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# Square-well potential by an algebraic approach

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The spectrum-generating algebra for the problem of a particle in a potential well is shown to be  $su(1,1)$ . Both the infinitely deep and finite square wells are considered. The generators can also be derived via a systematic procedure for determining the time-dependent constants of the motion. The coherent states are explicitly constructed.

## I. INTRODUCTION

This paper provides an algebraic approach to the celebrated quantum-mechanical problem of a particle in a box. There are two primary reasons for such a formulation. The first is that the potential and therefore the spectrum are quite anharmonic. Hence simpler algebraic techmques where the Hamiltonian is one of the group generators, which lead to, at best, a quasiharmonic spectrum, <sup>1,2</sup> will just not work for this potential. Systematic methods are, in principle, available for handling anharmonic sys $tems.<sup>2-4</sup>$  Also, model algebraic Hamiltonians which are bilinear in the generators have recently been extensively employed in both nuclear<sup>5</sup> and molecular<sup>6</sup> physics. It is therefore of interest to see whether these techniques will work for this benchmark problem. The second reason for our interest was the way most books solve the problem of the potential well. The procedures employed bear little relation to what will be done for other bound-state problems. Rather they have a distinct scattering theoretic flavor. Indeed, textbooks will often<sup>7</sup> use the discussion of the potential well as an introduction to the elementary techniques and concepts of scattering. We too propose to follow such a route but in its algebraic version. In this paper, however, we center attention on the bound spectrum. There is also a secondary reason for the present discussion. The problem is so elementary and serves as a simple model for such a host of phenomena that even for the sake of completeness one must not fail to provide an algebraic formulation.

#### II. THE GENERATORS

In a one-dimensional problem (say, the  $x$  coordinate), we expect a convenient realization of the relevant group in  $1 + 1$  variables. For the present application, x and the auxiliary coordinate (say,  $y$ ) can be taken real. If one allows them to be complex then one needs to consider the four-parameter Lie groups (or three if the group is to be unitary<sup>8</sup>). A convenient realization of such groups in two variables is as follows:<sup>9</sup> Let the four generators satisfy the commutation relations

$$
[J_+, J_-] = -2a^2 J_3 - bE , \qquad (2.1)
$$

$$
[J_3, J_{\pm}] = \pm J_{\pm} \tag{2.2}
$$

$$
[J_3, E] = [J_{\pm}, E] = 0 \tag{2.3}
$$

where  $a$  and  $b$  are complex numbers. Typically we shall be concerned with particular values of  $a$  and  $b$ . To realize the four generators as differential operators we use the ansatz

$$
J_3 = -i\partial/\partial y \tag{2.4}
$$

 $\epsilon$ 

$$
J_{\pm} = \exp(\pm iy) \left[ \pm k_0(x) \frac{\partial}{\partial x} - ik_1(x) \frac{\partial}{\partial y} + j(x) \right],
$$
 (2.5)

$$
E=\mu I\,\,,\tag{2.6}
$$

where I is the identity operator and  $\mu$  is a complex number. The three functions of x in (2.5)  $[k_0(x), k_1(x)]$  and  $j(x)$ , are to be determined by the condition that the four commutation relations  $(2.1)$ - $(2.3)$  are satisfied. It is only  $(2.1)$  that will not hold in general unless the three functions of  $x$  are related by (where the prime denotes a derivative with respect to  $x$ )

$$
k_1^2(x) - k_0(x)k_1'(x) = a^2,
$$
\n(2.7)

$$
k_0(x)j'(x) - k_1(x)j(x) = -b/2.
$$
 (2.8)

We shall be particularly concerned with the  $b = 0$  case when the choice  $j(x) \equiv 0$  is possible.

For future reference we also define the operator, bilinear in the generators

$$
C = J_{+}J_{-} + a^{2}J_{3}(J_{3} - 1) - bJ_{3}E
$$
  
=  $J_{-}J_{+} + a^{2}J_{3}(J_{3} + 1) - bJ_{3}E - bE$ , (2.9)

which commutes with every generator. It is often referred to as the Casimir invariant.

## III. THE INFINITELY DEEP WELL

For a particle of mass  $m$  in an infinitely deep well between  $0$  and  $a$ , the Schrödinger equation in scaled distance and energy units is

$$
-d^2\psi/dx^2 = E\psi . \tag{3.1}
$$

Here energy is measured in units of  $\varepsilon = (\hbar \pi/a)^2 /2m$  and the distance by  $(a/\pi)$  so that the range of the well in x is  $[0,\pi]$ . The eigenfunctions satisfying the boundary conditions  $\psi(0) = \psi(\pi) = 0$  are

$$
\psi_n = (2/\pi)^{1/2} \sin(nx), \ E_n = n^2. \tag{3.2}
$$

As a basis for the action of the generators we take

$$
f_n(x, y) = \psi_n(x) \exp(iny) \tag{3.3}
$$

The spectrum generating operators which shift  $n$ 

$$
T_{\pm}f_n(x,y) = nf_{n\pm1}(x,y)
$$
\n(3.4)

while maintaining the boundary conditions on the eigenfunctions are, from (3.2) and (3.3),

$$
T_{\pm} = \exp(\pm iy) \left[ -i(\cos x) \frac{\partial}{\partial y} \pm (\sin x) \frac{\partial}{\partial x} \right]
$$
 (3.5)

$$
T_3 = -i\frac{\partial}{\partial y} \tag{3.6}
$$

so that the commutation relations  $(2.1)$ - $(2.3)$  have the special form

$$
[T_+, T_-] = -2T_3 , \t\t(3.7)
$$

$$
[T_3, T_{\pm}] = \pm T_{\pm} \tag{3.8}
$$

i.e., that of the generators of  $SU(1,1)$ .

The generator  $T_3$  serves as the number operator

$$
T_3 f_n(x, y) = n f_n(x, y) . \t\t(3.9)
$$

The algebraic Hamiltonian is thus bilinear in the generators, i.e.,  $H \equiv T_3^2$ . It might appear that this identification is not unique in that the two relations

$$
T_{+}T_{-}f_{n}(x,y)=n (n - 1)f_{n}(x,y) ,
$$
  
\n
$$
T_{-}T_{+}f_{n}(x,y)=n (n + 1)f_{n}(x,y) ,
$$
\n(3.10)

enable us to propose another bilinear operator whose spectrum is also  $n^2$ ,

$$
\frac{1}{2}\left\{T_{+},T_{-}\right\}f_{n}(x,y)=n^{2}f_{n}(x,y) \ . \tag{3.11}
$$

Here the curly brackets denote the anticommutator,  ${A, B} = AB + BA$ . The difference is, however, only apparent. The (bilinear) operator that commutes with all three generators [i.e., the Casimir invariant<sup>8</sup> of  $SU(1,1)$ ] is, cf. (2.9),

$$
C = T_{-}T_{+} - T_{3}(T_{3} + 1)
$$
 satisfies  
=  $T_{+}T_{-} - T_{3}(T_{3} - 1)$ . (3.12)  $-i\partial \tilde{\psi}/\partial y = \tilde{n}\tilde{\psi}$  (4.3)

The representation is determined by the eigenvalue of the Casimir operator which is zero for our basis. Hence equivalent forms for the Hamiltoman are

$$
H = \frac{1}{2}(T_{-}T_{+} + T_{+}T_{-})
$$
\n(3.13)

$$
I = \frac{1}{2}(T_{-}T_{+} + T_{+}T_{-})
$$
\n
$$
= T_{+}T_{-} + \frac{1}{2}[T_{-},T_{+}]
$$
\n(3.13)\n(3.14)

$$
=C+T_3^2\tag{3.15}
$$

Note the formal similarity of (3.14) to the algebraic Hamiltonian

$$
H = a^{\dagger} a + \frac{1}{2} [a, a^{\dagger}] \tag{3.16}
$$

of the harmonic oscillator. Note that  $a^{\dagger}$  is (like  $T_{+}$ ) a raising operator and a (like  $T_{-}$ ) is a lowering operator. This analogy obtains also for other anharmonic potentials.<sup>10</sup>

In (3.5) and (3.6) we have provided a coordinate realization of the generators. An operator (Schwinger<sup>11</sup>) representation is introduced in terms of two  $(i = 1,2)$  boson creation  $(a_i^{\dagger})$  and annihilation  $(a_i)$  operators which are independent

$$
[a_i, a_j^{\dagger}] = \delta_{ij} \tag{3.17}
$$

In terms of the column vector a whose components are  $a_1$ and  $a_2$ , we have

and [cf. (2.4)]  

$$
T_{\pm} = \frac{i}{2} \mathbf{a}^{\dagger} \boldsymbol{\sigma}_{\pm} \mathbf{a} \tag{3.18}
$$

$$
T_3 = \frac{1}{2} \mathbf{a}^\dagger \boldsymbol{\sigma}_3 \mathbf{a} \tag{3.19}
$$

where the  $\sigma$ 's are the Pauli spin matrices with  $\sigma_{\pm} = (\sigma_1 \pm i \sigma_2)$ , or

$$
\boldsymbol{\sigma}_{+} = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}, \ \ \boldsymbol{\sigma}_{-} = \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix}, \ \ \boldsymbol{\sigma}_{3} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad (3.20)
$$

so that 
$$
[\sigma_+,\sigma_-]=4\sigma_3
$$
,  $[\sigma_3,\sigma_{\pm}]=\pm 2\sigma_{\pm}$ .

#### IV. TIME EVOLUTION

It is correct to think of the variable  $y$  in the basis states

$$
f_n(x,y) = \psi_n(x) \exp(iny)
$$

as "time." Seemingly that is not acceptable since the solutions  $\psi(t)$  of the time-dependent Schrödinger equation have the phase factor  $exp(-iE_n t/\hbar)$  so that the dimensionless time is  $y \in \ell \hbar$  with the phase factor  $\exp(-i n^2 y)$ . However, as discussed in detail in the Appendix we can subject the Schrödinger equation to a time dilation transformation<sup>3,4</sup>  $\widetilde{\psi} = D\psi$  using an operator  $\widetilde{n}$ , which is a function of the Hamiltonian, whose spectrum is linear,

$$
[\widetilde{n}(H) - n]\psi_n(x) = 0.
$$
 (4.1)

Hence  $\tilde{\psi}(y)$ 

$$
\widetilde{\psi} = D\psi(y) = \psi_n(x) \exp(iny) \tag{4.2}
$$

satisfies

$$
-i\partial \tilde{\psi}/\partial y = \tilde{n}\tilde{\psi} \tag{4.3}
$$

or

$$
[H - E(\tilde{n}(i\partial/\partial y))] \tilde{\psi}(y) = 0.
$$
 (4.4)

In the present problem (cf. the Appendix) (4.3) is equivalent to

$$
\left(-\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\widetilde{\psi}(y) = 0,
$$
\n(4.5)

with the solution

$$
\widetilde{\psi}(y) = \psi_n(x) \exp(iny) \equiv f_n(x, y) . \tag{4.6}
$$

 $[a^{\dagger}]$  (3.16) The equivalence between the eigenfunction  $\tilde{\psi}(y)$  of the

dilated equation (4.5) and the basis states  $f_n(x,y)$  is not accidental. Indeed, the systematic algebraic procedure<sup>2,3</sup> for obtaining the generators is to determine first the generators for (4.5) and then subject them to a similarity transformation by D. The details are provided in an appendix.

Coherent states<sup>12</sup> for the infinite square well can be obtained from the ground state by the action of a group element which acts as a displacement-type operator. For our purpose it is enough to "rotate" by the action of  $T_2$ ,  $where<sup>13</sup>$ 

$$
\exp(i\theta T_2) \begin{bmatrix} T_1 \\ T_3 \end{bmatrix} \exp(-i\theta T_2)
$$
  
= 
$$
\begin{bmatrix} \cosh\theta & -\sinh\theta \\ -\sinh\theta & \cosh\theta \end{bmatrix} \begin{bmatrix} T_1 \\ T_3 \end{bmatrix}.
$$
 (4.7)

Now

$$
U \equiv \exp(i\theta T_2) = \exp[-\theta(T_+ - T_-)/2]
$$
 (4.8)

or, in normal order

$$
U = \exp(-\xi T_+) \exp[\ln(1 - |\xi|^2)T_3] \exp(\xi T_-), \quad (4.9)
$$

with  $\xi = \tanh(\theta/2)$ . Since  $T - f_1 = 0$ , the operation by the first exponential in (4.9) on the ground state is equivalent to just the identity operator. The second exponential is diagonal. Hence, with  $1 - |\xi|^2 = \cosh(\theta/2)$ 

$$
Uf_1 = \cosh(\theta/2) \exp(-\xi T_+) f_1
$$
  
=  $\cosh(\theta/2) \sum_{n=0} \xi^n f_{n+1}$ , (4.10)

where we used  $T_{+}f_{n} = nf_{n+1}$ . The coherent states are normalized but different states (i.e., different values of  $\theta$ or equivalently of  $\xi$ ) are not orthogonal. They are linear combinations of eigenstates  $\psi_n(x)$  with the coefficient  $\left[\xi \exp(i y)\right]$ ".

Note that the coherent states are "coherent" in their evolution for the dilated equation (4.5}. States which remain coherent for the Schrödinger time evolution require an additional transformation by  $D^{-1}$ , cf. (4.2).

## V. THE SYMMETRIC WELL

Another version is an infinitely deep well where the potential is symmetric upon reflection  $V(-x)=V(x)$ , and the well extends from  $-a/2$  to  $a/2$ . That is just our previous problem but with the (reduced) distance shifted by  $\pi/2$ . Seemingly, there is no problem. Starting with (3.5), the new generators are

$$
P_{\pm} = \exp(\pm iy) \left[ -i(\sin x) \frac{\partial}{\partial y} \mp (\cos x) \frac{\partial}{\partial x} \right],
$$
 (5.1)

with the commutation relation between them

$$
[P_+, P_-] = -2T_3 \tag{5.2}
$$

being unchanged by the shift of the  $x$  coordinate.

Shifting the argument x of the basis  $f_n(x,y)$  by  $\pi/2$ shows that the functions split into two sets according to whether  $n$  is even or odd,

$$
f_n(x,y) = \begin{cases} (2/\pi)^{1/2} \exp(iny) \sin(nx), & n \text{ even} \\ (2/\pi)^{1/2} \exp(iny) \cos(nx), & n \text{ odd} \end{cases}
$$
(5.3)

$$
P_{\pm}f_n(x,y) = \mp n \, (-1)^n f_{n \pm 1}(x,y) \; . \tag{5.4}
$$

Note that  $P_{\pm}$  changes an even basis function into an odd one and vice versa. The  $\mp(-1)^n$  in (5.4) which is absent in (3.9) is just the phase change of  $f_n(x,y)$  when x is shifted by  $\pi/2$ .

In the algebraic approach, the generator of a shift in  $x$ is  $\partial/\partial x$ . Hence the transformation to the symmetric problem can also be carried out by computing  $\left[\frac{\partial}{\partial x}, T_{\pm}\right]$ when we find

$$
[P_3, T_{\pm}] = P_{\pm} \t\t(5.5)
$$

where

$$
P_3 = -\partial/\partial x \tag{5.6}
$$

Similarly

$$
[P_3, P_{\pm}] = -T_{\pm} \tag{5.7}
$$

and

$$
[T_3, P_{\pm}] = -P_{\pm} \ . \tag{5.8}
$$

The symmetric well problem can also be used to take the  $a \rightarrow \infty$  limit when the particle is free. For the dilated equation (4.5), the physical distance  $X$  ( $=ax \propto x/\epsilon$ ) and the physical time T,  $(Z = y/\varepsilon)$  scale with  $1/\varepsilon$  where  $\varepsilon \rightarrow 0$ in the  $a \rightarrow \infty$  limit. [See also (6.5) below.] Writing (3.5) in the physical variables and retaining only terms to lowest order in  $\varepsilon$  we have

$$
(T_{+} - T_{-})/2 \rightarrow \frac{1}{\varepsilon} \frac{\partial}{\partial X} , \qquad (5.9)
$$

$$
(T_{+} + T_{-})/2i \rightarrow \left[ X \frac{\partial}{\partial Z} - Z \frac{\partial}{\partial X} \right],
$$
 (5.10)

$$
iT_3 = \frac{1}{\varepsilon} \frac{\partial}{\partial Z} \ . \tag{5.11}
$$

The three operators (5.9)—(5.11) close an algebra and are the generators of the Euclidean group<sup>8,9</sup> appropriate for free motion. Note that (5.9} commutes with (5.11) while

if 
$$
L = X\partial/\partial Z - Z\partial/\partial X
$$
, then  
\n
$$
\left[L, \frac{1}{\epsilon} \frac{\partial}{\partial X}\right] = -\frac{1}{\epsilon} \frac{\partial}{\partial Z},
$$
\n(5.12)

$$
\left[L, \frac{1}{\varepsilon} \frac{\partial}{\partial Z}\right] = \frac{1}{\varepsilon} \frac{\partial}{\partial X},
$$
\n(5.13)

so that  $L$  need not have an  $\varepsilon$  dependence.

## VI. THE FINITE SQUARE WELL

For a particle in a well of a finite depth, the energy levels are the solution of a transcendental equation. We recover this result by imposing the condition that  $T_{+}f_{n}(x,y)$  be subject to the same boundary conditions as the basis functions themselves, namely, continuity at the two well boundaries at  $\pm a/2$ . In a sequel paper dealing with the continuous spectrum we shall obtain these levels as the poles of the scattering matrix on the negative real energy axis.

Using scaled coordinates and time as before, we have for a well of depth  $V_0$  over the range  $[-a/2, a/2]$  that

$$
-\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0 \t{,} \t(6.1)
$$

where

$$
\kappa^2 = [E - V(x)]/\varepsilon \tag{6.2}
$$

and  $-V_0 < E < 0$ ,

$$
V(x) = \begin{cases} -V_0, & |x| \le \pi/2 \\ 0, & \text{otherwise.} \end{cases}
$$
 (6.3)

Let  $f_{\kappa}(x,y) = \psi(x) \exp(i\kappa y)$  be a basis vector. The Schrödinger equation can be written in the form

$$
\frac{\partial^2 f_{\kappa}}{\partial x^2} = \frac{\partial^2 f_{\kappa}}{\partial y^2}
$$
 (6.4)

and  $f_{\kappa}$  is parametrized by the wave vector  $\kappa$ . The shift operators will change  $\kappa$ , say, by  $\delta$ . Now  $T_{\pm}f_{\kappa}$  are also to be solutions of (5.4). This condition plus the requirement that  $T_{\pm}$  be a first-order differential operator leads to

$$
T_{\pm} = \delta^{-1} \exp(\pm i\delta y) \left[ -i(\cos \delta x) \frac{\partial}{\partial y} \pm (\sin \delta x) \frac{\partial}{\partial x} \right]
$$
(6.5)

and

$$
[T_+, T_-] = (2i/\delta)\partial/\partial y \equiv -2T_3
$$
 (6.6)   
 will. CONCLUDING REMARKS

With the choice (6.6) for  $T_3$ ,  $[T_3 = -(i/8)\partial/\partial y]$ , we have recovered the  $SU(1,1)$  generators since

$$
[T_3, T_{\pm}] = \pm T_{\pm} \ . \tag{6.7}
$$

However, so far,  $\delta$  is arbitrary. If x is in the classically forbidden region then  $\kappa$  is purely imaginary and so is  $\delta$ . If one prefers a real parameter, the substitution  $\delta = i\gamma$  in the generators above leads to

$$
\tau_{\pm} = \pm \gamma^{-1} \exp(\mp \gamma y) \left[ \mp \cosh(\gamma x) \frac{\partial}{\partial y} + \sinh(\gamma x) \frac{\partial}{\partial x} \right],
$$
\n(6.8)

 $\tau_3 = -\gamma^{-1} \partial / \partial y$ . (6.9)

The commutation relations are unchanged

$$
[\tau_+, \tau_-] = -2\tau_3 \,, \tag{6.10}
$$

$$
[\tau_3, \tau_{\pm}] = \pm \tau_{\pm} \ . \tag{6.11}
$$

The basis vectors are again given by even and odd states

$$
f_{\kappa}(x,y) = \begin{cases} (2/\pi) \exp(i\kappa y) \sin(\kappa x) \\ (2/\pi) \exp(i\kappa y) \cos(\kappa x) \end{cases}
$$
 (6.12)

In the classically forbidden region,  $V(x)=0$ , the boundary conditions are

$$
\partial f_{\kappa}(x,y)/\partial x \pm ik f_{\kappa}(x,y) = 0, \quad x = \pm \pi/2 \tag{6.13}
$$

where  $k^2 = E/\varepsilon$ . Using (6.13) to evaluate the action of  $T_+$  on  $f_k$  at the boundary and the condition

$$
T_{+}f_{\kappa}=f_{\kappa+\delta} \tag{6.14}
$$

yields as the condition

$$
\tan(\kappa \pi/2) = \begin{cases} ik/\kappa, & \text{even states} \\ -ik/\kappa, & \text{odd states} \end{cases}
$$
 (6.15)

which is the familiar transcendental equation for  $\kappa$ . The number of bound states is finite and equals N when  $(N-1)\pi/2 < (V_0/\epsilon)^{1/2} \le N\pi/2$ . If  $V_0 \gg \epsilon$ ,  $\delta$  increases by almost two between successive eigenstates of the same symmetry. Since the even and odd levels interlace, the infinitely deep well limit is recovered as  $V_0 \rightarrow \infty$  (except that due to the shift in the origin of the energy axis, we now have  $E + V_0 = n^2 \varepsilon$ .

It is important to emphasize the essential difference between {3.5) and (6.5). For a particle in a fimte well, the bound states are finite in number and do not therefore belong to one irreducible representation of SU(1,1). Indeed, in (6.5) the value of  $\delta$  is different for different bound states. [Recall that  $\delta$  is the change in the wave vector between one bound state and the next. It is only for the infinitely deep well that  $\delta = 1$ . Otherwise it is to be determined using (6.15).] To get a set of states that do belong to one representation one will need to consider the socalled "potential" group. This is the group whose generators connect states of the same quantum number but in wells of different depths.

The quantum-mechanical problem of a particle in an infinite well was shown to admit raising and lowering operators which do not depend on the quantum number. In this it is similar to other anharmonic problems where the energy levels are analytic functions of the quantum numbers. Such problems are said to possess a "dynamical symmetry" in that the Hamiltonian can be written in terms of Casimir invariants of a chain of subgroups.<sup>5,6</sup> Here the chain is particularly simple

$$
U(1,1)\supset U(1) .
$$

In addition, however, rather than starting with an algebraic Hamiltonian and seeking its geometrical interpretation, the present problem is simple enough that one can start with the coordinate representation of the Hamiltonian and proceed, in a systematic fashion, to determine the corresponding algebra.

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# APPENDIX: CONSTANTS OF THE MOTION ENDIX: CONSTANTS OF THE MOTION<br>BY A SYSTEMATIC PROCEDURE  $D = \exp \left[ \ln \left( -\frac{\widetilde{n}(H)}{H} \right) \right]_L \frac{\partial}{\partial T}$

The operators that commute with the Hamiltonian when acting on an eigenstate generate states degenerate with it. To generate the entire spectrum one require time-dependent constants of the motion.<sup>4,14</sup> Such a generator Q, when acting on a solution  $\psi$  of the timedependent Schrödinger equation,

$$
(i\partial/\partial t - H)\psi = 0 \tag{A1}
$$

yields a solution of that equation

$$
(i\partial/\partial t - H)Q\psi = 0.
$$
 (A2)

The fact that  $Q$  is a constant of the motion follows upon taking the scalar product of  $(A2)$  with any solution  $\psi'$  of (Al).

$$
id \langle \psi' | Q | \psi \rangle / dt = - \langle \psi' | HQ | \psi \rangle
$$
  
+  $i \langle \psi' | \frac{\partial}{\partial t} (Q | \psi \rangle) = 0$ . (A3)

While both  $\psi$  and  $\psi'$  depend on time, so does Q with the net result that  $\langle \psi' | Q | \psi \rangle$  is time independent. If Q does not depend on time, (A3) reads

$$
\langle \psi' | [H,Q] | \psi \rangle = 0 \tag{A4}
$$

for any  $\psi'$ , showing that  $Q\psi$  is degenerate with  $\psi$ .

A formal construction of  $Q$ , even if time dependent, is immediate. Take X to be Q at time  $t = 0$ . Then

$$
Q = \exp(-iHt/\hbar)X\exp(iHt/\hbar)
$$
 (A5)

will satisfy (A3). In other words, Q is  $X_H(-t)$ , where  $X_H(t)$  is the Heisenberg picture operator. If the Hamiltonian is *linear* in the generators of some Lie group and  $X$ is a generator, then implementing  $(4.5)$  is straightforward. The outer automorphism of Lie groups<sup>8</sup> ensures that  $Q$  is but a linear combination of generators. Unfortunately, and as in the present problem, anharmonic systems are much better suited to an algebraic description by Hamiltonians which are *bilinear* in the generators.

In the systematic procedure,  $2^{-4}$  the Schrödinger equation  $(A1)$  is first subjected to a dilation transformation

$$
D(i\partial/\partial t - H)D^{-1}\widetilde{\psi} = 0 , \qquad (A6)
$$

where  $\tilde{\psi} = D\psi$  and the generator  $\tilde{Q}$  of the dilated problem is the solution of

$$
D(i\partial/\partial t - H)D^{-1}\widetilde{Q}\widetilde{\psi} = 0.
$$
 (A7)

The required generator  $Q$  can then be determined from

$$
Q = D^{-1} \widetilde{Q} D \tag{A8}
$$

Such a  $Q$  will then satisfy  $(A2)$ . We shall find, however, that  $\overline{Q}$  is all that we require.

Let  $\psi_n(x)$ exp( $-in^2y$ ) be a solution of (A1) for the square-well problem. As in the text,  $x$  is the reduced distance and y is the reduced time variable  $y = \varepsilon t / \hbar$ . Using the dilation operator

$$
D = \exp\left[\ln\left(\frac{\widetilde{n}(H)}{\lambda(\widetilde{n}(H))}\right)t\frac{\partial}{\partial t}\right],
$$
 (A9)

where  $\lambda(n)=E_n$  is the dependence of the energy on the quantum number with  $\lambda(n) = n^2$  in the present case. Under this transformation, (A 1) is transformed into

 $\sim$ 

$$
\left|H - \left|\frac{\lambda(\widetilde{n}(H))}{\widetilde{n}(H)}\right| i \frac{\partial}{\partial y} \right| \widetilde{\psi} = 0.
$$
 (A10)

We now seek a stationary solution of (Alo), i.e., one where  $\hat{\psi}(x,t)=\psi_n(x)exp(iny)$ . On these solutions we can write

$$
\left[\widetilde{n}(H) - i\frac{\partial}{\partial y}\right]\widetilde{\psi} = 0
$$
 (A11)

so that (A10) can be written as

 $\sim$ 

$$
\left(-\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi_n(x)\exp(iny) = 0.
$$
 (A12)

The generator  $\tilde{Q}$  is then the solution of

$$
\left(-\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \widetilde{Q} f_n(x, y) = 0.
$$
 (A13)

To solve (A13) we take as an ansatz that  $\tilde{Q}$  is a firstorder differential operator

$$
\widetilde{Q} = q^x \frac{\partial}{\partial x} + q^y \frac{\partial}{\partial y} + q^0 , \qquad (A14)
$$

where the three functions  $q^x$ ,  $q^y$ , and  $q^0$  are analytic functions of  $x$  and  $y$  to be determined by the condition that (A13) is satisfied.

Substituting (A14) in (A13) and since so far  $f_n(x,y)$  is undetermined we require that the coefficients multiplying  $f_n(x,y)$  or any one of its derivatives up to second order<sup>1</sup> vanish independently. This provides the following set of equations, where on the left we indicate the function whose coefficient is being set equal to zero,

$$
f: \quad q_{xx}^0 - q_{yy}^0 = 0 ,
$$
  
\n
$$
f_x: \quad 2q_x^0 + q_{xx}^x - q_{yy}^x = 0 ,
$$
  
\n
$$
f_y: \quad q_{xx}^y - 2q_y^0 - q_{yy}^y = 0 ,
$$
  
\n
$$
f_{xy}: \quad 2q_x^y - 2q_y^x = 0 ,
$$
  
\n
$$
f_{xx}: \quad 2q_x^x - 2q_y^y = 0 .
$$
\n(A15)

The subscripts denote a partial derivative with respect to the indicated variable.

There will be six integration constants required to specify the solution of (A15) which we denote by  $A_+$ ,  $A_-$ ,  $B_+$ ,  $B_-$ , C, and D. In terms of these

$$
q^{y} = -iA_{+}(\cos x)e^{iy} - iA_{-}(\cos x)e^{-iy} + iB_{+}(\sin x)e^{iy} - iB_{-}(\sin x)e^{-iy} - iC ,q^{x} = A_{+}(\sin x)e^{iy} - A_{-}(\sin x)e^{-iy} + B_{+}(\cos x)e^{iy} + B_{-}(\cos x)e^{-iy} + D , \qquad (A16)
$$
  

$$
q^{0} = 0 .
$$

The coefficient of  $A_+$  will be recognized as  $T_+$  as de-The coefficient of  $A_+$  will be recognized as  $I_+$  as d<br>fined in (3.5). Similarly,  $A_-$  yields  $T_-$ , and  $B_+$  and B yield  $P_{\pm}$  as defined in (4.1).  $T_3$  and  $P_3$  are the terms corresponding to  $C$  and  $D$ , respectively. Our six generators correspond to the six independent integration constants of (A15). Note also that in solving (A15) we have taken care to ensure that Qf will satisfy the required boundary conditions. Had we not, we could have obtained other solutions, e.g., those for a free particle, which were previously derived by Wulfman et  $al.$ <sup>3,4</sup> but without the dilation operation which was used here.

It also follows from (AS) that

$$
\langle \psi' | Q | \psi \rangle = \langle \widetilde{\psi}' | \widetilde{Q} | \widetilde{\psi} \rangle ,
$$

where, as before  $\tilde{\psi} = D\psi$ . Since any function of a constant of motion is a constant of motion (and  $[H,Q]$  and  $[Q',Q]$ as well) we have generated a large number of functionally dependent constants of the motion. Of the six we started with,  $T_3$  and  $P_3$  have an obvious geometrical significance. Not intuitive is the origin of the shift operators. Indeed they do not commute with  $H - E(\tilde{n}(i\partial/\partial y))$ . It is only when they act on  $f_n(x,y)$  that (A13) is satisfied.

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- <sup>15</sup>Seemingly, f has three independent second derivatives  $f_{xx}$ ,  $f_{xy}$ , and  $f_{yy}$ . But Q is to operate on solutions of (A12) which implies  $f_{yy} = -f_{xx}$ . Hence  $f_{yy}$  is linearly dependent on  $f_{xx}$  (or vice versa) and only the coefficients of two second-order derivatives can be independently put equal to zero. By taking partial derivatives of (A12) one can generate relations between higher-order derivatives. These are not required here but would restrict the number of independent functions had we allowed a more general form for  $\tilde{Q}$ , e.g., that of a differential operator up to second order.