Total time derivatives of operators in elementary quantum mechanics

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The use of a total time derivative of operators, that depends on the time evolution of the wave function as well as on any intrinsic time dependence in the operators, simplifies the formal development of quantum mechanics and allows its development to more closely follow the corresponding development of classical mechanics. We illustrate the use of the total time derivative for a free particle, the linear potential, the harmonic oscillator, and the repulsive inverse square potential. In these cases, operators whose total time derivative is zero can be found and yield general properties of wave packets and several useful time-dependent solutions of Schrödinger's equation, including the propagator. © *2003 American Association of Physics Teachers.*
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I. INTRODUCTION

The expectation value of any operator $\hat{A}$ changes with time according to[1]

$$\frac{d}{dt}\langle\hat{A}\rangle=\left\langle\frac{\partial}{\partial t}\hat{A}\right\rangle+\frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle. \tag{1.1}$$

The first term on the right-hand side comes from the intrinsic time dependence in $\hat{A}$, and the second from the way the states change with time. It has occasionally been suggested[2] that the *total time derivative* of any operator $\hat{A}$ be defined as

$$\frac{d}{dt}\hat{A}\equiv\dot{\hat{A}}:=\frac{\partial}{\partial t}\hat{A}+\frac{i}{\hbar}[\hat{H},\hat{A}]. \tag{1.2}$$

(The notation $X:=Y$ indicates that X is defined to be Y.) Then it is always true that

$$\frac{d}{dt}\langle\hat{A}\rangle=\left\langle\frac{d}{dt}\hat{A}\right\rangle, \tag{1.3}$$

and it can easily be seen that the definition implies that

$$\frac{d}{dt}(\hat{A}\hat{B})=\dot{\hat{A}}\hat{B}+\hat{A}\dot{\hat{B}} \tag{1.4}$$

and

$$\frac{d}{dt}(f(t)\hat{A})=\dot{f}\hat{A}+f\dot{\hat{A}}, \tag{1.5}$$

which implies that the total derivative obeys the same algebraic rules as ordinary derivatives.

Because this total time derivative is not defined to be a rate of change of anything, some may prefer to use a different symbol for it, for example, D_t instead of d/dt, but the latter notation will be used here. The context determines its meaning; when applied to an operator, its meaning is as in Eq. (1.2). Its use eliminates much of the tedious calculation of commutators in conventional treatments and allows calculations that closely follow those of classical mechanics. For many systems it also enables simple methods to be used to obtain the evolution of some wave packets and the propagator. It brings many of the advantages gained by moving to Heisenberg's picture of the time-evolution while actually remaining in the Schrödinger picture.

After showing how the formal development of quantum mechanics and its application to some systems can be simplified, we will find "invariant operators," that is, operators whose total time derivative is zero. This property is the appropriate generalization of "constant of the motion" to operators that depend on the time. Invariant operators are used here to find general properties and specific examples of the evolution of wave packets and to find the energy eigenvalues of the harmonic oscillator.

II. FORMAL DEVELOPMENT FOR SYSTEMS DESCRIBED BY A POTENTIAL

We first consider Hamiltonians of the form

$$\hat{H}=\frac{1}{2m}\hat{p}^2+V(\hat{\mathbf{r}}). \tag{2.1}$$

In this case all the operators are independent of the time, so calculating the total time derivative requires only the commutator with the Hamiltonian. A calculation of these commutators gives

$$m\dot{\hat{\mathbf{r}}}=\hat{\mathbf{p}}\quad\text{and}\quad\dot{\hat{\mathbf{p}}}=-\nabla\hat{V}, \tag{2.2}$$

as in classical mechanics.

Ehrenfest's theorem for the time evolution of expectation values follows immediately from Eq. (1.3):

$$m\frac{d}{dt}\langle\hat{\mathbf{r}}\rangle=\langle\hat{\mathbf{p}}\rangle\quad\text{and}\quad\frac{d}{dt}\langle\hat{\mathbf{p}}\rangle=-\langle\nabla\hat{V}\rangle. \tag{2.3}$$

The virial theorem also follows easily using Eq. (1.4) from the expectation value of

$$\frac{d}{dt}(\hat{\mathbf{r}}\cdot\hat{\mathbf{p}})=\dot{\hat{\mathbf{r}}}\cdot\hat{\mathbf{p}}+\hat{\mathbf{r}}\cdot\dot{\hat{\mathbf{p}}}=\frac{1}{m}\hat{\mathbf{p}}^2-\hat{\mathbf{r}}\cdot\nabla\hat{V}. \tag{2.4}$$

The time derivative of the angular momentum is

$$\frac{d}{dt}\hat{\mathbf{L}}=\frac{d}{dt}(\hat{\mathbf{r}}\times\hat{\mathbf{p}})=\dot{\hat{\mathbf{r}}}\times\hat{\mathbf{p}}+\hat{\mathbf{r}}\times\dot{\hat{\mathbf{p}}}=-\hat{\mathbf{r}}\times\nabla\hat{V}, \tag{2.5}$$

because $\hat{\mathbf{p}}\times\hat{\mathbf{p}}=0$. For a central potential, $\nabla V=r^{-1}(dV/dr)\mathbf{r}$ and therefore $\dot{\mathbf{L}}=0$, and $\mathbf{L}$ is a constant of the motion.

These calculations are not only simpler, because the commutators were used only for the equations of motion (2.2), but easier for students because the calculations closely follow the corresponding classical calculations.

Next consider how the spread of the position and momentum change with time for a free wave packet in one dimension. There is no force, so $m\dot{\hat{x}}=\hat{p}$ and $\dot{\hat{p}}=0$. To obtain the spread in position, we use the operator $(\hat{x}-\langle\hat{x}\rangle)^2$. Unlike the above operators, this operator is time dependent. Up to now $\dot{a}$ has just been a convenient shorthand for $i\hbar^{-1}[\hat{H},\hat{a}]$, but now the intrinsic time dependence will also play a role. We use the operator equations of motion to find

$$m\frac{d}{dt}(\hat{x}-\langle\hat{x}\rangle)^2=(\hat{x}-\langle\hat{x}\rangle)(\hat{p}-\langle\hat{p}\rangle)+(\hat{p}-\langle\hat{p}\rangle)(\hat{x}-\langle\hat{x}\rangle),$$

(2.6)

$$m^2\frac{d^2}{dt^2}(\hat{x}-\langle\hat{x}\rangle)^2=2(\hat{p}-\langle\hat{p}\rangle)^2.$$

(2.7)

If we define $(\Delta x)^2:=\langle(\hat{x}-\langle\hat{x}\rangle)^2\rangle$ and $(\Delta p)^2:=\langle(\hat{p}-\langle\hat{p}\rangle)^2\rangle$, then Δp is constant and

$$m^2\frac{d^2}{dt^2}(\Delta x)^2=2(\Delta p)^2.$$

(2.8)

[Note that $d^2\langle\hat{A}\rangle/dt^2=d(d\langle\hat{A}\rangle/dt)/dt=d(\langle d\hat{A}/dt\rangle)/dt=\langle d^2\hat{A}/dt^2\rangle$, where $d^2\hat{A}/dt^2$ means the result of the action in Eq. (1.2) applied twice to $\hat{A}$.] Therefore, Δx must have the form

$$\Delta x=\Delta x_0\sqrt{1+(t-t_0)^2/\tau^2},$$

(2.9)

where $\tau=m\Delta x_0/\Delta p$. Hence, for a free wave packet, the spread Δx goes through a minimum Δx_0 and approaches a linear increase with time at large distances from the minimum.

A similar, but slightly lengthier, calculation can be carried out for the harmonic oscillator to show the centroid of every wave packet not only follows the classical oscillation, but its width oscillates at twice the frequency. For a linear potential (motion under gravity or a uniform electric field) the width behaves exactly as for the free case.

A comparison of these calculations with the conventional methods[3] will show how much simpler this approach is.

III. INVARIANT OPERATORS

An operator is "invariant" if its total time derivative is zero. This definition includes the usual "constant of the motion," that is, a time-independent operator that commutes with the Hamiltonian. It will be seen below that time-dependent invariant operators are especially interesting. It is easy to see that if $\hat{a}$ and $\hat{b}$ are invariant then so are $\hat{a}+\hat{b}$, $\hat{a}\hat{b}$, the adjoints $\hat{a}^\dagger$ and $\hat{b}^\dagger$, and $\lambda\hat{a}$ if λ is a constant.

If an invariant operator $\hat{a}$ is applied to any solution ψ of Schrödinger's equation

$$\hat{H}\psi=i\hbar\frac{\partial\psi}{\partial t},$$

(3.1)

it will produce another solution, because

$$\left(\hat{H}-i\hbar\frac{\partial}{\partial t}\right)\hat{a}\psi=\left(\hat{H}\hat{a}-i\hbar\frac{\partial\hat{a}}{\partial t}-\hat{a}\hat{H}\right)\psi=-i\hbar\dot{\hat{a}}\psi$$

(3.2)

and $\dot{\hat{a}}=0$. Invariant operators will be used in this way to produce different solutions of Schrödinger's equation for several systems.

Now consider whether eigenstates of an invariant operator will satisfy Eq. (3.1). The operators (in Schrödinger's representation) involve differentiation by position only, so if $\phi(\mathbf{r},t)$ is a solution of $\hat{a}\phi=\alpha\phi$, then $f(t)\phi(\mathbf{r},t)$ also will be a solution. Thus it is not true that every eigenfunction will satisfy Schrödinger's equation. However, if $\phi(\mathbf{r},t)$ is an eigenfunction at a particular time t_0, then there will be a unique solution $\psi(\mathbf{r},t)$ of Schrödinger's equation (for all t) such that $\psi(\mathbf{r},t_0)=\phi(\mathbf{r},t_0)$ and, from Eq. (3.2), $(\hat{a}-\alpha)\psi$ will satisfy Schrödinger's equation and therefore will remain zero. That is, $\psi(\mathbf{r},t)$ will be both an eigenfunction of $\hat{a}$ (with constant eigenvalue α) and a solution of Schrödinger's equation. Thus, if there is only one eigenfunction of $\hat{a}$, it must satisfy Eq. (3.1), apart from a time-dependent factor. If there are several linearly independent eigenfunctions of $\hat{a}$, then linear combinations with time-dependent coefficients may be required to satisfy Eq. (3.1).

Invariant operators will now be found for some simple one-dimensional systems.

IV. A FREE PARTICLE

The operator equations of motion are $m\dot{\hat{x}}=\hat{p}$ and $\dot{\hat{p}}=0$. Classically, $mx-pt$ is constant and similarly $m\hat{x}-\hat{p}t$ is invariant. A constant can be added to t, even a complex one; but a real constant just changes the origin of time, and we take

$$\hat{a}:=m\hat{x}-\hat{p}(t-i\tau)\quad(\tau\text{ real}).$$

(4.1)

To find an eigenstate ψ_α of $\hat{a}$ with eigenvalue α, we first find the real values $\bar{x}_0$, $\bar{p}_0$ such that $\alpha=m\bar{x}_0+i\bar{p}_0\tau$. Then $\alpha=m\bar{x}-\bar{p}(t-i\tau)$ for all time, where $\bar{x}$, $\bar{p}$ are the solutions of the classical equations of motion with initial values $\bar{x}_0$, $\bar{p}_0$. Next define

$$\hat{a}_\alpha:=\hat{a}-\alpha=m(\hat{x}-\bar{x})-(\hat{p}-\bar{p})(t-i\tau).$$

(4.2)

Now ψ_α will have $\hat{a}_\alpha\psi_\alpha=0$ and therefore $\langle\hat{a}_\alpha\rangle=0$, $\langle\hat{x}\rangle=\bar{x}$, and $\langle\hat{p}\rangle=\bar{p}$ for an eigenstate of $\hat{a}$. Furthermore

$$\hat{a}_\alpha-\hat{a}_\alpha^\dagger=2i\tau(\hat{p}-\bar{p}),$$
$$\tfrac{1}{2}(\hat{a}_\alpha+\hat{a}_\alpha^\dagger)=m(\hat{x}-\bar{x})-(\hat{p}-\bar{p})t,$$

(4.3)

and therefore

$$2m(\hat{x}-\bar{x})=\hat{a}_\alpha(1-it/\tau)+\hat{a}_\alpha^\dagger(1+it/\tau).$$

(4.4)

Hence, using $[\hat{a}_\alpha,\hat{a}_\alpha^\dagger]=[\hat{a},\hat{a}^\dagger]=2\hbar m\tau$, we have

$$4\tau^2\langle(\hat{p}-\bar{p})^2\rangle=\langle\hat{a}_\alpha\hat{a}_\alpha^\dagger\rangle=\langle\hat{a}_\alpha^\dagger\hat{a}_\alpha+2\hbar m\tau\rangle=2\hbar m\tau,$$

(4.5)

$$4m^2\langle(\hat{x}-\bar{x})^2\rangle=\langle\hat{a}_\alpha\hat{a}_\alpha^\dagger\rangle(1+t^2/\tau^2)=2\hbar m\tau(1+t^2/\tau^2).$$

(4.6)

Thus, for any eigenstate of $\hat{a}$,

$$\Delta p=\sqrt{\hbar m/2\tau}\quad\text{and}\quad\Delta x=\sqrt{\hbar\tau/2m}\sqrt{1+t^2/\tau^2},$$

(4.7)

consistent with Eq. (2.9). Note that the minimum value of the uncertainty product $\Delta x\Delta p$ is $\tfrac{1}{2}\hbar$; so at its minimum this eigenfunction is a minimum uncertainty wave packet.

It is easy to find the form of the wave function $\psi_\alpha(x,t)$. From $\hat{a}_\alpha\psi_\alpha=0$, we have

$$\frac{\partial \psi}{\partial x} = \frac{i}{\hbar}\left[\bar{p} + \frac{m(x-\bar{x})}{t-i\tau}\right]\psi, \tag{4.8}$$

and hence

$$\psi_\alpha(x,t) = \exp\frac{i}{\hbar}\left[\vartheta(t) + \bar{p}x + \frac{m(x-\bar{x})^2}{2(t-i\tau)}\right], \tag{4.9}$$

where $\vartheta(t)$ can be determined by substituting $\psi_\alpha(x,t)$ into Schrödinger's equation. This substitution gives

$$\vartheta = \tfrac{1}{2}i\hbar/(t-i\tau) - \bar{E}, \tag{4.10}$$

where $\bar{E} := \tfrac{1}{2}\bar{p}^2/m$, and therefore

$$\psi_\alpha(x,t) = \frac{1}{\sqrt{t-i\tau}}e^{i(\bar{p}x-\bar{E}t)/\hbar}\exp\left(\frac{im(x-\bar{x})^2}{2\hbar(t-i\tau)}\right). \tag{4.11}$$

Equation (4.11) represents the moving Gaussian wave function found in most texts, but here its expectation values ($\langle\hat{x}\rangle,\langle\hat{p}\rangle,\Delta x,\Delta p$) are known without any further integration.

The eigenfunction $\psi_\alpha(x,t)$, with $\bar{p}=0$ and $\tau=0$, must (when appropriately normalized) be the propagator for the free particle. The propagator is just the evolution of the δ function, and the eigenfunction (with eigenvalue $\bar{x}$) of $\hat{x}$ is $\delta(x-\bar{x})$. Therefore, the eigenfunction of $\hat{x}-\hat{p}t/m$ must approach $\delta(x-\bar{x})$ as $t\to0$. Thus the propagator $K(x,x',t)$, such that

$$\int_{-\infty}^{\infty} K(x,x',t)\psi(x',t_0)dx' = \psi(x,t_0+t) \tag{4.12}$$

for any wave function $\psi(x,t)$, can differ only by a constant factor from

$$\Psi(x,x',t) := \frac{1}{\sqrt{t}}\exp\left(\frac{im}{2\hbar t}(x-x')\right). \tag{4.13}$$

To determine the factor, use the integral

$$\int_{-\infty}^{\infty} \Psi(x,x',t_1)\Psi(x',x'',t_2)dx'$$
$$= \sqrt{2\pi i\hbar/m}\,\Psi(x,x'',t_1+t_2), \tag{4.14}$$

which is easily calculated by direct integration. Because the propagator must propagate itself, it must be $K(x,x',t) = \Psi(x,x',t)/\sqrt{2\pi i\hbar/m}$.

Other invariants: For the free particle, $\hat{p}$ is also invariant (but independent of t). Thus the spatial derivative of any solution of the free Schrödinger equation is also a solution, as are all higher derivatives as follows directly from Schrödinger's equation. A similar property holds for indefinite spatial integrals and time derivatives and integrals of any solution of the free Schrödinger equation. The spatial derivatives of the propagator are the evolutions of the derivatives of the δ function, and can be related[4] to Hermite polynomials using

$$(d/d\xi)^n e^{-x^2} = (-1)^n H_n(\xi)e^{-x^2}. \tag{4.15}$$

The integral of the δ function is a step function and the integral of the propagator can be expressed in terms of the Fresnel integrals

$$C(y) + iS(y) = \int_0^y \exp(\tfrac{1}{2}i\pi z^2)dz. \tag{4.16}$$
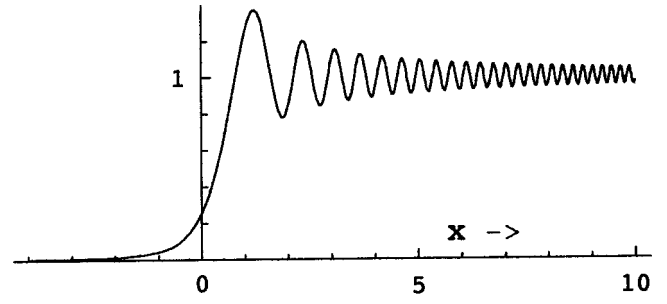
Fig. 1. The free evolution of the step function. The graph shows $|\phi^2|$ where $\phi(x)$ is initially the step function. The shape is valid for all times $t>0$; all that changes is the scale on the x-axis. The values of x shown are for $t = m/\pi\hbar$.

Thus $C(y)+iS(y)$ satisfies the free Schrödinger equation if $y = \sqrt{m/\pi\hbar t}\,x$, and $\phi := \tfrac{1}{2}+\tfrac{1}{2}(1-i)[C(y)+iS(y)]$ is the time evolution of the step function and also satisfies $\hat{a}\hat{p}\varphi = 0$. [If $\chi := \hat{p}\phi$, then $\hat{a}\chi = 0$, so that $\chi = f(t)\psi$, where ψ is the propagator, and therefore $\phi(x,t) = (i/\hbar)f(t) \times \int^x \psi(x',t)dx'$.] Figure 1 shows $|\phi^2|$. Many other invariants can be made from powers, sums, and products of $\hat{a}$ and $\hat{p}$. These can be used to create a vast variety of solutions of the free Schrödinger equation, but they will not be pursued further here.

V. UNIFORM BUT TIME-VARYING FORCE

The Hamiltonian is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 - \mathcal{E}(t)\hat{x}, \tag{5.1}$$

which could represent a charged particle in a time-varying electric field. The operator equations of motion are $m\dot{\hat{x}} = \hat{p}$, $\dot{\hat{p}} = \mathcal{E}(t)$ which differ from the free case only in that $\dot{\hat{p}}$ varies with time, but is still independent of $\hat{x}$ and $\hat{p}$. Thus, all we need to do is change the invariant $\hat{a}$ by adding a suitable time-varying multiple of the unit operator:

$$\hat{a} := m\hat{x} - \hat{p}(t-i\tau) + \sigma(t). \tag{5.2}$$

Then $\dot{\hat{a}} = -\mathcal{E}(t)(t-i\tau) + \dot{\sigma}$, so that

$$\sigma(t) = \int_0^t (t'-i\tau)\mathcal{E}(t')dt'. \tag{5.3}$$

To generalize this invariant to refer to an arbitrary trajectory, we define

$$\hat{a}_\alpha := m(\hat{x}-\bar{x}) - (\hat{p}-\bar{p})(t-i\tau) = \hat{a}-\alpha, \tag{5.4}$$

where $\bar{x}$, $\bar{p}$ satisfy the classical equations of motion $m\dot{\bar{x}} = \bar{p}$ and $\dot{\bar{p}} = \mathcal{E}(t)$ to ensure that $\hat{a}_\alpha$ is invariant. Here $\alpha = m\bar{x} - \bar{p}(t-i\tau) + \sigma(t)$ and the real and imaginary parts of the constant α give the classical motion

$$\bar{p} = \bar{p}_0 + \int_0^t \mathcal{E}(t')dt',$$

$$m\bar{x} = m\bar{x}_0 + \bar{p}_0 t + \int_0^t (t-t')\mathcal{E}(t')dt'. \tag{5.5}$$

As before $\langle \hat{a}_\alpha \rangle = 0$ gives $\langle \hat{p} \rangle = \bar{p}$ and $\langle \hat{x} \rangle = \bar{x}$. Thus $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$ exactly follow the classical trajectory. The widths Δx, Δp are not affected by $\sigma(t)$ and therefore evolve exactly as they would if no force were acting. The wave function has the same form as for the free particle [see Eq. (4.11)], except that $\bar{x}$, $\bar{p}$ now follow a trajectory that depends on the field $\mathcal{E}(t)$.

VI. THE SIMPLE HARMONIC OSCILLATOR

The Hamiltonian is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2 \hat{x}^2, \tag{6.1}$$

and the operator equations of motion are $m\dot{\hat{x}} = \hat{p}$, $\dot{\hat{p}} = -m\omega^2 \hat{x}$. From these equations, we have $\dot{\hat{x}} + i\dot{\hat{p}}/m\omega = -i\omega(\hat{x} + i\hat{p}/m\omega)$, and therefore

$$\hat{a} := e^{i\omega t}(\hat{x} + i\hat{p}/m\omega)/L \tag{6.2}$$

is invariant. The divisor $L := \sqrt{2\hbar/(m\omega)}$ is inserted to make $[\hat{a}, \hat{a}^\dagger] = 1$, as usual.

Energy eigenstates: Using this invariant operator allows a slightly different approach to finding the energy eigenstates. When multiplied by $\exp(-iEt/\hbar)$, an eigenstate with energy E satisfies Schrödinger's equation and therefore if $\hat{a}$ is applied to such an energy eigenstate, it either gives zero or a solution of Schrödinger's equation with its only time dependence in the factor $\exp[-i(E-\hbar\omega)t/\hbar]$, that is, an eigenstate with E lower by $\hbar\omega$. Similarly $\hat{a}^\dagger$, which is also invariant, raises the energy by $\hbar\omega$. Because the energy eigenvalues must be positive, if we repeatedly apply $\hat{a}$ to any energy eigenstate, we must eventually reach a ground state ψ_0 such that $\hat{a}\psi_0 = 0$. Then $\hat{a}^\dagger \hat{a}\psi_0 = 0$, and

$$\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + \tfrac{1}{2}), \tag{6.3}$$

so the lowest energy eigenvalue is $E_0 = \tfrac{1}{2}\hbar\omega$, and every eigenvalue must be of the form $(n + \tfrac{1}{2})\hbar\omega$ with $n = 0,1,2,\dots$. The spatial dependence of the wave function $\psi_0(x,t)$ is found from $\hat{a}\psi_0 = 0$, which gives

$$\psi_0(x,t) = e^{-i\omega t/2}\exp(-x^2/L^2). \tag{6.4}$$

Applying $\hat{a}^\dagger$ repeatedly to $\psi_0(x,t)$ gives the excited states, in the usual way.

Coherent states: To deal with an eigenstate of $\hat{a}$ with eigenvalue α, we first find the classical motion $\bar{x}$, $\bar{p}$ that has real initial values $\bar{x}_0$, $\bar{p}_0$ such that $\alpha = (\bar{x}_0 + i\bar{p}_0/m\omega)/L$. Then $e^{i\omega t}(\bar{x} + i\bar{p}/m\omega)/L$ will be constant (and equal to α) for all time. Now we define

$$\hat{a}_\alpha := \hat{a} - \alpha = e^{i\omega t}[(\hat{x} - \bar{x}) + i(\hat{p} - \bar{p})/m\omega]/L. \tag{6.5}$$

Then the solutions of $\hat{a}_\alpha\psi = 0$ will have $\langle \hat{a}_\alpha \rangle = 0$, and therefore $\langle \hat{x} \rangle = \bar{x}$ and $\langle \hat{p} \rangle = \bar{p}$; that is, the wave packet evolves with its centroid at $\bar{x}$, $\bar{p}$ following a sinusoidal oscillation. To find the spread in position, we use

$$\hat{x} - \bar{x} = \tfrac{1}{2}L(\hat{a}_\alpha e^{-i\omega t} + \hat{a}_\alpha^\dagger e^{i\omega t}), \tag{6.6}$$

and obtain

$$\langle(\hat{x} - \bar{x})^2\rangle = \tfrac{1}{4}L^2\langle \hat{a}_\alpha \hat{a}_\alpha^\dagger \rangle. \tag{6.7}$$

Then using $[\hat{a}_\alpha, \hat{a}_\alpha^\dagger] = [\hat{a}, \hat{a}^\dagger] = 1$, we get $\Delta x = \tfrac{1}{2}L$. This result is the same as for the ground state energy eigenstate,

which corresponds to $\bar{x} = \bar{p} = 0$. Similarly, $\Delta p = \hbar/L$, so these states always have the minimum uncertainty product.

The differential equation $\hat{a}_\alpha\psi = 0$ yields

$$\psi = \exp\left[\frac{i}{\hbar}(\vartheta(t) + \bar{p}x) - (x - \bar{x})^2/L^2\right], \tag{6.8}$$

and $\vartheta(t)$ can be found by inserting Eq. (6.8) into Schrödinger's equation. The result is

$$\dot{\vartheta} = -\frac{1}{2}\hbar\omega - \frac{1}{2m}\bar{p}^2 + \frac{1}{2}m\omega^2\bar{x}^2, \tag{6.9}$$

so that

$$\vartheta = -\tfrac{1}{2}\hbar\omega t - \tfrac{1}{2}\bar{x}\bar{p}. \tag{6.10}$$

These states, which follow the classical oscillation without change of width, are known as coherent states. The "raising operator" $\hat{a}_\alpha^\dagger$ can be applied to these states to obtain displaced excited states that are essentially Hermite–Gaussians that also follow a classical oscillation.[4]

Squeezed states: The operator $\hat{a}$ in Eq. (6.2) is not the most general invariant that is linear in $\hat{x}$ and $\hat{p}$. The form

$$\hat{b} = \mu\hat{a} + \nu\hat{a}^\dagger \tag{6.11}$$

will be invariant if μ and ν are constants. To set the scale of $\hat{b}$, we also take $[\hat{b}, \hat{b}^\dagger] = 1$, which implies that $\mu^*\mu - \nu^*\nu = 1$. In terms of $\hat{x}$ and $\hat{p}$,

$$\hbar\hat{b} = \xi(t)\hat{p} - \pi(t)\hat{x}, \tag{6.12}$$

where

$$\xi = \tfrac{1}{2}iL(\mu e^{i\omega t} - \nu e^{-i\omega t}), \pi = -\hbar(\mu e^{i\omega t} + \nu e^{-i\omega t})/L. \tag{6.13}$$

Note that ξ and π have the dimensions of length and momentum, respectively, and satisfy the classical equations of motion, $m\dot{\xi} = \pi$, $\dot{\pi} = -m\omega^2\xi$, but can be complex. The phase assigned to $\hat{b}$ is not important, so we take μ to be real. Then adding a constant phase ϑ to ν is equivalent to shifting the time by $\tfrac{1}{2}\vartheta/\omega$ [because $\mu a(t) + \nu e^{i\vartheta}a^\dagger(t) = \mu e^{i\omega t}a(0) + \nu e^{-i(\omega t - \vartheta)}a^\dagger(0) = e^{1/2i\vartheta}\hat{b}(t - \tfrac{1}{2}\vartheta/\omega)]$. Thus, we can also take ν to be real. Instead of the two parameters μ and ν, it is sometimes convenient to use the "squeezing factor" $s := \mu + \nu$. Then $\mu^2 - \nu^2 = 1$ leads to $\mu - \nu = 1/s$ and $s \geq 1$. The coherent states correspond to $\mu = 1$, $\nu = 0$, or $s = 1$.

Next we introduce

$$\hbar\hat{b}_\alpha := \xi(t)(\hat{p} - \bar{p}) - \pi(t)(\hat{x} - \bar{x}), \tag{6.14}$$

where $\bar{x}$, $\bar{p}$ is a classical oscillation and again the solution of $\hat{b}_\alpha\psi = 0$ (and therefore any eigenstate of $\hat{b}$) will follow the classical motion in the sense that $\langle \hat{x} \rangle = \bar{x}$ and $\langle \hat{p} \rangle = \bar{p}$. From Eq. (6.14) and using $\mathrm{Im}(\xi^*\pi) = \tfrac{1}{2}\hbar$, we find

$$\hat{x} - \bar{x} = i(\xi^*\hat{b}_\alpha - \xi\hat{b}_\alpha^\dagger), \quad \hat{p} - \bar{p} = i(\pi^*\hat{b}_\alpha - \pi\hat{b}_\alpha^\dagger), \tag{6.15}$$

and therefore, similarly to the derivation of Eq. (6.7), $\Delta x = |\xi|$ and $\Delta p = |\pi|$. From Eq. (6.13), at $t = 0$, $\Delta x = \tfrac{1}{2}L(\mu - \nu) = \tfrac{1}{2}L/s$, and $\Delta p = \hbar s/L$. Then $2\Delta x/L$ and $L\Delta p/\hbar$ oscillate between the two extremes of s and $1/s$, each taking its maximum value when the other takes its minimum. The differential equation corresponding to $\hat{b}_\alpha\psi = 0$ is easily solved

[similarly to Eq. (6.8)] and the squeezed states of the oscillator are also moving Gaussians.

The propagator requires $\xi = 0$ to ensure that the eigenfunctions of $\hat{b}$ will be $\delta(x - \bar{x})$ and ξ will be zero at $t = 0$ if $s = \infty$. (A factor of s must be removed from $\hat{b}_\alpha$ to keep it finite in this limit.)

VII. REPULSIVE INVERSE SQUARE POTENTIAL

The Hamiltonian is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + c/x^2. \tag{7.1}$$

Only the repulsive case ($c > 0$) will be considered because the attractive case is too singular and requires special treatment.[5] Such a potential arises, with $c = \hbar^2 \ell(\ell+1)/2m$, for the radial part of the wave function (multiplied by r) for a spherically symmetric system in three dimensions, and the spherical Bessel functions are familiar as the radial part of the energy eigenfunctions for the free particle. We will treat the general case of arbitrary $c > 0$ in one dimension. The repulsive hill is impenetrable so there can be no tunneling through the origin. Therefore, only $x > 0$ need be considered, and we expect the wave function to vanish as $x \to 0$.

The operator equations of motion are $m\dot{\hat{x}} = \hat{p}$, $\dot{\hat{p}} = 2c/x^3$. Therefore

$$\frac{d}{dt}(\hat{x}\hat{p}) = \frac{d}{dt}(\hat{p}\hat{x}) = \frac{1}{m}\hat{p}^2 + 2c/x^2 = 2\hat{H} \tag{7.2}$$

and

$$\hat{a} := \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}) - 2t\hat{H} \tag{7.3}$$

is invariant. (We have used the symmetrized form to keep it Hermitean.) Furthermore,

$$\frac{1}{2}m\frac{d}{dt}(\hat{x}^2) = \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}) = \hat{a} + 2t\hat{H}, \tag{7.4}$$

so that

$$\hat{b} := \frac{1}{2}m\hat{x}^2 - t\hat{a} - t^2\hat{H} = \frac{1}{2}m\hat{x}^2 - \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}) + t^2\hat{H} \tag{7.5}$$

is also invariant. It follows that $\langle x^2 \rangle$ is quadratic in t for any state.

Also the eigenfunction of $\hat{b}$, with arbitrary eigenvalue β, will give the propagator for the system because as $t \to 0$, it must approach an eigenfunction of $\hat{x}^2$, that is, $\delta(x^2 - 2\beta/m)$ apart from a factor. (The variable x^2 is just as good as x for this system because we need only consider positive values of x.)

The solution of the differential equation $\hat{b}\varphi = \beta\varphi$ is

$$\varphi = \exp(i\tfrac{1}{2}mx^2/\hbar t)\sqrt{x}J_\nu(\sqrt{2m\beta/\hbar^2}x/t), \tag{7.6}$$

where $\nu^2 = \frac{1}{4} + 2cm/\hbar^2$. A discussion of how to find this solution is given in the Appendix. The positive value of ν gives the regular solution; the negative value also gives a solution, but it is singular at $x = 0$. As before, this eigenfunction requires a time-dependent factor to also satisfy Schrödinger's equation. The factor can be found to be $\exp(i\beta/\hbar t)/t$ by inserting φ in Eq. (7.6) into Schrödinger's equation. Thus

$$\psi = \exp[i(\beta + \tfrac{1}{2}mx^2)/\hbar t](\sqrt{x}/t)J_\nu(\sqrt{2m\beta/\hbar^2}x/t) \tag{7.7}$$

is the eigenfunction of $\hat{b}$ that also evolves as a wave function.

As before, a more general wave function will be obtained by replacing t by $t - i\tau$. The propagator results from the limit $\tau \to 0$, while for sufficiently large τ, the wave function corresponds to a localized "particle" coming toward the origin, being slowed to a standstill by the repulsive force and then retreating, as in the classical case. The details of this calculation, and the exact normalization and calculation of $\langle x^2 \rangle$, $\langle \hat{H} \rangle$, and $\langle \hat{a} \rangle$, will be pursued in the Appendix.

VIII. RELATION TO THE HEISENBERG PICTURE

For the operator $\hat{A}$, the equivalent in the Heisenberg picture[6] is $\hat{A}_H := \hat{T}^\dagger \hat{A}\hat{T}$, where $\hat{T}$ is the time-evolution operator such that $\psi(t) = \hat{T}\psi(0)$ and $i\hbar d\hat{T}/dt = \hat{H}\hat{T}$. It follows that

$$ih\frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}_H] + ih\hat{T}^\dagger\frac{\partial\hat{A}}{\partial t}\hat{T}. \tag{8.1}$$

That is,

$$\frac{d\hat{A}}{dt} = \hat{T}\frac{d\hat{A}_H}{dt}\hat{T}^\dagger. \tag{8.2}$$

(Note that where d/dt is applied to an operator in Heisenberg's picture, it does not have the special meaning it has when applied to an operator in Schrödinger's picture).

Thus the total time derivative of any operator is the Schrödinger picture version of the time derivative of its Heisenberg picture version, which implies that the operator equations of motion will have the same form in the Heisenberg picture as they have in Schrödinger picture using the total time derivative.

The formal development in Sec. II and the determination and application of the invariant operators could therefore be presented in the Heisenberg picture, but the advantage of using the total time derivative in an elementary course is that the Heisenberg picture requires much more mathematical machinery. One must deal with exponentials of operators and, for Hamiltonians that depend on the time, the determination of the explicit form of the transformation is often quite difficult.

IX. DISCUSSION

Time-dependent invariant operators that are linear in $\hat{x}$ and $\hat{p}$ can be found[4] for any Hamiltonian that is quadratic (or linear) in $\hat{x}$ and $\hat{p}$, even with arbitrary time dependence in the Hamiltonian. These systems include, for example, harmonic oscillators that are driven (a time-varying linear term in H) or have varying frequency, as well as the cases treated previously. The case of $V = c/x^2$ shows that the method is not restricted to quadratic Hamiltonians. However, I have not found a useful invariant for the important case of $V = c/x$. An indication that this potential might be more difficult can be seen from the corresponding classical system. For all classical one-dimensional potentials, an integral gives the time as a function of x and the energy. In the previous examples, the time (or some function of the time) can be expressed in a form that is linear in the velocity and the energy and then the eigenfunctions of the corresponding quantum operator can be found easily. But for $V = c/x$, the classical result is highly non-linear in the energy.

In summary, the use of the total derivative of operators (in Schrödinger's picture of the time evolution) simplifies the formal development of quantum mechanics and its application to particular systems. This approach eliminates many of the tedious calculations of commutators that are required in the usual treatment and allows a development that more closely follows the familiar classical treatment. Furthermore, it makes it easy to use the simple invariant operators that can be found for many of the systems often studied in elementary quantum mechanics to find simple wave packets that illustrate the dynamics of the system and to find the propagator.

APPENDIX: ANALYSIS OF THE WAVE FUNCTION FOR THE POTENTIAL $V = c/x^2$

The equation $\hat{b}\varphi = \beta\varphi$ is, in Schrödinger's representation, an ordinary differential equation (ODE) in x with t as a parameter. Its solution, apart from a possible time-dependent factor, will satisfy Schrödinger's equation, which is a partial differential equation (PDE). But $\hat{b}\varphi = \beta\varphi$ is not easy to solve even though it is only an ODE. [The solution was given in Eq. (7.7).] Equation-solving programs such as Maple or Mathematica will probably not solve it because they will not attempt to factor out the required factor of $\sqrt{x}\,\exp(\frac{1}{2}imx^2/\hbar t)$ to reduce the equation to Bessel's form.

Surprisingly, one way to obtain the solution is to convert the equation to a PDE using the requirement that the solution also satisfy Schrödinger's equation. First write $\hat{b} := \frac{1}{2}m\hat{x}^2 - t(\hat{x}\hat{p} - \frac{1}{2}i\hbar) + t^2\hat{H}$, and then insert $\hat{p} = -i\hbar\,\partial/\partial x$ and $\hat{H} = i\hbar\,\partial/\partial t$ to give the PDE,

$$tx\frac{\partial\varphi}{\partial x} + t^2\frac{\partial\varphi}{\partial t} + \left[\frac{1}{2}t + \frac{i}{\hbar}\left(\beta - \frac{1}{2}mx^2\right)\right]\varphi = 0. \tag{A1}$$

Such first-order, linear PDEs can be solved easily by standard methods (or using equation-solving programs), and it is easy to verify directly that $\varphi = \exp[i(\beta + \frac{1}{2}mx^2)/(\hbar t)]f(x/t)/\sqrt{x}$ satisfies Eq. (A1), if f is an arbitrary function of x/t. If we substitute this form of φ into Schrödinger's equation, we see that $f(u)$, with $u = x/t$, must satisfy the ODE

$$u^2 f'' - u f' + (c_1 + c_2 u^2)f = 0, \tag{A2}$$

where $c_1 = \frac{3}{4} - 2cm/\hbar^2$ and $c_2 = 2m\beta/\hbar^2$. It is not difficult to recognize that Eq. (A2) can be converted to Bessel's equation by dividing $f(u)$ by u. Thus

$$\varphi = \exp[i(\beta + \frac{1}{2}mx^2)/(\hbar t)]u J_\nu(\sqrt{2m\beta/\hbar^2}u)/\sqrt{x}, \tag{A3}$$

where $\nu^2 = 1 - c_1 = \frac{1}{4} + 2cm/\hbar^2$. The form of Eq. (A3) agrees with Eq. (7.7).

Expectation values: As before, t can be complex and the function

$$\psi = \exp\left[\frac{i}{\hbar}\frac{\beta + \frac{1}{2}mx^2}{t - i\tau}\right]\frac{\sqrt{x}}{t - i\tau}J_\nu\left(\sqrt{\frac{2m\beta}{\hbar^2}}\frac{x}{t - i\tau}\right) \tag{A4}$$

is the eigenfunction, with eigenvalue β, of the invariant operator

$$\hat{B} := \frac{1}{2}m\hat{x}^2 - \frac{1}{2}(t - i\tau)(\hat{x}\hat{p} + \hat{p}\hat{x}) + (t - i\tau)^2\hat{H}, \tag{A5}$$

and ψ satisfies the time-dependent Schrödinger equation for the potential $V = c/x^2$.

To calculate expectation values, we first normalize the wave function using

$$\psi^*\psi = \exp\left[-\frac{2}{\hbar}\frac{\tau(\beta_r + \frac{1}{2}mx^2) + \beta_i t}{t^2 + \tau^2}\right]$$

$$\times\frac{x}{t^2 + \tau^2}J_\nu(a^*x)J_\nu(ax), \tag{A6}$$

where $a := \sqrt{2m\beta/\hbar^2}/(t - i\tau)$ and $\beta = \beta_r + i\beta_i$. Now apply the integral

$$\int_0^\infty \exp(-\frac{1}{2}\lambda x^2)J_\nu(ax)J_\nu(bx)x\,dx$$

$$= \lambda^{-1}\exp[-\frac{1}{2}\lambda^{-1}(a^2 + b^2)]I_\nu(ab/\lambda) \tag{A7}$$

[for $\mathrm{Re}(\nu) > -1$] given by Weber in 1868.[7] We substitute $b = a^*$ and $\lambda = 2\tau m/\hbar(t^2 + \tau^2)$, and obtain

$$\int_0^\infty \psi^*\psi\,dx = \frac{\hbar}{2\tau m}\exp\left(-\frac{\beta_r}{\hbar\tau}\right)I_\nu\left(\frac{|\beta|}{\hbar\tau}\right). \tag{A8}$$

To determine $\langle\hat{x}^2\rangle$ we differentiate Weber's integral in Eq. (A7) with respect to λ to obtain[8]

$$\int_0^\infty \exp(-\frac{1}{2}\lambda x^2)J_\nu(ax)J_\nu(bx)x^3\,dx$$

$$= 2\lambda^{-2}e^{-w}\{(\nu + 1 - w)I_\nu(z) + zI_{\nu+1}(z)\}, \tag{A9}$$

where $w := \frac{1}{2}(a^2 + b^2)/\lambda$ and $z := ab/\lambda$. Equation (A9) implies that

$$\frac{1}{2}m\langle\hat{x}^2\rangle = \beta_r + \frac{t}{\tau}\beta_i + (t^2 + \tau^2)\frac{\hbar}{2\tau}\left[\nu + 1 + z\frac{I_{\nu+1}(z)}{I_\nu(z)} - \frac{\beta_r}{\hbar\tau}\right], \tag{A10}$$

and $z = |\beta|/\hbar\tau$. But Eq. (A5) can be written as

$$\hat{B} := \frac{1}{2}m\hat{x}^2 - (t - i\tau)\hat{a} - (t^2 + \tau^2)\hat{H}, \tag{A11}$$

and therefore, taking the real and imaginary parts of the expectation value of $\hat{B}$, $\beta_i = \tau\langle\hat{a}\rangle$, and

$$\frac{1}{2}m\langle\hat{x}^2\rangle = \beta_r + (t/\tau)\beta_i + (t^2 + \tau^2)\langle\hat{H}\rangle. \tag{A12}$$

If we compare this form with Eq. (A10), we see that

$$\langle\hat{H}\rangle = \frac{\hbar}{2\tau}\left[\nu + 1 + z\frac{I_{\nu+1}(z)}{I_\nu(z)} - \frac{\beta_r}{\hbar\tau}\right]. \tag{A13}$$

The propagator: A more symmetrical form for the eigenfunction of $\hat{b}$, with eigenvalue $\frac{1}{2}mx'^2$, is

$$\Psi(x, x', t) = \frac{\sqrt{xx'}}{t}\exp\left[\frac{im}{2\hbar t}(x^2 + x'^2)\right]J_\nu\left(\frac{mxx'}{\hbar t}\right). \tag{A14}$$

As shown in Sec. V, this eigenfunction must be the propagator apart from a factor independent of x and t that will now be determined. The eigenfunction satisfies Schrödinger's equation and therefore should propagate itself. If we use the integral in Eq. (A7), we can evaluate the relevant integral to give

$$\int_0^\infty \Psi(x, x', t_1)\Psi(x', x'', t_2)dx'$$

$$= i^{\nu+1}(\hbar/m)\Psi(x, x'', t_1 + t_2), \tag{A15}$$

where the relation $I_\nu(iz) = i^\nu J_\nu(z)$ [for $\mathrm{Im}(z) > 0$] has been used. Hence the propagator K, such that

$$\int_0^\infty K(x,x',t)\psi(x',t_0)dx' = \psi(x,t_0+t) \qquad (A16)$$

for any wave function $\psi(x,t)$, is

$$K(x,x',t) = i^{-(\nu+1)}(m/\hbar)\Psi(x,x',t). \qquad (A17)$$

The single-hump regime: The argument $u := ax$ of the Bessel function in ψ has $|u^2| = z\lambda x^2$. But $\psi^*\psi$ contains a factor $\exp(-\frac{1}{2}\lambda x^2)$. Hence if $|\beta| \ll \hbar\tau$, that is $z \ll 1$, then $|\psi|$ will become small (because of the exponential factor) before the argument of the Bessel function leaves the region where $|u| \ll 1$, and therefore[8] $J_\nu(u) \approx (\frac{1}{2}u)^\nu/\Gamma(\nu+1)$. In this regime the spatial form of ψ is $x^{\nu+1/2}\exp[\frac{1}{2}im\hbar^{-1}x^2/(t-i\tau)]$, and $|\psi|$ has just a single hump. If we substitute $I_\nu(z) \approx (\frac{1}{2}z)^\nu/\Gamma(\nu+1)$ into Eq. (A13), we obtain $\langle \hat{H} \rangle \approx \frac{1}{2}\hbar\tau^{-1}(\nu+1)$, and

$$\tfrac{1}{2}m\langle \hat{x}^2 \rangle \approx \langle \hat{H} \rangle(t^2+\tau^2). \qquad (A18)$$

Equation (A18) can be compared with the classical motion

$$\tfrac{1}{2}mx^2 = Et^2 + \tfrac{1}{2}mc/E. \qquad (A19)$$

The first term Et^2 corresponds as closely as possible to the quantum term $\langle \hat{H} \rangle t^2$, while the second term, specifying the closest approach to the origin, is $\langle \hat{H} \rangle \tau^2 \approx \frac{1}{4}\hbar^2(\nu+1)^2/\langle \hat{H} \rangle$ in the quantum case. This quantity is to be compared with $\frac{1}{2}mc/E$ noting that $\frac{1}{2}mc = \frac{1}{4}\hbar^2(\nu^2 - \frac{1}{4})$. The closest approach in the quantum case has a lower limit for $\frac{1}{2}m\langle \hat{x}^2 \rangle$ of $\frac{9}{16}\hbar^2/\langle \hat{H} \rangle$ for a very weak potential ($c \approx 0$) and is always greater than in the classical case with the same energy. This behavior is due to the existence of a completely repulsive barrier at $x=0$ (because ψ is always zero there), and therefore ψ is squeezed against this barrier, whereas the classical particle will approach the origin arbitrarily closely for sufficiently small c. In this regime, the wave packet motion is similar to that of the classical particle coming toward the origin, slowing to a standstill, and then retracing its inward trajectory; however, there are quantum effects that are greatest near the closest approach to the origin.

Figure 2 shows two examples of the evolution of this wave function; one has $z \ll 1$ and therefore has a single hump while the other has $z \gg 1$ and is shown at a time when it has two maxima.
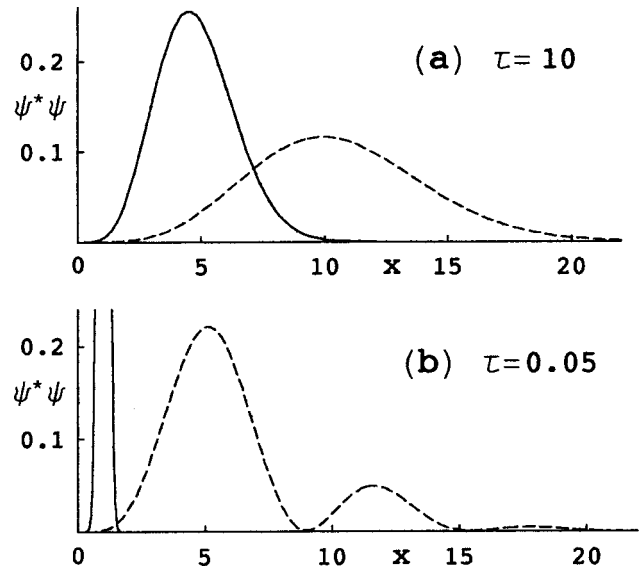

Fig. 2. Two wave packets for the potential $V = c/x^2$. In each case the wave function is as in Eq. (A4); $|\psi^2|$ is plotted with $m = \hbar = c = 1$ and eigenvalue $\beta = \frac{1}{2}$. In case (a), $\tau = 10$ and the wave function is shown for $t=0$ (solid) and for $t=20$ (dashed). This case is in the "single-hump" regime. In case (b), $\tau = 0.05$ and the wave function is shown for $t=0$ (solid line) and for $t=2$ (dashed line). For $t=0$, the maximum value is about 2.5. This case is in the regime where the Bessel function gives rise to multiple maxima.

[1] Eugen Merzbacher, *Quantum Mechanics*, 2nd ed. (Wiley, New York, 1970), p. 165.

[2] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1958), Chap. 9. Also see Ref. 1, p. 337, Eq. (15.13).

[3] Eugen Merzbacher, *Quantum Mechanics*, 3rd ed. (Wiley, New York, 1998), p. 49, Problems 2 and 3.

[4] Mark Andrews, "Invariant operators for quadratic Hamiltonians," Am. J. Phys. **67**, 336–343 (1999).

[5] For a recent discussion of the attractive case (in three dimensions), see Sydney A. Coon and Barry R. Holstein, "Anomalies in quantum mechanics: The $1/r^2$ potential," Am. J. Phys. **70**, 513–519 (2002).

[6] See Ref. 3, Chap. 14, Sec. 2.

[7] G. N. Watson, *Theory of Bessel Functions*, 2nd ed. (Cambridge University Press, Cambridge, 1944), Chap XIII, Sec. 13.31, p. 395.

[8] For relations involving Bessel's functions, see Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions* (NBS, Washington, DC, 1964), Chap. 9.