\ . \qquad (31)$$

Three features of this expression are noteworthy. First, $T_{nm}(t)$ has the same periodicity as the surface. In addition, once the normalization has been introduced, $T_{nm}(t)$ is a numerical function of n and m, with the "dimensionless" parameter $g^{1/3}h_0$. That is, $T_{nm}(t)$ does not depend on g and h_0 separately, but only on this combination (Appendix, Sec. 5). Finally, although this expression has been derived for $\Delta \ll \Sigma$, it is clear that T does not decay exponentially with Δ. We believe this feature will survive a more detailed analysis of Eq. (26), and it indicates consistency with the absence of Kolmogorov-Arnold-Moser (KAM) trajectories for the classical problem [1,2]. At present we are not sure, however, whether the periodicity of T is a reflection of the existence of a Poincaré-Cartan integral invariant [1].

Figures 1–3 illustrate numerical evaluations of the normalized estimate of $T_{nm}(t)$. For the purpose of these illustrations, we have set $g=\omega=1$ and $h_0=5$ in Figs. 1 and 2, corresponding to a "stochasticity parameter" [1–3] $4\omega^2 h_0/g=20$, well into the classically chaotic region. Figure 3 corresponds to a stochasticity parameter twice as large. Given an initial mode, the computer program searched for a range of modes such that the parameter ρ^2 remained smaller than approximately 1/16, while parameter $\Sigma \gg 1$. In all cases, the second half-period just reverses the evolution during the initial half-period, and so is not displayed.

Throughout this work I have employed units $h/2\pi=1$, where h is Planck's constant. We may, however, consider the progression to higher values of m to correspond to approaching the semiclassical limit. Figures 1 and 2 clearly indicate that as m increases, the structure of $T_{nm}(t)$ becomes more richly detailed. [Some of the "filigree" in the vicinity of the maximum is due to numeric or graphic artifacts. The larger scale "peacock" structures survive enhanced computational resolution.]

We will defer to later work attempts to quantify the observed structure and to discuss it in terms of quantal manifestations of classical chaos. Qualitatively, however, we offer this conjecture. For large mode numbers, the Airy functions $\phi_n(x)$ are sharply peaked at the classical turning point. The "trajectory" of maximal values of $T_{nm}(t)$ "drags" the spatial maximum of the wave func-

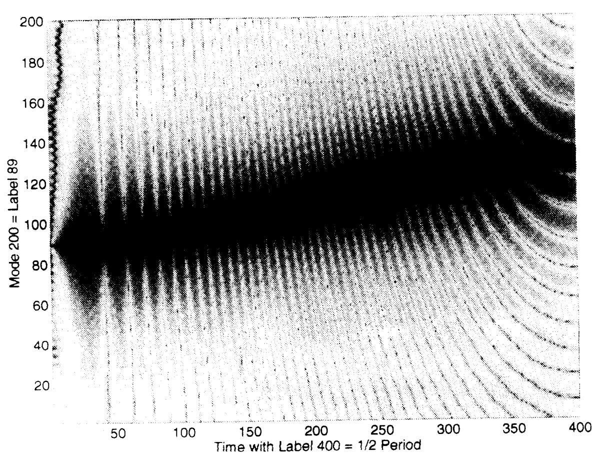

FIG. 1. Magnitude of the coupling (natural logarithm of the absolute value) of the initial state mode 200 to nearby modes over $\frac{1}{2}$ cycle of the perturbation. The motion reverses over the second $\frac{1}{2}$ cycle. The dark curve and the striations are maxima. In this and the other figures, the range is from order 1 to e^{-12}. The parameters are $g=\omega=1$ and $h_0=5$. Due to the details of the graphics package employed, the point where the "intense" curve intersects the ordinate indicates the *sequential label* for the initial mode. That is to say, mode 200 has a label corresponding to the intersection. Mode 300 is 100 axis units above this, etc. Similarly, the time is in units 1 to 400 with 400 corresponding to $\frac{1}{2}$ period.

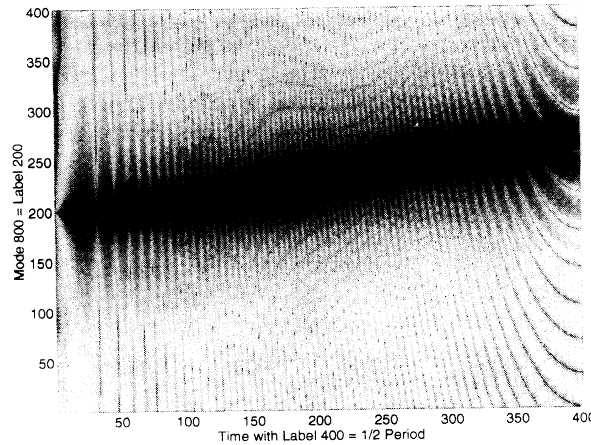

FIG. 2. Same as Fig. 1 with initial state mode 800. Increasing the initial mode number may be viewed as effectively decreasing Planck's constant in the quantal context.

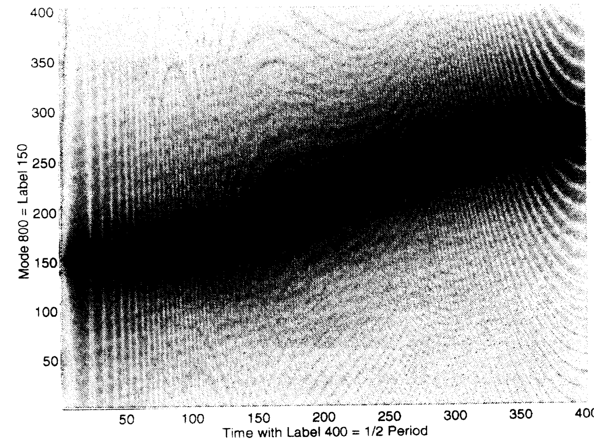

FIG. 3. Same as Fig. 1 with initial state mode 800, but $h_0=10$. Classically, this increases the stochasticity of the ray trajectories.

tion up and down with the periodicity of the wall (in its rest frame). There are, however, a large number of weaker maxima that have a more complicated and intricate time dependence, suggesting rapid spatial jumps. Nothing requires that individual jumpers take short leaps, so long as their total number follows the pattern. It is easy to envision chaotic trajectories.

In conclusion, we reiterate that Eq. (7) is the central result of this paper, although the integral expression given for $T_{nm}(t)$ is also exact for Σ positive. Approximations to T were described and the results were displayed graphically. It is evident that the wave mechanics of the bouncing ball develops interesting structure. The coordinate representation of the solution will be employed to investigate the quantal manifestations of classical chaos further, and the results will be reported elsewhere.

ACKNOWLEDGMENTS

I thank Mike Brown and Fred Tappert for helpful remarks in the course of this work. I also thank Jorge Jose for many instructive discussions, Yoichiro Nambu for encouragement, Michael Berry for pressing me on details, and Richard Eykholt for demanding rigor. This work was supported in part through NSF Grant No. OCE-9115949.

APPENDIX

1. Representation of T_{nm} as a single integral

For the moment, neglect the normalization factor $\mathcal{N}$ appearing in Eq. (13). Noting that the functions $\phi_n(x)$ are real, insert that representation into Eq. (26) to obtain

$$T_{nm}(t)=\int_{h(t)}^{\infty}dx\int_{-\infty}^{\infty}dk\,\exp\left[i\left(\frac{k^3}{6g}+k(x-x_n)\right)\right]\int_{-\infty}^{\infty}dk'\exp\left[i\left(\frac{k'^3}{6g}+k'(x-h(t)-x_m)\right)\right].$$

The x integration can be performed directly (and we neglect $i\varepsilon$ prescriptions, as they are not necessary for what follows):

$$\int_{h(t)}^{\infty}dx\,\exp[i(k+k')x]=\frac{i\exp[i(k+k')h(t)]}{(k+k')}.$$

Let

$$k=\frac{\sigma+\delta}{2},\quad k'=\frac{\sigma-\delta}{2},\quad \Sigma=\frac{x_n+x_m-h(t)}{2},\quad \text{and finally,}\quad \Delta=\frac{x_n-x_m-h(t)}{2}.$$

These changes result in

$$T_{nm}(t)=\frac{i}{2}\int_{-\infty}^{\infty}\frac{d\sigma}{\sigma}\exp\left[\frac{i\sigma^3}{24g}\right]e^{-i\sigma\Sigma}\int_{-\infty}^{\infty}d\delta\,\exp\left[\frac{i\sigma\delta^2}{8g}\right]e^{-i\delta\Delta}.$$

The δ integral can be done at once, producing

$$T_{nm}(t)=\frac{i}{2}\int_{-\infty}^{\infty}\frac{d\sigma}{\sigma}\left[\frac{8\pi g}{-i\sigma}\right]^{1/2}\exp\left[\frac{i\sigma^3}{24g}\right]e^{-i\sigma\Sigma}\exp\left[\frac{-2ig\Delta^2}{\sigma}\right].$$

In this expression, we *have* exercised caution regarding placement of the factor $(-i)^{-1/2}$, for we now introduce $w=\sigma^{-1}$ and end up with an expression involving only non-negative w. Keeping careful track of the phase,

$$T_{nm}(t)=\frac{i}{2}\int_0^{\infty}dw\left[\frac{8\pi g}{-iw}\right]^{1/2}e^{i\chi(w)}+\frac{i}{2}\int_0^{\infty}dw\left[\frac{8\pi g}{iw}\right]^{1/2}e^{-i\chi(w)}=\frac{i}{2}(2i)\,\mathrm{Im}\int_0^{\infty}dw\left[\frac{8\pi g}{w}\right]^{1/2}e^{i\chi(w)}e^{i\pi/4}.$$

The function $\chi(w)$ is simply the preceding exponent expressed in terms of $w=\sigma^{-1}$. Finally, let $v=\sqrt{\Sigma}w$, under the assumption that Σ is positive. The integral representation Eq. (27) follows.

2. Implementation of the stationary phase estimate

We are interested in approximating the integral $K=\int_0^{\infty}(dv/\sqrt{v})e^{i\chi(v)}$, with $\chi(v)$ as described above and written out in the text after Eq. (27). The stationary points of the phase are the solutions of $\chi'(v)=0$, which is a quadratic equation in the variable v^2. However, the integration has been restricted to the positive v axis, so the stationary points of interest are just the pair indicated in Eq. (28), $v_{\pm}=\{[1\pm(1-\rho^2)^{1/2}/4g\rho^2\}^{1/2}$. As noted there, v_+ is not small. That is, recall that parameter

$$\rho=\Delta/\Sigma=\frac{x_n-x_m-h(t)}{x_n+x_m-h(t)}.$$

The function $h(t)$ is of order 1 for all t. In the semiclassical limit, we are interested in at least one of the classical turning points to be located at $x\gg 1$, and so also $\Sigma\gg 1$. "Small ρ" then means a band of neighboring large energies, and in this circumstance $v_+\approx[2g\rho^2]^{-1/2}\gg 1$. Thus about this stationary point,

$$K(v_+)\approx\left[\frac{2\pi}{-iv_+\chi''(v_+)}\right]^{1/2}e^{i\chi(v_+)}$$
$$\Longrightarrow \mathrm{Im}\,e^{i\pi/4}K(v_+)$$
$$\approx-\frac{\sqrt{\pi}\sin(2\sqrt{2g}\,\rho\Sigma^{3/2})}{\sqrt{2g}\,\rho\Sigma^{3/4}} .$$

On the other hand, with the same approximation, $v_-\approx[8g]^{-1/2}$, and this can be sufficiently close to zero so that respect for $v^{-1/2}$ in the denominator of the integrand is required. Following Ref. [10], Taylor expand the phase but work a bit further:

$$K(v_-)\approx e^{i\chi(v_-)}\int_0^\infty\frac{dv}{\sqrt{v}}\exp[i(8g\Sigma)^{3/2}(v-v_-)^2] .$$

Change the contour according to

$$v=\frac{\eta e^{i\pi/4}}{\sqrt{2}(8g\Sigma)^{3/4}}$$

and introduce $z=e^{3i\pi/4}(32g\Sigma^3)^{1/4}$. This produces

$$K(v_-)\approx C(\Sigma,g)\int_0^\infty\frac{d\eta}{\sqrt{\eta}}\exp[-\eta^2/2-\eta z] ,$$

where C is a messy complex expression.

The remaining integral can be expressed in terms of the parabolic cylinder function $D_{-1/2}(z)$. For Σ large, use the approximation appropriate for $\arg(z)=3\pi/4$,

$$D_{-1/2}(z)\to\frac{1}{\sqrt{z}}[\exp(-z^2/4)+i\sqrt{2}\exp(z^2/4)] .$$

Insert this result into the expression for $K(v_-)$, take the required imaginary part, add $K(v_+)$, and insert the prefactors relating T to K. Equation (31) then follows. (These steps require nothing more than arithmetic, so the full details will not be displayed.)

3. Normalization integral

Equation (29) is most easily obtained by setting $n=m$, $h(t)=0$, in Eq. (31). Then $\Delta\to0$, while $\Sigma=x_n$. We have

$$T_{nm}(t)\to(\phi_n,\phi_n)=4\pi\sqrt{2gx_n}-O(1/x_n) ,$$

from which Eq. (29) follows for large x_n.

4. Eigenvalue condition

If $f(+t)=-f(-t)$, $\int_{-\infty}^{\infty}dt\,e^{if(t)}=2\int_0^\infty dt\cos f(t)$. Thus through a rescaling of the integration variable, the representation Eq. (13) may be written $\phi_n(x)\propto\int_0^\infty dt\cos(t^3-zt)$, where $z=(6g)^{1/3}(x_n-x)$, and as $x\to0$, $z>0$. In this situation,

$$\int_0^\infty dt\cos(t^3-zt)=(\pi z^{1/2}/3^{3/2})\{J_{1/3}[2(z/3)^{3/2}]+J_{-1/3}[2(z/3)^{3/2}]\} .$$

Application of an asymptotic formula for J_ν with large argument leads to the condition $\phi_n(0)=0\Longrightarrow\cos(\alpha x_n^{3/2}-\pi/4)=0$, where $\alpha=(8g)^{1/2}/3$. Equation (30) follows. The result is identical to a WKB estimate neglecting terms of 0(1).

5. Formula for the normalized transition amplitudes

The stationary phase estimates cited above for $T_{nm}(t)$ did not take the normalization of the ϕ_n into account. A "normalized" version within the present notation reads $T_{nm}(t)=T_{nm}(t)/\sqrt{(\phi_n,\phi_n)(\phi_m,\phi_m)}$. To simplify the formula for $T_{nm}(t)$ examine first the expression $(2g\Sigma^3)^{1/2}$, which appears in Eq. (31). Using the asymptotic approximation for the eigenvalues,

$$(2g\Sigma^3)^{1/2}=(3/2^{5/2})\{[(n-\tfrac14)\pi]^{2/3}+[(m-\tfrac14)\pi]^{2/3}-h_0\alpha^{2/3}[1-\cos(\omega t)]\}^{3/2} ,$$

with $\alpha=(8g)^{1/2}/3$ as before. [The function $h(t)$ has been evaluated to obtain this result.] This encourages us to denote

$$\Sigma_{nm}\{\Delta_{nm}\}\equiv\{[(n-\tfrac14)\pi]^{2/3}+\{-\}[(m-\tfrac14)\pi]^{2/3}-h_0\alpha^{2/3}[1-\cos(\omega t)]\} .$$

Similarly, from the normalization factors, we have

$$(x_nx_m)^{-1/4}=\alpha^{1/3}\{[(n-\tfrac14)\pi][(m-\tfrac14\pi]\}^{-1/6}\equiv\alpha^{1/3}N_{nm}^{-1/6} .$$

Assemble the pieces to obtain

$$T_{nm}(t)=(2N_{nm}^{-1/6}/3)((1/\Delta_{nm})\sin([3/2^{3/2}]\Delta_{nm}\sqrt{\Sigma_{nm}})-(\sqrt{2}/4\Sigma_{nm})\{\sin(\Sigma_{nm}/2)^{3/2}+\sqrt{2}\cos[2(\Sigma_{nm}/2)^{3/2}]\}) .$$

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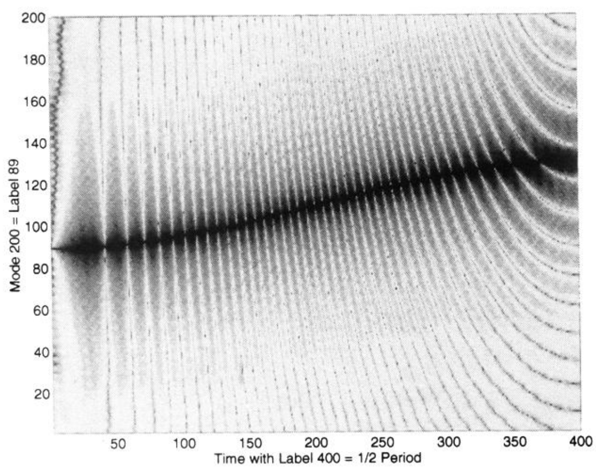

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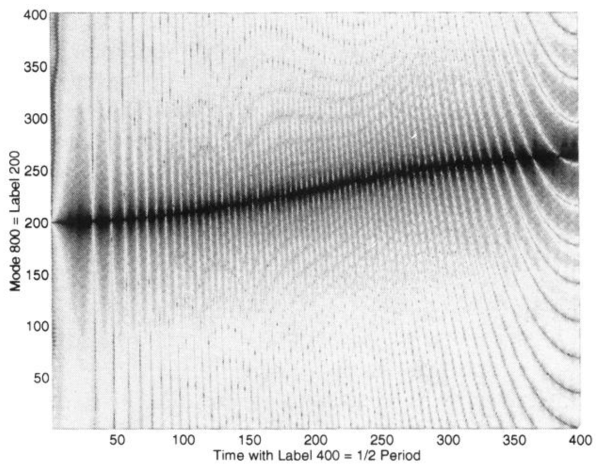

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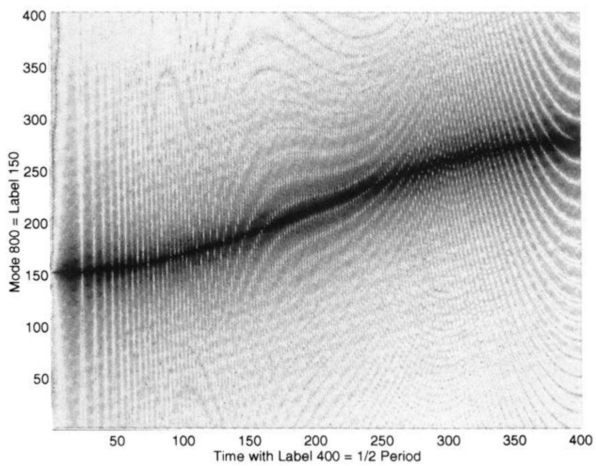

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