Integration of the Heisenberg equations of motion for quartic potentials

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A direct integration of the Heisenberg equations of motion yields expansions of the position and momentum operators $x(t)$ and $p(t)$, each as an infinite series in terms of the initial Weyl-ordered basis set $\{S_{m,n}\}$ formed from $x(0)$ and $p(0)$, with c-number time-dependent coefficients. This method is applied to the problem of tunneling in a symmetric and an asymmetric quartic potential. The expectation values of the position and momentum operators with minimum uncertainty wave packet $\langle 0|x(t)|0\rangle$ and $\langle 0|p(t)|0\rangle$ can be calculated accurately for a maximum time that is short compared to the period of oscillation of the wave packet. From the result of this calculation, with the help of Prony's method one can determine the level spacings for the low-lying states. In addition, in this formulation the wave packet retains its shape; therefore, one can study the trajectory $\langle 0|x(t)|0\rangle$ and $\langle 0|p(t)|0\rangle$ as the quantal analogue of the motion of the system in phase space.

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I. INTRODUCTION

Klein and co-workers in a series of papers have studied the possibility of using Heisenberg's equation of motion to obtain the eigenvalues of simple one-dimensional systems such as those of quartic symmetric potentials [1–3]. From the equations of motion, the Hamiltonian operator, and the canonical commutation relations they have found that for these potentials the eigenvalues can be determined very accurately for weak as well as strong potentials from the solution of a set of nonlinear algebraic equations. This approach is different from the classical way of solving these problems since it is formulated in terms of a time-independent set of equations. A method of integration of the operator equations, as an initial value problem, has been recently proposed by Bender and co-workers [4–8], where the position and momentum of the particle at time t is expressed in terms of an infinite series of Weyl-ordered operators at $t=0$, with time-dependent c-number coefficients. The integration of these operator equations enables one to investigate the details of the motion of a wave packet describing the particle as it tunnels between two potential wells or jumps over a barrier [9–10].

In this work, we study some aspects of the solution of the Heisenberg equations of motion for confining double well potentials. In Sec. II we write the equations of motion for a general quartic potential in terms of a dimensionless parameter that measures the strength of the potential. The Hamiltonian operator in this case is the generator of the unfolding of the system in the dimensionless time variable θ. In Sec. III, we study the motion of a Gaussian wave packet, which initially has its center at the position of the minimum of one of the wells of the double well potential. We determine the inequality that must be satisfied by the potential parameter so that the energy associated with the wave packet is less than the height of the central maximum of the potential. Thus we study the motion of the packet as it tunnels through the barrier. Having obtained this condition, we find the equation of motion for quartic potentials satisfied by the Weyl-ordered set of operators $\{S_{m,n}(\theta)\}$ of which the Heisenberg equations are special cases. By integrating the differential operator equations $dS_{mn}(\theta)/d\theta$, we obtain the expectation values of position and momentum operators of the center of the Gaussian wave packets as a function of θ, but only for times short compared to the period of oscillation of the wave packet between the two wells, if quantum tunneling can take place. From this partial knowledge of the motion of the wave packet we want to obtain information about the observables of the system. To this end we use the simplest version of the Prony method [11] of determining the frequencies of a finite sum of sinusoidal functions of time which gives us the position of the center of the wave packet (Sec. IV). Before applying this technique to our problem we test its accuracy on an exactly solvable bistable potential. For this potential we determine the matrix element of the position operator for a time that is short compared to the known period of oscillation. Then we use Prony's method to invert the process and find the level spacings from the time dependence of the matrix element. We observe that only for very strong potentials when the level spacing is very small, the Prony method fails to give accurate results (Sec. V). In Sec. VI, we apply this method of inversion to quartic symmetric and asymmetric potentials and obtain the level spacing for the low-lying states. In addition to the matrix elements of x and p, in this approach, those of $S_{m,n}(\theta)$ are found. This enables us to obtain the time dependence of the uncertainty product $\Delta x \Delta p$ and also study the quantal analogue of the motion of the classical particle in the phase space.

II. EQUATIONS OF MOTION

Consider a typical asymmetric potential given by

$$V(x)=(1/2)m\omega^2x^2[(x/a)^2-A(x/a)+B]\ , \qquad (2.1)$$

where A and B are dimensionless constants and ω and a are constants having the dimensions of (time)$^{-1}$ and length, respectively. This potential has two minima one at $x=x_0=0$, where $V(x=x_0)=0$, and the other at $x=x_2=[3A+(9A^2-32B)^{1/2}](a/8)$, where $V_{\min}=V(x=x_2)$. These two minima are separated by a barrier with a maximum at $x=x_1=[3A-(9A^2-32B)^{1/2}](a/8)$, where the height of the barrier is $V(x=x_1)$. The Hamiltonian for this system is

$$H=p_x^2/(2m)+V(x) , \tag{2.2}$$

where p_x and x satisfy the commutation relation

$$[x,p_x]=i\hbar . \tag{2.3}$$

To simplify the problem let us first consider the dimensionless coordinate ξ, and its conjugate momentum p_ξ defined by

$$\xi=x/a \quad \text{and} \quad p_\xi=ap_x , \tag{2.4}$$

and then replace p_ξ by a dimensionless momentum operator p, where

$$p=p_\xi/(m\omega a^2) . \tag{2.5}$$

With these changes the commutation relation (2.3) is replaced by

$$[\xi,p]=i/\beta^2 , \quad \beta^2=m\omega a^2/\hbar , \tag{2.6}$$

where β^2 is also dimensionless. In terms of these dimensionless operators the Hamiltonian (2.2) becomes

$$H=(m\omega^2a^2/2)[p^2+\xi^2(\xi^2-A\xi+B)] . \tag{2.7}$$

Finally let us introduce a dimensionless time by $\theta=\omega t$ and its conjugate Hamiltonian by $K=H/(\hbar\omega)$ so that

$$K=(\beta^2/2)[p^2+\xi^2(\xi^2-A\xi+B)] . \tag{2.8}$$

The Heisenberg equations of motion derived from Eqs. (2.6) and (2.8) are

$$i d\xi/d\theta=[\xi,K]=[\xi,\beta^2p]=ip , \tag{2.9}$$

and

$$\begin{aligned} i\,dp/d\theta&=[p,K]=[p,-\beta^2\xi^2(\xi^2-A\xi+B)] \\ &=-i[2\xi^3-(3/2)A\xi^2+B\xi] . \end{aligned} \tag{2.10}$$

III. MOTION OF A GAUSSIAN WAVE PACKET

From Eq. (2.8) it is clear that around $\xi=x/a\approx 0$, the potential can be approximated by a harmonic-oscillator potential

$$V(\xi)\approx(1/2)\beta^2B\xi^2 . \tag{3.1}$$

The ground-state wave function for this potential is a Gaussian wave packet;

$$\psi(\xi)=(\nu/\pi)^{1/4}\exp[-(1/2)\nu\xi^2] , \tag{3.2}$$

where

$$\nu=\sqrt{B}\,\beta^2 . \tag{3.3}$$

The momentum p is given by the differential operator

$$p=-(i/\beta^2)d/d\xi , \tag{3.4}$$

therefore, K in (2.8) can be written as

$$K=(\beta^2/2)[-(1/\beta^4)(d^2/d\xi^2)+\xi^2(\xi^2-A\xi+B)] . \tag{3.5}$$

The expectation value of this Hamiltonian with the wave function ψ, Eq. (3.2) is

$$\langle 0|K|0\rangle=[\sqrt{B}/2+3/(8\beta^2B)] . \tag{3.6}$$

If the center of the wave packet (3.2) is displaced by ξ_0, i.e., for the wave function $\psi(\xi-\xi_0)$ the expectation value of K is given by

$$\begin{aligned} \langle 0|K|0\rangle_{\xi_0}&=\sqrt{B}/2+3/(8\beta^2B) \\ &\quad+\xi_0[(\beta^2\xi_0/2)(\xi_0^2-\xi_0A+B) \\ &\quad+(3/2\sqrt{B})(\xi_0-A/2)] . \end{aligned} \tag{3.7}$$

For quantum tunneling, the expectation value of K which is related to the energy of the wave packet (3.2) representing the particle should be less than the height of the barrier at $x_1=a\xi_1$, i.e.,

$$\langle 0|K|0\rangle < V(\xi_1) . \tag{3.8}$$

Now let us consider two specific cases:

(1) If $A=2$ and $B=1$, we have a symmetric double well, $V(\xi)=(\beta^2/2)[\xi^2(\xi-1)^2]$. The maximum height of the barrier is at $\xi=(1/2)$, and $V_{\max}=\beta^2/32$. From Eq. (3.6) and (3.8) it follows that for this case $\beta^2>16.72$.

(2) When $A=14$ and $B=45$, we have an asymmetric well with a local maximum at $\xi=3$, and $V_{\max}=45\beta^2$. For this case from (3.8) we find that β^2 must satisfy the inequality $\beta^2>0.0645$. Similar results can be found from (3.7) and (3.8) when $\xi_0\neq 0$.

If the particle is initially located at $\xi=0$, then the classical motion will be oscillations about this point as long as the kinetic energy $p^2/2$ is less than the height of the barrier $(1/2)\xi_1^2(\xi_1^2-A\xi_1+B)$. For the kinetic energies larger than this the particle passes over the barrier and enters the second well. Thus

$$p_c=\xi_1(\xi_1^2-A\xi_1+B)^{1/2} \tag{3.9}$$

defines the separatrix for this motion. In the case of the symmetric double well with $\beta^2=20$ the value of p_c is (1/4) with the corresponding energy $K_c=0.51875$. For an asymmetric well ($\beta^2=0.1$), $p_c=6\sqrt{3}$, with $K_c=3.4374$.

For integrating the operator equations of motion we start with the wave packet (3.2) and calculate the expectation values of K, Eq. (3.7), $p(\theta=0)$ and $\xi(\theta=0)$,

$$\langle 0|p(0)|0\rangle=0 , \tag{3.10}$$

and

$$\langle 0|\xi(0)|0\rangle=0 . \tag{3.11}$$

Then we introduce the Weyl-ordered operator basis $\{S_{k,n}\}$ which is defined in terms of powers of $p(\theta)$ and $\xi(\theta)$,

$$S_{m,n}=(1/2)^m \sum_{j=0}^{m} \{m!/[(m-j)!j!]\} p^j \xi^n p^{m-j} . \tag{3.12}$$

We note that $S_{k,n}$ form an algebra closed under multiplication [7,8], and that the properties of this algebra can be derived from the product formula

$$S_{m,n}S_{r,s}=\sum_{j=0}^{\infty}(i/2)^j \sum_{k=0}^{j} \{(-1)^{j-k}[1/(j-k)!k!]\beta^{-2j}S_{m+r-j,n+s-j}\} \times \frac{[\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)]}{[\Gamma(n-k+1)\Gamma(m+k-j+1)\Gamma(r-k+1)\Gamma(s+k-j+1)]} . \tag{3.13}$$

From this relation we calculate the commutation relation between two members of the set

$$[S_{m,n},S_{r,s}]=2\sum_{j=0}^{\infty}(i/2)^{2j+1}\sum_{k=0}^{2j+1}\{(-1)^k[1/(2j+1-k)!k!]\beta^{-2j}S_{m+r-2j-1,n+s-2j-1}\} \times\{[\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)]/ [\Gamma(m-k+1)\Gamma(n+k-2j)\Gamma(r+k-2j)\Gamma(s-k+1)]\} . \tag{3.14}$$

We note that ξ and p are expressible in terms of $S_{k,n}$, i.e.,

$$\xi(\theta)=S_{0,1}(\theta) \quad \text{and} \quad p(\theta)=S_{1,0}(\theta) . \tag{3.15}$$

Since K is the generator of motion in time (or $\theta=\omega t$), according to Eqs. (2.9) and (2.10), we can write $\xi(\theta+\Delta\theta)$ as a Taylor series using the time derivatives given by these equations, i.e.,

$$\xi(\theta+\Delta\theta)=\xi(\theta)+[(-i\Delta\theta)/1!][\xi,K]_\theta+[(-i\Delta\theta)^2/2!][[\xi,K],K]_\theta+[(-i\Delta\theta)^3/3!][[[\xi,K],K],K]_\theta+\cdots \tag{3.16}$$

Next we replace the commutators in this expansion in terms of $S_{0,1}$ and $S_{1,0}$ as given by Eq. (3.16). We also choose a step size $\Delta\theta$ and write $\theta=j\Delta\theta$, where j is an integer. With these changes we can write

$$\xi(\theta_{j+1})=\xi(\theta_j)+(\Delta\theta/1!)S_{1,0}(\theta_j)+[(\Delta\theta)^2/2!]f(S_{0,1}(\theta_j))+(1/2)[(\Delta\theta)^3/3!]\{S_{1,0}f'(S_{0,1})+f'(S_{0,1})S_{1,0}\}_{\theta_j}+\cdots \tag{3.17}$$

and

$$p(\theta_{j+1})=S_{1,0}(\theta_j)+(\Delta\theta/1!)f(S_{0,1}(\theta_j))+(1/2)[(\Delta\theta)^2/2!]\{S_{1,0}f'(S_{0,1}(\theta_j))+f'(S_{0,1}(\theta_j))S_{1,0}\}+\cdots , \tag{3.18}$$

where

$$f(\xi)=-[2\xi^3-(3/2)A\xi^2+B\xi] , \tag{3.19}$$

and primes denote derivatives with respect to the argument.

From the definition (3.12), we can calculate the matrix elements of $S_{m,n}$ with the wave function $\psi(\xi)$,

$$\langle 0|S_{m,n}|0\rangle=\begin{cases}[a^{m-n}\beta^{-(m+n)}(B)^{(m-n)/4}(m-1)!!(n-1)!!]/2^{(m+n)/2} , & m \text{ and } n \text{ even}\\ 0 , & \text{otherwise} .\end{cases} \tag{3.20}$$

Thus we have

$$\langle 0|S_{2,0}|0\rangle=a^2\sqrt{B}/(2\beta^2) , \tag{3.21}$$

$$\langle 0|S_{0,2}|0\rangle=1/(2B^{1/2}a^2\beta^2) , \tag{3.22}$$

$$\langle 0|S_{0,4}|0\rangle=3/(4a^4\beta^4B) . \tag{3.23}$$

In our calculations we choose $\hbar=1$ and $a=1$.

From the commutation relation (3.14) we can determine the time derivative of any member of the set $S_{m,n}$ of the ordered operators. To this end we note that

$$i\,dS_{m,n}/d\theta=[S_{m,n},K] . \tag{3.24}$$

Now according to (2.8), K can also be written in terms of $S_{m,n}$

$$K=(\beta^2/2)[S_{2,0}+S_{0,4}-AS_{0,3}+BS_{0,2}] . \tag{3.25}$$

Using the commutators

$$[S_{m,n},S_{2,0}]=(2in/\beta^2)S_{m+1,n-1}\ , \tag{3.26}$$

$$[S_{m,n},S_{0,2}]=-(2im/\beta^2)S_{m-1,n+1}\ , \tag{3.27}$$

$$[S_{m,n},S_{0,3}]=(1/\beta^2)\{-3imS_{m-1,n+2}+(i/4\beta^2)[m!/(m-3)!]S_{m-3,n}\} \tag{3.28}$$

and

$$[S_{m,n},S_{0,4}]=(1/\beta^2)\{-4imS_{m-1,n+3}+(i/\beta^2)[m!/(m-3)!]S_{m-3,n+1}\}\ , \tag{3.29}$$

we find $dS_{m,n}/d\theta$;

$$dS_{m,n}/d\theta=nS_{m+1,n-1}-2mS_{m-1,n+3}+(1/2\beta^2)[m!/(m-3)!][S_{m-3,n+1}-(A/4)S_{m-3,n}] \tag{3.30}$$
$$+(3/2)mAS_{m-1,n+2}-mBS_{m-1,n+1}\ .$$

Thus using (3.30), the equations of motion can be written in terms of $S_{m,n}$ in the following way:

$$dS_{0,1}/d\theta=S_{1,0}\ , \tag{3.31}$$

and

$$dS_{1,0}/d\theta=(1/2)(-4S_{0,3}+3AS_{0,2}-2BS_{0,1})\ . \tag{3.32}$$

These are the same as Eqs. (2.9) and (2.10). Using Eq. (3.30), we can also show that K defined by (3.25) is a constant of motion.

IV. DETERMINATION OF THE EIGENVALUES FOR THE LOW-LYING STATES

Suppose that by the integration of equations of motion, we have obtained $\langle 0|x(t)|0\rangle$ as a function of time. This time dependence of $\langle 0|x(t)|0\rangle$ can directly be related to the low-lying eigenvalues of the bound-state problem. Let us consider the expectation value of the position operator in the Schrödinger picture, i.e., start with a real normalized time-dependent wave packet that describes the motion

$$\Psi(x,t)=\sum_{\nu=0}^{\infty}c_n\psi_n(x)\exp(-iE_nt/\hbar)\ . \tag{4.1}$$

Here E_n and $\psi_n(x)$ denote the eigenvalues and the eigenfunctions of the Hamiltonian H. Using this wave packet we calculate $\langle\Psi(x,t)|x|\Psi(x,t)\rangle$ in terms of the matrix elements $\langle\psi_j|x|\psi_n\rangle$,

$$\langle\Psi(x,t)|x|\Psi(x,t)\rangle=\sum_{n=0}^{\infty}\sum_{j=0}^{\infty}c_nc_j\exp(-i\omega_{nj}t)\langle\psi_j|x|\psi_n\rangle$$
$$=\sum_{n=0}^{\infty}\sum_{j=0}^{\infty}c_nc_j\cos(\omega_{nj}t)\langle\psi_j|x|\psi_n\rangle\ , \tag{4.2}$$

where we have used the well-known fact that for this one-dimensional problem the eigenfunctions are real. Now let us assume that the initial wave packet $\Psi(x,0)$ is given by a Gaussian wave packet, Eq. (3.2). Thus c_n are the coefficients of expansion of $\Psi(x,0)$ in terms of the set of $\psi_n(x)$,

$$\Psi(x,0)=\sum_{n=0}^{\infty}c_n\psi_n(x)\ . \tag{4.3}$$

In this expansion only the first few terms are important, i.e., for large n, c_n tend to zero rapidly. In fact for the case of the wave functions of an exactly solvable double-well potential one can show that in the expansion of a Gaussian wave packet of the type given by Eq. (3.2) only the first three or four terms in the infinite series (4.3) contribute significantly to the sum. Thus we can define a function $f(t)$ in the following way:

$$f(t)=\langle 0|x(t)|0\rangle=\langle\Psi(x,t)|x|\Psi(x,t)\rangle$$
$$\approx c_0c_1\langle\psi_0|x|\psi_1\rangle\cos(\nu_1\theta)$$
$$+c_0c_2\langle\psi_0|x|\psi_2\rangle\cos(\nu_2\theta)$$
$$+c_2c_1\langle\psi_2|x|\psi_1\rangle\cos(\nu_3\theta)+\cdots\ , \tag{4.4}$$

where $\theta=\omega t$ and ν_k is the dimensionless frequency defined by

$$\nu_1=\omega_{10}/\omega\ ,\quad \nu_2=\omega_{20}/\omega\ ,\quad \nu_3=\omega_{21}/\omega\ ,$$
$$\nu_4=\omega_{30}/\omega,\ldots\ . \tag{4.5}$$

Here the matrix element $\langle 0|x(t)|0\rangle$ is calculated by the integration of the Heisenberg equations of motion for a finite time interval $0\le t\le t_N$ or in terms of θ, for $0\le\theta\le\theta_N$. The time dependence of the left-hand side of Eq. (4.4) enables us to determine the approximate frequencies ν_1, ν_2, ν_3, ... and hence obtain the low-lying energy eigenvalues measured relative to the ground-state energy E_0. For obtaining the unknown frequencies ν_k we use the simplest version of Prony's method [11]. If we know the N values

$$f_0=f(0)\ ,\quad f_1=f(1)\ ,\quad f_2=f(2),\ldots,$$
$$f_{N-1}=f(N-1)\ , \tag{4.6}$$

of a function $f(\theta)$ which is expressible as

$$f(\theta)=A_1\cos(\nu_1\theta)+B_1\sin(\nu_1\theta)+A_2\cos(\nu_2\theta)$$
$$+B_2\sin(\nu_2\theta)+\cdots+A_m\cos(\nu_m\theta)$$
$$+B_m\sin(\nu_m\theta)\ ,\quad 3m=N \tag{4.7}$$

then $\cos(\nu_1),\cos(\nu_2),\ldots,\cos(\nu_m)$ are the roots of the algebraic equation [11]

$$\cos(m\nu)-\alpha_1\cos[(m-1)\nu]-\cdots-\alpha_{m-1}\cos(\nu)$$
$$-(\alpha_m/2)=0\ . \tag{4.8}$$

In Eq. (4.8) α_m are defined as the solutions of the set of linear equations

$$\sum_{k=1}^{m-1}(f_{i+k-1}+f_{2m+i-k-1})\alpha_k+f_{m+i-1}\alpha_m +f_{i-1}+f_{2m+i-1}=0\ ,\quad i=1,2,\ldots,N-2m\ . \tag{4.9}$$

Equations (4.9) form a set of m linear equations for m unknowns (α_k), and from α_k and Eq. (4.8) we find $\nu_1,\nu_2,\ldots\nu_m$. Note that in an exact calculation ν_k are not all independent since we have relations of the form

$$\omega_{ij}=\omega_{jk}-\omega_{ik}\ ,\quad k<i,k<j\ . \tag{4.10}$$

These relations help us to connect all ω_{ij} to ω_{j0} and ω_{i0}, etc., which we have determined earlier.

V. A TEST OF PRONY'S METHOD FOR OBTAINING THE EIGENVALUES

In this section, we will show that if the matrix elements of the position or the momentum operators are known very accurately for a short time, then Prony's method can be used to find level spacings for the low-lying eigenvalues. To this end let us consider the double-well potential

$$V_D(x)=(1/8)b^2\cosh(4x)-4b\cosh(2x) -(1/8)b^2+V_0\ , \tag{5.1}$$

where we have set $(\hbar^2/2m)=1$, x is a dimensionless variable, and V_0 is a constant determined by the requirement that the minimum of $V_D(x)$ is zero. Note that $V_D(x)$ has the dimension of L^{-2}, where L is an arbitrary unit of length. The eigenfunctions for the four low-lying states of this potential and their corresponding eigenvalues are known analytically [12]:

$$\psi_j(x)=N_j\exp[-(b/4)\cosh(2x)]\phi_j(x)\ , \quad j=0,1,2,3\ , \tag{5.2}$$

where

$$\phi_0=3b\cosh(x) +[4-b+2(4-2b+b^2)^{1/2}]\cosh(3x)\ , \tag{5.3}$$

$$\phi_1=3b\sinh(x) +[4+b+2(4+2b+b^2)^{1/2}]\sinh(3x)\ , \tag{5.4}$$

$$\phi_2=3b\cosh(x) +[4-b-2(4-2b+b^2)^{1/2}]\cosh(3x)\ , \tag{5.5}$$

$$\phi_3=3b\sinh(x) +[4+b-2(4+2b+b^2)^{1/2}]\sinh(3x)\ . \tag{5.6}$$

In these relations N_j are the normalization constants. The eigenvalues for these four states are given by [12]

$$E_0=-[5+b+2(4-2b+b^2)^{1/2}]+V_0\ , \tag{5.7}$$

$$E_1=-5+b-2(4+2b+b^2)^{1/2}+V_0\ , \tag{5.8}$$

$$E_2=-5-b+2(4-2b+b^2)^{1/2}+V_0\ , \tag{5.9}$$

$$E_3=-5+b+2(4+2b+b^2)^{1/2}+V_0\ , \tag{5.10}$$

where all E_j have the dimension L^{-2}. Using these four wave functions we can construct a wave packet localized around one of the minima of the potential $V_D(x)$ which we denote by x_m, where

$$x_m=(1/2)\cosh^{-1}(8/b)\ . \tag{5.11}$$

Around the point $x=-x_m$ we expand $V_D(x)$ with the result that

$$V_a(x)=(1/2)\Omega^2(x+x_m)^2\ , \tag{5.12}$$

where Ω is a function of the parameter b of the potential. The form of the potential $V_a(x)$ suggests that a Gaussian wave packet of the form

$$\Psi_g(x)=(\Omega/\pi)^{1/4}\exp[-(\Omega/2)(x+x_m)^2] \tag{5.13}$$

can be used to study oscillations about $x=-x_m$. The wave packet (5.13) can be approximated by $\Psi_a(x)$ which is a linear combination of $\psi_j(x)$

$$\Psi_a(x)=\sum_{j=0}^{3}c_j\psi_j(x)\ . \tag{5.14}$$

Thus the time evolution of this wave packet is given by Eq. (4.1), and the matrix element $\langle\Psi_a(x,t)|x|\Psi_a(x,t)\rangle$ is found from (4.2), but now the sums are finite

$$g(t)=\langle\Psi_a(x,t)|x|\Psi_a(x,t)\rangle =\sum\sum_{n,j=0}^{3}c_nc_j\cos[(E_n-E_j)t]\langle\psi_j|x|\psi_n\rangle\ , \tag{5.15}$$

where ψ_j and ψ_n are given by Eqs. (5.2)–(5.6). For $x_m=1$, i.e., $b=[8/\cosh(2)]$, the two wave packets are shown in Fig. 1.

First we compute $g(t)$ for the time interval $0\le t\le 1.1$, where t is in the units of L^2. This time interval is much shorter than the period of oscillation of the wave packet which is about $2\pi/(E_1-E_0)\approx 5.08L^2$. Using Prony's method with 12 points in this range we find

$$E_1-E_0=1.2368\ ,\quad E_2-E_1=7.0277\ ,$$

$$E_3-E_0=15.5334\ .$$

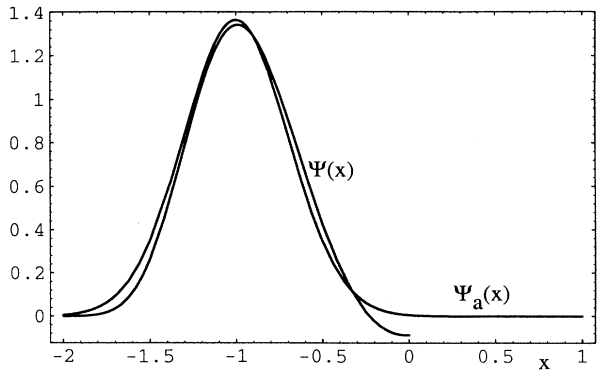

FIG. 1. The exact Gaussian wave packet $\Psi_g(x)$ and its approximate form $\Psi_a(x)$ obtained from the superposition of four eigenstates, Eqs. (5.2)–(5.6).

These energy differences agree with the exact result to the last decimal point given above. However, the potential given by the Hamiltonian (2.7) and (2.8) with $\beta=20$ is by a factor 0.07 smaller than $V_D(x)$. Let us consider the accuracy of Prony's inversion when it is applied to a smaller potential (or a set of eigenvalues). For this purpose we replace $g(t)$, Eq. (5.15) by $f(t)$ in which the eigenvalues are five times smaller, viz.,

$$f(t)=\sum_{n,j=0}^{3} c_n c_j \cos\{[(E_n-E_j)/5]t\}\langle\psi_j|x|\psi_n\rangle \quad (5.16)$$

but at the same time we consider the interval $0\le t\le 2.2L^2$. Again this time interval is much shorter than the period of oscillation of the wave packet which is about $26L^2$ (see Fig. 2). By first calculating $f(t)$ and then inverting the process using Prony's method with $N=12$, we find

$$E_1-E_0=1.2101\ ,\quad E_2-E_1=7.3296\ ,$$
$$E_3-E_0=15.5334\ .$$

Thus for smaller eigenvalues the method is not as reliable as with the larger eigenvalues; nevertheless the differences between the energies of the lowest states are predicted reasonably well by this method.

Before leaving this discussion let us also use the semiclassical method of obtaining the level spacing E_1-E_0. This is given by the expression [13]

$$E_1-E_0=(2E_0/\pi)\exp\{-\int_{x_1}^{x_2}[V_D(x)-E_0]^{1/2}dx\}\ , \quad (5.17)$$

where x_1 and x_2 are the two classical turning points. Using the potential (5.1) and E_0 given by (5.7) we find

$$E_1-E_0=1.0919$$

which is smaller than the exact result.

VI. LEVEL SPACING OBTAINED FROM THE MOTION OF THE CENTER OF THE WAVE PACKET

Let us now return to the solution of the Heisenberg equations of motion. These equations can be integrated for a maximum time θ_m, which is considerably shorter than the period of the oscillation of the wave packet. For longer times, accumulation of round-off errors makes the solution unstable. We have two tests to verify the accuracy of the integration; the energy $\langle 0|K|0\rangle$ obtained from Eq. (3.25) and the expectation value of the commutator given by Eq. (2.6). These are calculated at each stage of integration, and as long as they remain close to their initial values (here within one part in 10^3), we consider the result of integration acceptable. We start this calculation with Eqs. (3.17) and (3.18) with $j=0$, and we use either the fourth-order expansion, i.e., by keeping terms up to and including $(\Delta\theta)^4$ or the sixth-order expansion with terms including $(\Delta\theta)^6$. The results of calculation of the matrix elements $\langle 0|\xi(\theta)|0\rangle$ and $\langle 0|p(\theta)|0\rangle$ for the symmetric quartic potential

$$V(\xi)=10\xi^2(1-\xi)^2 \quad (6.1)$$

are shown in Fig. 3. Up to a maximum time of about $\theta\approx 1.8$ the energy $\langle 0|K|0\rangle$ and the commutator $\langle 0|[\xi(\theta),p(\theta)]|0\rangle=i/\beta^2$ do not change. Substituting these results in the Prony method, Eq. (4.9) with 36 input points (i.e., $N=12$), at the intervals $\Delta\theta=0.05$, we find the following values for v_i:

$$v_1=0.2618\ ,\quad v_2=0.7933\ ,\quad v_3=1.2803\ ,$$

and

$$v_4=1.5579\ .$$

For comparison we note that the semiclassical approximation for the splitting of the lowest level is given by [13]

$$v_1=(1/\pi)\exp\{-\beta^2\int_{x_1}^{x_2}[x^2(1-x)^2-(1/\beta^2)]^{1/2}dx\}\ , \quad (6.2)$$

where x_1 and x_2 are the two turning points. This approximation yields a value of $v_1=0.1806$ which is smaller than the value calculated by Prony's method. The exact solution of the Schrödinger equation with the quartic potential (6.1) yields the following results for the first three eigenvalues:

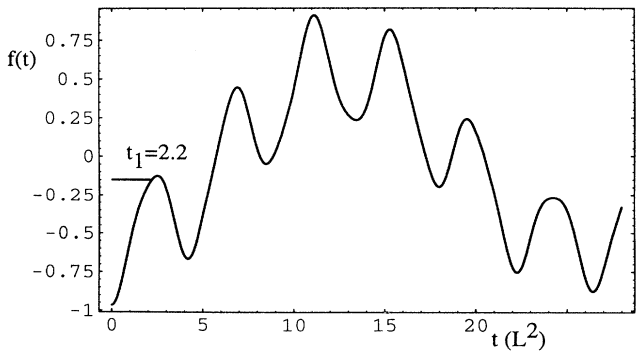

FIG. 2. The time dependence of the center of the wave packet Eq. (5.16) for the period $10\pi/(E_1-E_0)$. Only the part shown in the interval $0\le t\le 2.2(L^2)$ is used to test Prony's inversion. Thus if $f(t)$ is known accurately in this interval then the complete curve can be constructed.

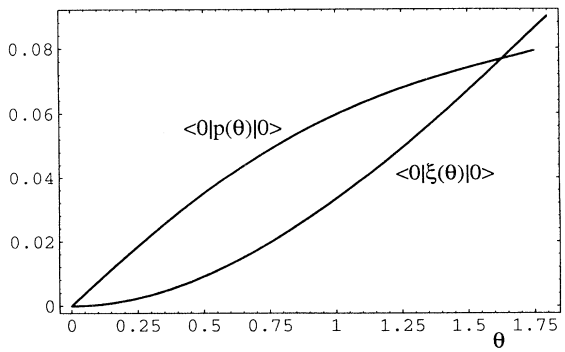

FIG. 3. The position and the momentum of the center of the wave packet for symmetric potential plotted as a function of the dimensionless time θ. For the values of θ shown here the matrix elements have been determined very accurately.

$$\lambda_0=0.7701\ ,\quad \lambda_1=0.9927\ ,\ \text{and}\ \lambda_2=2.1239\ .$$

Hence the lowest-level splitting is given by $\lambda_1-\lambda_0=0.2226$. Noting that Eq. (4.8) has multivalued solutions, therefore, only when we have accurate results from Prony's inversion, we can associate each ν_k with the corresponding $\lambda_{k+1}-\lambda_k$ as we did in the last section. For higher barriers, i.e., for larger β^2, the splitting becomes smaller, and when ν_0 is very small, then the simple Prony's method discussed here fails to predict the energy differences accurately, and a more elaborate method such as the one discussed by Whittaker and Robinson [14] must be utilized.

For the asymmetric potential

$$V(\xi)=0.05\xi^2(\xi^2-14\xi+45) \tag{6.3}$$

the integration of the Heisenberg equations of motion yields the time evolution of the position and momentum of the wave packet as is shown in Fig. 4. Again using Prony's method with 36 points of the values of the matrix element $\langle 0|\xi(\theta)|0\rangle$ calculated at intervals $\theta=0.01$ we obtain the following values for level spacings:

$$\nu_1=0.1309\ ,\quad \nu_2=0.3921\ ,\quad \nu_3=1.0480\ ,$$

and

$$\nu_4=1.3494\ .$$

However, in this case, the semiclassical method, Eq. (6.2) is not valid and we can only compare our results with the exact solution. The exact results for the first few eigenvalues are given by

$$\lambda_0=-13.177\ ,\quad \lambda_1=1.175\ ,\quad \lambda_2=6.060\ ,$$

$$\lambda_3=11.946\ ,\ \text{and}\ \lambda_4=17.187\ .$$

Here we note that

$$\nu_2'=2\pi-(\lambda_3-\lambda_2)=0.387\ ,$$

$$\nu_3'=2\pi-(\lambda_4-\lambda_3)=1.042\ ,$$

and

$$\nu_4'=4\pi-(\lambda_4-\lambda_2)=1.4290\ .$$

as the exact frequencies associated with the ν_k obtained from the solution to the Heisenberg equations. However, in this case unlike the symmetric potential the difference between the two lowest eigenvalues λ_0, and λ_1 does not appear in the first few terms of the expansion (4.4). The reason for this seems to be that whereas in the symmetric potential $\lambda_{k+1}-\lambda_k$ increases as the integer k becomes larger, for the asymmetric potential this is not the case, and thus in Prony's inversion ν_1 which is large can only show up if we include many more points in our calculation, i.e., extend the range of integration of the operator equation.

The essential difference between the motion of the wave packet in the symmetric and asymmetric double-well potentials is that in the former case the position of the center of the wave packet oscillates between the two wells with an approximate period of $2\pi/\nu_1$, but for the latter except for "resonance" cases such an oscillation does not take place [15]. Thus for the potential (6.1), $\langle 0|\xi(\theta)|0\rangle$ moves from the first minimum, i.e., $\langle 0|\xi(\theta)|0\rangle=0$, to the second at $\langle 0|\xi(\theta)|0\rangle=1$. However, for the asymmetric potential Eq. (6.3) the motion is confined in the first well and $\langle 0|\xi(\theta)|0\rangle$ cannot reach the other side of the barrier. By comparing the level spacings for these two potentials, we observe that from these data alone we cannot infer whether or not a wave packet tunnels through the barrier. In fact it can be shown that this difference persists even for symmetric and asymmetric potentials with identical sets of energy levels [16]. Among other features of the present approach is the possibility of the calculation of some of the other time-dependent physical quantities such as the rate of change of the kinetic or the potential energy as a function of time, and the time dependence of the uncertainty relation $\Delta p\Delta\xi$. These are calculated along with the matrix elements of p and ξ from the integration of the Weyl-ordered products $S_{m,n}(\theta)$, Eq. (3.30) which is the basic equation in our approach. Figure 5 shows how the uncertainty relation $\Delta p\Delta\xi$ changes as a function of θ for the symmetric double well. We have a similar time dependence for the asymmetric well. Finally, we note that in this approach the wave packet does not change with

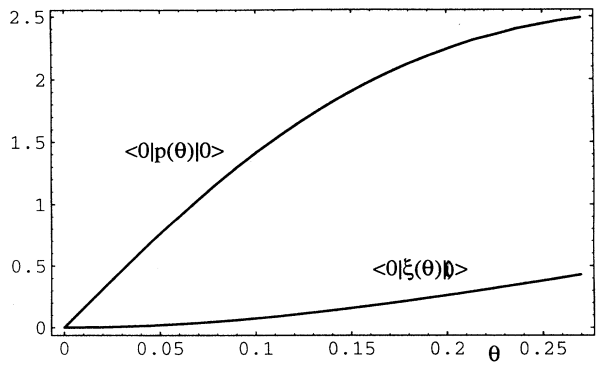

FIG. 4. The position and the momentum of the center of the Gaussian wave packet for the case of asymmetric potential is given as a function of dimensionless time θ.

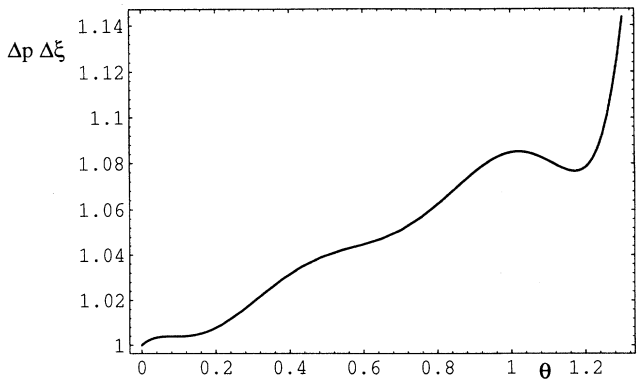

FIG. 5. The time dependence of the uncertainty $\Delta p\Delta\xi$ obtained from the solution of the Heisenberg equations. This uncertainty is normalized so that its value at $t=0$ is one.

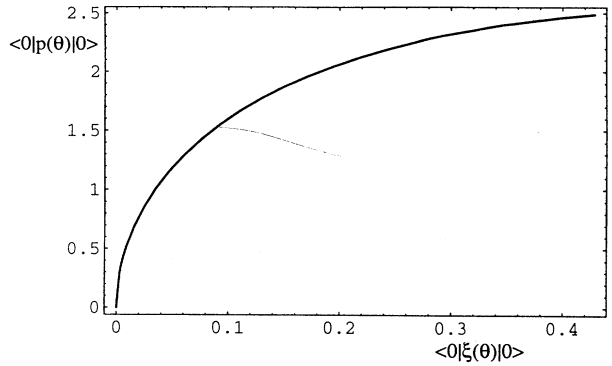

FIG. 6. Parametric plot of $\langle 0|p(\theta)|0\rangle$ versus $\langle 0|\xi(\theta)|0\rangle$ which shows the motion of the center of the wave packet in "phase space" for asymmetric potential.

time; therefore, the parametric curve $\{\langle 0|\xi(\theta)|0\rangle, \langle 0|p(\theta)|0\rangle\}$ can be regarded as the quantal analogue of the motion of a classical particle in phase space. Figure 6 shows this motion for the asymmetric potential, given by Eq. (6.3).

VII. CONCLUSION

As we have seen in the preceding sections the operator equations of motion can be integrated very accurately for a maximum time θ_m which is much smaller than the period of oscillation of the wave packet in the symmetric potential (6.1). These accurate results enable us to use the inversion method of Prony to find the level spacings at least for low-lying states. By comparing Figs. 3 and 4, we observe that this θ_m is much smaller for a strong and asymmetrical well than the weak symmetric quartic potential. Because of this limitation on the range of integration, we cannot give a definite answer to the interesting question raised and discussed by Nieto *et al.* [15] concerning the possibility of tunneling in an asymmetric potential. However an extrapolation of our best fit to the position of the center of the wave packet in the range $0 \leq \theta \leq 0.3$ using four level spacings obtained in the last section showed that $\langle 0|\xi(\theta)|0\rangle$ does not pass the center of the barrier, i.e., $\xi = 3$. But because of the extrapolation this result is not conclusive. We hope that by improving the method of integration we can study this feature of quantum tunneling and also the motion of the localized and time-independent wave packet in the phase space.

ACKNOWLEDGMENT

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