Integration of the Heisenberg equations for inverse power-law potentials

M. Hron and M. Razavy
Theoretical Physics Institute, Department of Physics, The University of Alberta, Edmonton, Alberta, Canada T6G 2J1
(Received 5 March 1996; revised manuscript received 16 July 1996)

The direct method of integration of the operator Heisenberg equations of motion is extended to the solution of quantum tunneling when the central potential is a sum of inverse powers of the radial distance. By obtaining the equation of motion for the Weyl-ordered basis set $\{S_{m,n}(t)\}$ formed from $r(t)$ and $p_r(t)$, one can express the time evolution of any member of the set as an infinite sum involving the operators $\{S_{m,n}(0)\}$. The direct integration enables one to find the expectation values of the radial position operator and its conjugate momentum and higher moments of these operators as functions of time. [S1050-2947(96)04511-8]

PACS number(s): 03.65.Ca, 03.65.Bz

I. INTRODUCTION

This is the third in a series of papers devoted to the study of the problem of integration of the Heisenberg equations based on ideas suggested by Bender and collaborators [1–3]. In the earlier papers we discussed the solution of the initial value operator equations of motion for cubic [4] and quartic [5] potentials, respectively. In both cases we observed that the time evolution of the operators can be determined only for relatively short times. The nonlinearity of the problem combined with the operator nature of the solution of the differential equations for position and momentum restricted the number of steps in the integration process. Nonetheless, by calculating the constants of motion we showed that for a short time interval the result of integration is very accurate, and the result enabled us to find (a) the lifetime of a quasi-stationary wave packet trapped by a cubic potential and (b) the energy differences for quartic potentials. The present work is concerned with the more interesting problem, viz., how one can extend the idea of Bender and collaborators to the central, inverse law potentials, and solve the three-dimensional problem of bound state or resonance tunneling using Heisenberg's equations. In Sec. II we write the Hamiltonian for the radial motion of a particle in terms of the basis set $\{S_{m,n}(t)\}$ of the Weyl-ordered operators. These operators are constructed from $r(t)$ and $p_r(t)$ and form an algebra which is closed under multiplication [1,2]. Then we derive and solve the Heisenberg equation of motion for $S_{m,n}(t)$. As a special case we observe that if the potential is proportional to the inverse square of the radial distance, then the exact solution for the operator $S_{0,2}$ can be obtained as a function of time (Sec. III). In Sec. IV we find the expectation values of the operators $S_{m,-n}(0)$ for a simple wave packet and calculate the quantities $\langle r(t)\rangle$, $\langle p_r(t)\rangle$, and in general $\langle S_{m,n}(t)\rangle$ as functions of time. In Sec. V we present the results of our calculation for a tunneling problem and a bound state problem. We discuss the special case of the Coulomb problem with the Rydberg wave packet in Sec. VI. We show in Sec. VII that the same method can be used for a sum of exponential potentials, such as the Morse potential. Finally we conclude the paper with a discussion of the merits and also the problems of the present approach.

II. BENDER AND DUNNE ALGEBRA FOR THE RADIAL COORDINATE AND ITS CONJUGATE MOMENTUM

In their work on the integration of an operator differential equation, Bender and Dunne introduced a set of Weyl-ordered operators corresponding to the classical product $p^m q^n$ (m and n are integers) by

$$T_{m,n}=\frac{1}{2^n}\sum_{k=0}^{n}\frac{n!}{(n-k)!k!}\,q^k p^m q^{n-k}, \tag{2.1}$$

and showed that the basis elements $T_{m,n}$ form an algebra closed under multiplication. Here we consider a trivial modification of this product rule for the radial coordinate r and its conjugate p_r, where

$$p_r=-\left(\frac{i}{r}\frac{\partial}{\partial r}\right)r \tag{2.2}$$

and satisfies the commutation relation

$$[r,p_r]=i. \tag{2.3}$$

Here we have set $\hbar=1$.

We replace $T_{m,n}$ as defined above by $S_{m,n}$ where

$$\begin{aligned}S_{m,n}&=\frac{1}{2^n}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\,r^k\left(-\frac{i}{r}\frac{\partial}{\partial r}\right)^m r^{n-k}\\&=\frac{1}{r}\left[\frac{1}{2^n}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\,r^k\left(-i\,\frac{\partial}{\partial r}\right)^m r^{n-k}\right]r\\&=\frac{1}{r}\,T_{m,n}r.\end{aligned} \tag{2.4}$$

Then the product rule becomes

$$S_{m,n}S_{k,l}=\frac{1}{r}\,T_{m,n}T_{k,l}r=\sum_{j=0}^{\infty}\frac{(i/2)^j}{j!}\sum_{s=0}^{j}(-1)^{j-s}\left(\frac{j!n!m!k!l!}{s!(j-s)!(n-s)!(m+s-j)!(k-s)!(l+s-j)!}\,S_{m+k-j,n+l-j}\right), \tag{2.5}$$

and the commutation relation between two members of the set of $S_{m,n}$'s can be obtained from (2.5);

$$[S_{m,n},S_{r,s}]=2\sum_{j=0}^{\infty}\frac{(i/2)^{2j+1}}{(2j+1)!}\sum_{k=0}^{2j+1}(-1)^k\frac{(2j+1)!}{k!(2j+1-k)!}\,S_{m+r-2j-1,n+s-2j-1}\times\frac{\Gamma(m+1)\Gamma(n+1)\Gamma(r+1)\Gamma(s+1)}{\Gamma(m-k+1)\Gamma(n+k-2j)\Gamma(r+k-2j)\Gamma(s-k+1)}. \tag{2.6}$$

The two equations (2.5) and (2.6) are the basic relations which enable us to find the equations of motion for any operator $S_{m,n}$ from the Hamiltonian H. The Heisenberg equation of motion for the operator $S_{m,n}$ is

$$i\,\frac{dS_{m,n}}{dt}=[S_{m,n},H], \tag{2.7}$$

where H is the Hamiltonian of the system. The reduced Hamiltonian for the radial motion of a particle of mass $M=1$ is

$$H=\tfrac{1}{2}p_r^2+V_{\rm eff}(r)=\tfrac{1}{2}S_{2,0}+V_{\rm eff}(S_{0,n}), \tag{2.8}$$

where the effective potential $V_{\rm eff}\,(r)$ is the sum of the centrifugal potential $l(l+1)/r^2$ and the external force. In this work we are interested in potentials of the type

$$V_{\rm eff}(r)=\sum_{k=1}^{J}\frac{A_k}{r^k} \tag{2.9}$$

and in particular we want to consider a potential of the form

$$V_{\rm eff}(r)=\sum_{k=1}^{3}\frac{A_k}{r^k}, \tag{2.10}$$

where we have included $l(l+1)/r^2$ as a part of A_2/r^2. With this type of potential, the Hamiltonian H can be written as

$$H=\tfrac{1}{2}S_{2,0}+\sum_{k=1}^{J}A_kS_{0,-k}\,. \tag{2.11}$$

In order to calculate the time development of $S_{m,n}$ for this system we need the following two commutators that we can find from (2.6):

$$[S_{m,n},S_{2,0}]=2inS_{m+1,n-1}, \tag{2.12}$$

$$[S_{m,n},S_{0,-s}]=2\sum_{j=0}^{\infty}\left(\frac{i}{2}\right)^{2j+1}\frac{m!(s+2j)!}{(m-2j-1)!(s-1)!}\times S_{m-2j-1,n-s-2j-1}\,. \tag{2.13}$$

The last commutator is found by calculating the limit of Eq. (2.6) when the argument of the Γ functions becomes negative. Note that the sum in Eqs. (2.13) is finite, i.e., for odd m, $j_{\max}=\frac{1}{2}(m-1)$ and for even m, $j_{\max}=\frac{1}{2}(m-2)$.

From Eqs. (2.12) and (2.13) we find $dS_{m,n}/dt$;

$$\begin{aligned}i\,\frac{dS_{m,n}}{dt}&=[S_{m,n},H]\\&=inS_{m+1,n-1}\\&\quad+2\sum_{j=0}^{\infty}\left(\frac{i}{2}\right)^{2j+1}\frac{m!}{(m-2j-1)!(2j+1)!}\\&\quad\times\left(\sum_{k=1}^{J}A_k\,\frac{(k+2j)!}{(k-1)!}\,S_{m-2j-1,n-k-2j-1}\right).\end{aligned} \tag{2.14}$$

In particular, the equations of motion for $S_{1,0}$ and $S_{0,1}$ are the Heisenberg equations for r and p_r, i.e., they reduce to two real equations,

$$\frac{dr}{dt}=p_r \tag{2.15}$$

and

$$\frac{dp_r}{dt}=\sum_{k=1}^{J}\frac{kA_k}{r^{k+1}}=-\frac{\partial V_{\rm eff}}{\partial r}. \tag{2.16}$$

We can write Eq. (2.16) also as an equation with real coefficients,

$$\frac{dS_{m,n}}{dt}=nS_{m+1,n-1}+\sum_{j=0}^{\infty}\left(-\frac{1}{2}\right)^{j}\frac{m!}{(m-2j-1)!}\times\left(\sum_{k=1}^{J}A_k\,\frac{(k+2j)!}{(k-1)!}\,S_{m-2j-1,n-k-2j-1}\right). \tag{2.17}$$

Now we write $S_{m,n}(\Delta t)$ as a Taylor expansion,

$$S_{m,n}(\Delta t)=S_{m,n}(0)+\frac{\Delta t}{1!}\left(\frac{dS_{m,n}}{dt}\right)_0+\frac{(\Delta t)^2}{2!}\left(\frac{d^2S_{m,n}}{dt^2}\right)_0+\cdots\,. \tag{2.18}$$

The second term $(dS_{m,n}/dt)_0$ can be calculated from (2.17) in terms of $S_{m-2j-1,n-2j-2}(0)$, etc. By differentiating $dS_{m,n}/dt$, Eq. (2.17), we find $d^2S_{m,n}/dt^2$, but this is also

expressible in terms of $S_{m-2j-1,n-2j-3},\ldots$ if we substitute for $dS_{m-2j-1,n-2j-2}/dt$ and similar terms from (2.18). Thus $S_{m,n}(\Delta t)$ can be written as an expansion involving $S_{m,n}$'s all at $t=0$. By repeating this process we find that $S_{m,n}(2\Delta t)$, $S_{m,n}(\Delta t),\ldots$ can all be expressed in terms of $S_{m,n}(0)$, $S_{m+1,n-1}(0),\ldots,S_{m-2j-1,n-2j-s}(0),\ldots$ where s is a large positive integer. The final result can be written as an operator equation

$$S_{m,n}(N\Delta t)=\sum_{j,k} C_{j,k}(N,\Delta t)S_{m-j+1,n-k}(0). \quad (2.19)$$

Here the coefficients $C_{j,k}(N,\Delta t)$ are determined numerically for a given N and Δt. Once $S_{m,n}(N\Delta t)$ is determined as an operator, we can find the expectation value of $r(N\Delta t)$, $p_r(N\Delta t)$, $r^2(N\Delta t)$, $p_r^2(N\Delta t),\ldots$ directly from (2.19) by calculating $S_{0,1}$, $S_{1,0}$, $S_{0,2}$, $S_{2,0}$, etc. all at $N\Delta t$. For instance, let us consider the radial position operator $r=S_{0,1}$ at Δt;

$$S_{0,1}(\Delta t)=S_{0,1}(0)+\frac{\Delta t}{1!}\left(\frac{dS_{0,1}(t)}{dt}\right)_0+\frac{(\Delta t)^2}{2!}\left(\frac{d^2S_{0,1}(t)}{dt^2}\right)_0 +\cdots . \quad (2.20)$$

Using Eq. (2.17) repeatedly we find that

$$\begin{aligned}S_{0,1}(\Delta t)=&S_{0,1}(0)+\frac{\Delta t}{1!}S_{1,0}(0)+\frac{(\Delta t)^2}{2!}\sum_{k=1} kA_kS_{0,-(k+1)}(0)\\ &-\frac{(\Delta t)^3}{3!}\sum_{k=1} k(k+1)A_kS_{1,-(k+2)}(0)\\ &-\frac{(\Delta t)^4}{4!}\sum_{k=1} k(k+1)A_k\Bigg(-(k+2)S_{2,-(k+3)}(0)\\ &+\sum_{j=1} jA_jS_{0,-(k+j+3)}(0)\Bigg)+\cdots . \quad (2.21)\end{aligned}$$

In Sec. IV we will see how the expectation values of these operators can be calculated if we choose a suitable wave function.

III. A SIMPLE EXAMPLE

Let us consider the special case where

$$H=\frac{1}{2}p_r^2+\frac{A}{r^2}=\frac{1}{2}S_{2,0}+A_2S_{0,-2}. \quad (3.1)$$

We calculate $S_{0,2}(t)$ from the Taylor expansion

$$S_{0,2}(t)=S_{0,2}(0)+\frac{t}{1!}\left(\frac{dS_{0,2}}{dt}\right)_0+\frac{t^2}{2!}\left(\frac{d^2S_{0,2}}{dt^2}\right)_0+\cdots . \quad (3.2)$$

But

$$\frac{dS_{0,2}}{dt}=\frac{1}{i}[S_{0,2},H]=2S_{1,1} \quad (3.3)$$

and

$$\frac{d^2S_{0,2}}{dt^2}=\frac{1}{i}[S_{1,1},H]=2S_{2,0}+4A_2S_{0,-2}. \quad (3.4)$$

Finally we calculate

$$\frac{d^3S_{0,2}}{dt^3}=\frac{d}{dt}\{2S_{2,0}+4A_2S_{0,-2}\}=\frac{d(4H)}{dt}=0. \quad (3.5)$$

Hence the series (3.2) terminates after the third term

$$\begin{aligned}S_{0,2}(t)=&S_{0,2}(0)+\frac{2t}{1!}S_{1,1}(0)+\frac{t^2}{2!}\\ &\times\{2S_{2,0}(0)+4A_2S_{0,-2}(0)\}. \quad (3.6)\end{aligned}$$

This is the exact solution for the operator equation for $r^2(t)$.

IV. CALCULATION OF THE EXPECTATION VALUES

Suppose that we want to calculate $\langle r(t)\rangle$ or $\langle r^2(t)\rangle$, then we divide t into N equal intervals $\Delta t=t/N$. Now we need to choose a narrow wave packet which gives us finite result for the matrix element

$$\langle\psi|S_{m+j,n-k}|\psi\rangle=\int_0^\infty r\psi^*S_{m+j,n-k}(r\psi)dr, \quad (4.1)$$

when k is large. Therefore we seek a wave packet with the property that

$$\lim r^{-n}[r\psi(r)]\to 0 \quad \text{as } r\to 0 \quad \text{for all } n. \quad (4.2)$$

This condition guarantees that the matrix elements of $S_{m,-n}$ are finite.

Now let us consider the operator $S_{m,-n}$ given by

$$S_{m,-n}=\frac{1}{2^m}\sum_{j=0}^{m}\frac{m!}{j!(m-j)!r}p_r^j\left(\frac{1}{r^n}\right)p_r^{m-j}r, \quad n>0 \quad (4.3)$$

which is equivalent to the definition (2.4) (see Bender and Dunne). Using the wave packet (4.2), we find that

$$\langle\psi|S_{2m+1,-n}|\psi\rangle=0 \quad (4.4)$$

and

$$\begin{aligned}\langle\psi|S_{2m,-n}|\psi\rangle=&\frac{(-1)^m}{2^{2m}}\sum_{j=0}^{2m}\frac{(2m)!}{(2m-j)!j!}(-1)^j\\ &\times\int_0^\infty\frac{\partial^j(r\psi)}{\partial r^j}\frac{1}{r^n}\left(\frac{\partial^{2m-j}(r\psi)}{\partial r^{2m-j}}\right)dr. \quad (4.5)\end{aligned}$$

Thus all the matrix elements of $S_{m,-n}$ are real.

A simple and analytically tractable wave packet with the property (4.2) is

$$r\psi(r)=N\exp\left[-\frac{1}{2}\left(\frac{a}{r}+br\right)\right], \quad (4.6)$$

which is shown in Fig. 1.

Here N is the normalization constant and is given by

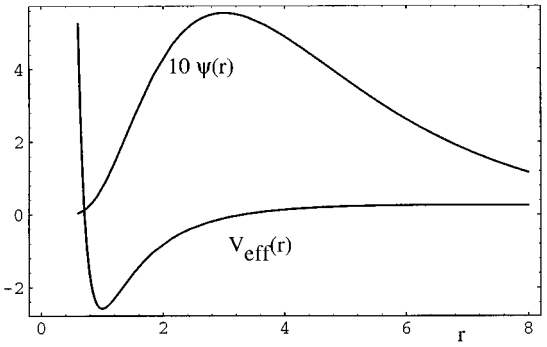

FIG. 1. The wave packet, Eq. (4.6), and the effective potential, Eq. (2.10), are shown as functions of r. The minimum and the maximum of the potential are at $r=1L$ and $7L$, respectively, and the center of the wave packet is at $r=3.7769L$.

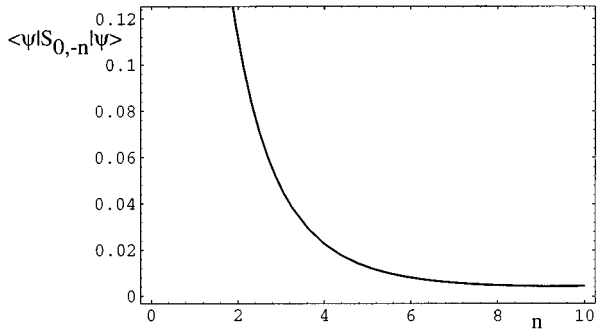

FIG. 2. The expectation value of $\langle\psi|S_{0,-n}|\psi\rangle$ as a function of n, where ψ is the wave packet defined by Eq. (4.6). For $n>15$, this expectation value starts increasing monotonically as n becomes larger.

$$N=\frac{1}{\sqrt{2}}\left(\frac{b}{a}\right)^{1/4}\{K_1(2\sqrt{ab})\}^{-1/2}, \tag{4.7}$$

where $K_v(x)$ is the modified Bessel function. Equation (4.6) is the ground state wave function for the potential

$$V_e(r)=\frac{(a^2-4ar-2abr^2)}{8r^4}, \tag{4.8}$$

with the corresponding eigenvalue

$$\varepsilon=-\frac{b^2}{8}. \tag{4.9}$$

The form of the potential (4.8) is similar to the general type of the potential (2.9) and (2.10). The center of the wave packet (4.6) is at r_0 where

$$r_0=\left(\frac{a}{b}\right)^{1/2}\frac{K_2(2\sqrt{ab})}{K_1(2\sqrt{ab})}. \tag{4.10}$$

Using this wave function we find

$$\langle\psi|S_{0,-n}|\psi\rangle=\frac{(b/a)^{n/2}K_{n-1}(2\sqrt{ab})}{K_1(2\sqrt{ab})}. \tag{4.11}$$

In solving the Heisenberg equations we follow the position of the center of the wave packet, i.e., $\langle\psi|r(t)|\psi\rangle$ as it moves through the potential barrier. In some problems particularly in quantum tunneling the motion of the point $r_c(t)$ where $r_c(t)$ is defined by

$$P_-[r_c(t)]=\int_0^{r_c}|r\psi(r,t)|^2dr=\tfrac{1}{2} \tag{4.12}$$

is of interest. Here $P_-[r_c(t)]$ is the probability of finding the particle to the left of the point $r=r_c$. Thus if $P_-[r_c(t)]>\frac{1}{2}$, the probability of the particle being in the range $0<r<r_c$ is greater than finding the particle between r_c and infinity. However, in the case of Heisenberg's equations we seek a solution of the operator equation for $r(t)$ and therefore it is easier to follow the motion of the center of the wave packet, i.e., $\langle\psi|r(t)|\psi\rangle$. To test our method, let us again consider the solvable example given by the potential (4.8) and the wave function (4.6). From Eq. (2.20) we find the expectation value of $S_{0,1}(\Delta t)$ with the wave packet (4.6), i.e.,

$$\langle\psi|r(\Delta t)|\psi\rangle=\langle\psi|S_{0,1}(\Delta t)|\psi\rangle. \tag{4.13}$$

This involves calculating terms like $\langle\psi|S_{2,-(k+3)}(0)(t)|\psi\rangle$ etc. all at $t=0$. We have calculated the coefficients of $(\Delta t)^2$ and $(\Delta t)^4$ analytically and found that these coefficients are identically zero independent of the values of the parameters a and b.

V. MOTION OF THE CENTER OF THE WAVE PACKET

Our choice of the wave packet Eq. (4.6) not only gives us analytic expectation values, Eq. (4.11), but also guarantees that these expectation values remain finite for all integers n. In this case the expectation value at first decreases as a function of n (Fig. 2) but eventually starts increasing. Noting that the wave packet does not change its shape in the course of time, one is tempted to choose a narrow wave packet and follow the motion of this wave packet through the interaction region. However, for the rapid convergence of the iterative method of integration outlined in Sec. II, the ratio of (a/b) and the product (ab) both must be large, and the potential must not be too deep. Choosing $b=1L$, where L is an arbitrary unit of length, we first tried to find a so that the wave packet has minimum uncertainty, i.e., $(\Delta p_r)^2(\Delta r)^2$ is minimum. But this uncertainty turns out to be a monotonic function of a which is nearly flat for $5<a<20$. Therefore the value of $a=9$ was used in all our calculations. Using these parameters we have found the values of r_0 and r_c to be 3.7769 and 3.513, respectively.

We have studied two special cases: (a) the case of quantum tunneling and (b) the bound state of the potential (2.10). For the former case we have chosen

$$A_1=3.872, \quad A_2=-15.488, \quad \text{and} \quad A_3=9.0349.$$

This potential is shown in Fig. 1, together with the wave packet (4.6). By calculating the total energy $\langle\psi|H|\psi\rangle$, where H is the Hamiltonian (2.11) we have found that the total energy is zero. The potential $V_{\text{eff}}(r)$ has a minimum at $r=1L$ and a maximum at $r=7L$, where $V_{\max}=0.2634$. Since

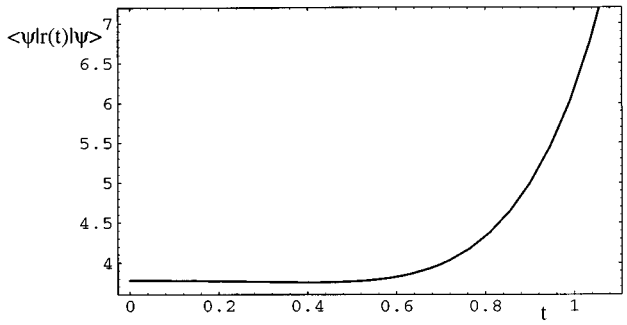

FIG. 3. The position of the center of the wave packet as a function of time (measured in units of L^2). At $t=0.4$ it reaches a minimum of $3.755L$ before changing its direction.

the energy associated with the wave packet is less than the height of the potential, this case corresponds to quantum tunneling. To verify the accuracy of the integration of the differential equation, at each interval $j\Delta t$, $j=1,2,\ldots$ we have obtained the expectation values of the energy, $\langle\psi|H|\psi\rangle$, and the commutator $\langle\psi|[r,p_r]|\psi\rangle$. Both of these quantities remain constant over a time interval of about $1L^2$ for the tunneling problem with an error of about one part in 10 000. The expectation value of $\langle\psi|r(t)|\psi\rangle=\langle\psi|S_{0,1}(t)|\psi\rangle$ is shown in Fig. 3. Here we observe that the center of the wave packet first moves toward the minimum of the potential, but then changes its direction and escapes the barrier. A plot of $\langle\psi|p_r(t)|\psi\rangle$ vs $\langle\psi|r(t)|\psi\rangle$, which is the analog of the classical motion in phase space, is displayed in Fig. 4, again showing penetration through the barrier. We have also studied the motion of the wave packet when the total energy of the wave packet is negative, i.e., a bound state. For this case using the same wave packet as before we have chosen

$$A_1=49.579, \quad A_2=-235.474, \quad \text{and} \quad A_3=187.895,$$

corresponding to the expectation value of $\langle\psi|H|\psi\rangle=-2L^{-2}$. The wave function is not an eigenstate of H, but a superposition of bound states and continuum wave functions. For this case the motion of the center of the wave packet is shown in Fig. 5. Here because of the depth of the

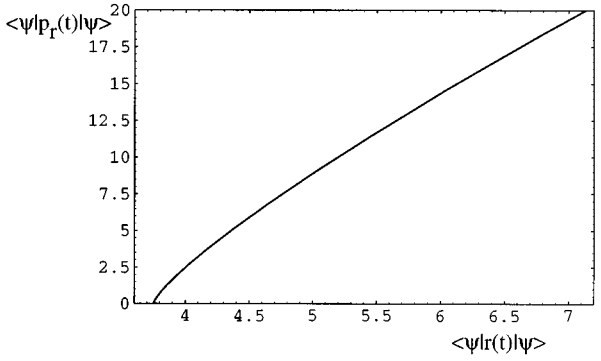

FIG. 4. The expectation value of momentum versus the expectation value of the position indicating the escape through the barrier.

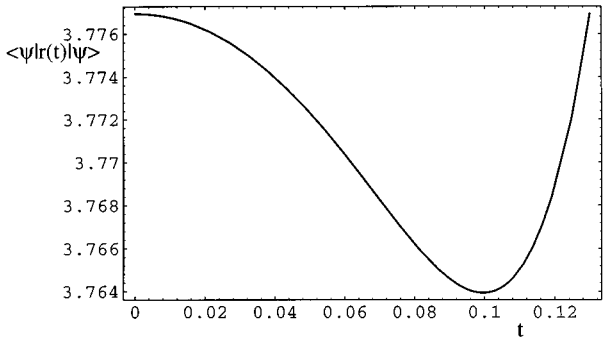

FIG. 5. The expectation value of the position of the particle as a function of time when the total energy of the wave packet is negative $\langle\psi|H|\psi\rangle=-2L^{-2}$. Here the minimum of $\langle\psi|r(t)|\psi\rangle=3.763$ is reached at $t=0.1L^2$.

potential, the integration is accurate only for a short time, about 0.13 in units of L^2. Figure 5 shows the motion of the center of the wave packet.

VI. RYDBERG WAVE PACKET

Rydberg wave packets, in their simplest form, are superpositions of many eigenstates with different principle quantum numbers and are well localized in the radial coordinate r. These wave packets are of great interest in studying the classical limit of the problem of interaction between atoms and an external electromagnetic field [6,7]. Let $u_{n',l}(r)$ be the radial wave function for a hydrogenlike atom,

$$u_{n',l}(r)=\left[\left(\frac{2Z}{n'}\right)^3\frac{(n'-l-1)!}{2n'n'!}\right]^{1/2}\exp\left(-\frac{Z}{n'}r\right)\times\left(\frac{2Zr}{n'}\right)^l L^{2l+1}_{n'-l-1}\left(\frac{2Zr}{n'}\right), \quad n'=1,2,\ldots \tag{6.1}$$

where r is measured in units of the Bohr radius $a_0=\hbar^2/(Me^2)$, and Z is the nuclear charge. From the set of $u_{n',l}$'s we can construct a Rydberg wave packet in the following way: For the central force problems, we fix l and write

$$\psi_l(r)=\sum_{n'} C_{n'}u_{n',l}(r). \tag{6.2}$$

We want the matrix element $\langle\psi|S_{2m,-n}|\psi\rangle$ to remain finite for $n\leqslant K$, therefore we choose $C_{n'}$ such that

$$\lim \psi_l(r)\to r^K \quad \text{as} \quad r\to 0. \tag{6.3}$$

To this end we expand the right hand side of (6.2) in powers of r and equate the coefficients of r^s, $s=0,1,\ldots,K-1$ equal to zero and the coefficients of r^K equal to unity. This gives us a set of $K+1$ linear equations for $C_{n'}$'s. For instance, a normalized Rydberg wave function for the S wave obtained by the superposition

$$\psi_R(r)=\sum_{n'}^{K} C_{n'}u_{n'}(r) \tag{6.4}$$

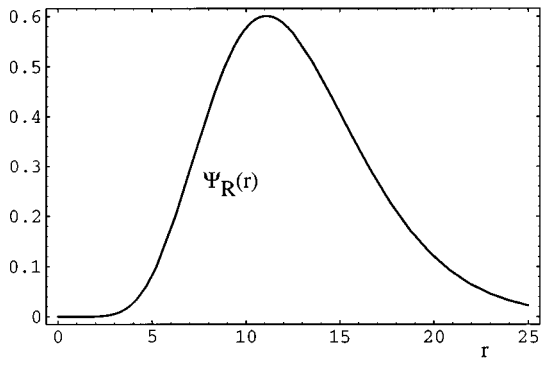

FIG. 6. The Rydberg wave packet for the S wave obtained by superposition of five n' values [see Eq. (6.4)].

is displayed in Fig. 6 for the values of $K=6$ and $Z=3$. The potential in this case is just the Coulomb potential $-Z/r=-3/r$ in atomic units ($a_0=1$), and the calculation is done exactly as before. The result for the expectation value of the position of the center of the wave packet is shown in Fig. 7. For this problem the motion of the center of the wave packet can be found directly from the solution of the Schrödinger equation, i.e.,

$$\langle \psi_l(r,t)|r|\psi_l(r,t)\rangle=\sum_{n,j}^{K} C_n C_j^* \exp[i(E_j-E_n)t] \times\langle u_{j,l}(r)|r|u_{n,l}(r)\rangle. \tag{6.5}$$

This result should be the same as $\langle \psi_l(r)|r(t)|\psi_l(r)\rangle$ found from the solution of the Heisenberg equation with appropriate A_i's, and with Rydberg wave packet. The results obtained by these two approaches completely overlap for $0\leqslant t\leqslant 7$ as is shown in Fig. 7. Thus we have another way of verifying the accuracy of the method developed in the present work.

VII. APPLICATION TO OTHER SYSTEMS

In addition to the power law and inverse power law potentials, the method described in this paper can be applied to

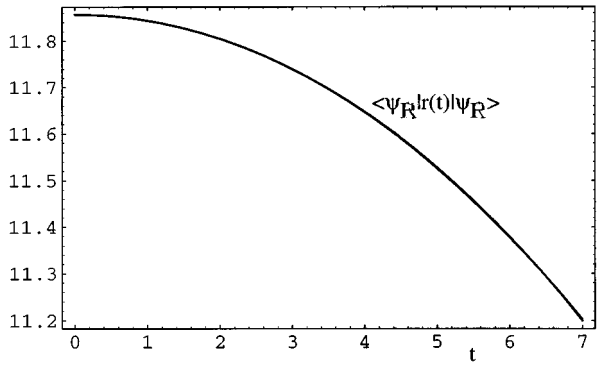

FIG. 7. The position of the center of the Rydberg wave packet as a function of time found by the integration of the Heisenberg equations and also from the solution of the Schrödinger equation. For $t\leqslant 7$ (in units of $Ma^2\hbar$) the two results overlap.

a number of other types of potentials. For instance, let us consider the Morse potential in one dimension,

$$V(x)=V_0\left[\exp\left(-\frac{2(x-x_0)}{c}\right)-2\exp\left(-\frac{(x-x_0)}{c}\right)\right]. \tag{7.1}$$

If we change x to q where q is defined by

$$q=\exp\left(-\frac{(x-x_0)}{c}\right), \tag{7.2}$$

then the Hamiltonian for this system can be written as (in units of $\hbar=M=1$)

$$H=\left(\frac{1}{c}\right)^2\left[-\frac{1}{2}\left(q^2\frac{d^2}{dq^2}+q\frac{d}{dq}\right)+v_0(q^2-q)\right], \tag{7.3}$$

where $v_0=c^2V_0$ is a dimensionless variable. Writing H in terms of $T_{m,n}$, Eq. (2.1), we find

$$H=\frac{1}{c^2}\left(\frac{1}{2}(T_{0,2}T_{2,0}-iT_{0,1}T_{1,0})+v_0(T_{0,2}-2T_{0,1})\right). \tag{7.4}$$

With the help of the product formula, Eq. (2.5), we can write H as an operator which is linear in $T_{m,n}$'s,

$$H=\frac{1}{c^2}\left(\frac{1}{2}T_{2,2}+iT_{1,1}+v_0(T_{0,2}-2T_{0,1})\right). \tag{7.5}$$

From this Hamiltonian we obtain the equation of motion for $T_{m,n}$,

$$\begin{aligned} i\frac{dT_{m,n}}{dt}&=[T_{m,n},H]\\ &=\left(\frac{i}{4}\right)mn(m-n)T_{m-1,n-1}+(m-n)T_{m,n}\\ &\quad+i(n-m)T_{m+1,n+1}\\ &\quad+2mv_0(T_{m-1,n}-T_{m-1,n+1}). \end{aligned} \tag{7.6}$$

The Heisenberg equations of motion for q and p are the special cases of Eq. (7.6) for $(m=0,n=1)$ and $(m=1,n=0)$, respectively. We can solve these equations by the method discussed in Sec. II, however, in this case only $T_{m,n}$ with $m\geqslant 0$ and $n\geqslant 0$ will contribute.

VIII. CONCLUSION

In this paper we have tried to show that the method of integration of the operator Heisenberg equations can be extended to the inverse power law potentials. In particular, we have studied the problem of quantum tunneling in a central field of force, and the time development of the Rydberg wave packet. There are certain advantages in this approach as compared to the conventional method of solving the Schrödinger equation. First the shape of the wave packet will not change in the course of motion, therefore it is easier to define a tunneling time by finding the time that the position of the center of wave packet r_0 [or r_c, Eq. (4.12)] passes through the maximum point of the barrier. For the calculation of the tunneling time a narrow wave packet is prefer-

able, however, for a narrow wave packet the main contribution will come from continuum states, furthermore, the expectation value of $\langle\psi|S_{0,-n}(t)|\psi\rangle$ which appears in the calculation of $\langle\psi|r(t)|\psi\rangle$ grows very rapidly with n even for small n. Therefore the rapid convergence of the expectation value $S_{m,n}(N\Delta t)$, Eq. (2.19), is not assured when $N\Delta t$ is large. For the times that the result of integration is valid (Sec. V), this method gives us not only the expectation values of r and p_r, but generally the expectation value of any Weyl-ordered product $S_{m,n}(t)$. For instance as a byproduct one can calculate the time evolution of the uncertainty $(\langle S_{2.0}-\langle S_{1.0}\rangle^2\rangle)^2(\langle S_{0.2}-\langle S_{0.1}\rangle^2\rangle)^2$ for any power law or inverse power law potentials, or operator integrals of motion such as Eq. (3.6). As we have emphasized before in the integration of the Heisenberg equations, the choice of the wave packet is crucial in getting a rapidly converging series. If we want to use a minimum uncertainty wave packet we can transform the original Hamiltonian by a unitary transformation so that the resulting equation for $T_{m,n}$ involves $m\geqslant 0$ and $n\geqslant 0$ terms as was done for the Morse potential. Another approach which has been recently proposed by Pen and Jiang to study the scattering by a one-dimensional Coulomb potential uses a finite-dimensional matrix method together with a minimum uncertainty wave packet to solve the Heisenberg equation [8].

ACKNOWLEDGMENT

This work is supported in part by a grant from the Natural Sciences and Engineering Council of Canada.

[1] C. M. Bender, F. Cooper, V. P. Gutschick, and M. M. Nieto, Phys. Rev. D **32**, 1486 (1985).
[2] C. M. Bender and G. V. Dunne, Phys. Rev. D **40**, 2739 (1989).
[3] C. M. Bender and G. V. Dunne, Phys. Rev. D **40**, 3504 (1989).
[4] Martin Kamela and M. Razavy, Phys. Rev. A **45**, 2695 (1992).
[5] M. Hron and M. Razavy, Phys. Rev. A **51**, 4365 (1995).
[6] M. Mallalieu and C. R. Stroud, Jr., Phys. Rev. A **51**, 1827 (1995).
[7] G. Alber and P. Zoller, Phys. Rep. **199**, 231 (1991).
[8] Ue-Li Pen and T. F. Jiang, J. Phys. B **28**, L69 (1995).