Relation between the solutions of Newton's and Heisenberg's equations of motion

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(Received 19 April 1978)

For a class of problems it is shown that a solution to Newton's equation of motion may be interpreted as the generating function for the matrix elements of the coordinate operators in the Heisenberg representation. For three one-dimensional problems, the harmonic oscillator, the particle in a box, and the x^4 anharmonic oscillator, solutions to the quantum-mechanical problem are given in terms of the classical solution. A brief examination is made of a two-dimensional problem in which the angular momentum is conserved.

I. INTRODUCTION

In a series of earlier papers attempts have been made to solve anharmonic-oscillator-type problems[1] based on the following pair of assumptions:

(i) Matrix elements decrease rapidly as the difference between indices (distance from the main diagonal) increases.

(ii) Matrix elements vary slowly parallel to the principal diagonal. The experience gained in the application of these ideas to oscillator problems has led to modifications in these ideas.

The solution of a quantum-mechanical problem in the matrix form involves the construction of pairs of operators q_i, p_i such that

(i) the commutation rules are satisfied,

(ii) the Hamiltonian operator H expressed as a function of the p_i and the q_i is diagonal.

In terms of the type of approximation referred to above it is possible to separate these two aspects of the problem. The diagonalization of H may be treated primarily as a problem in the difference of the matrix indices while the commutation relations primarily involve the dependence of matrix elements on the sum of the indices. The part of the problem that depends on the difference of the indices, the diagonalization of H, can be reduced to the solution of Newton's equation: $F = ma$.

The demonstration that the diagonalization of H can be approximately achieved in terms of a solution of $F = ma$ will first be carried out in Sec. II for a one-dimensional problem for which the motion is periodic and for which the potential is assumed to be expressed in terms of powers of the coordinate. The generalization to a many-degree-of-freedom problem is straightforward and is carried out in Sec. III. To complete the solution of the quantum-mechanical problem the commutation conditions are introduced in Sec. IV. In Sec. V the application of the method to the harmonic oscillator, the particle in a box, and the x^4 anharmonic oscillator are treated.

The demonstration that a solution of Newton's equation can be used to find approximate matrix elements has previously been given by Klein[2] in the course of a derivation of the WKB method. The derivation presented here grew out of attempts to solve Eq. (1) as a set of coupled algebraic equations to which it reduces if the sum (2) is truncated. The truncated-sum point of view gives insight into the sizes of the various matrix elements which may be particularly useful guidance in treating nonseparable problems. Several two-dimensional problems are mentioned.

II. THE DIAGONALIZATION OF THE HAMILTONIAN IN A ONE-DEGREE-OF-FREEDOM PROBLEM

The Newton and Heisenberg equations both have the form

$$m\frac{d^2x}{dt^2} = F(x),$$

where in Newton's equation x is a number while in Heisenberg's it is a matrix. The time derivative of a Heisenberg matrix element is given by

$$\left(\frac{d^2x}{dt^2}\right)_{ab} = -[(E_a - E_b)/\hbar]^2 x_{ab}.$$

The equation becomes

$$-m\left(\frac{E_a - E_b}{\hbar}\right)^2 x_{ab} = [F(x)]_{ab}. \tag{1}$$

This is a set of coupled algebraic equations usually nonlinear since F will in general be a complicated function of x. The computation of $[F(x)]_{ab}$ presents computational problems, and before attempting this calculation the first assumption will be introduced:

(i) The dependence of the matrix element x_{ab} on the sum of the indices is weak enough so that the approximation

$$x_{ab} = \sum \alpha_r(\delta_{a,b+r} + \delta_{a,b-r}) \tag{2}$$

is adequate to treat the diagonalization of H. The

assumed weak dependence of x_{ab} on $a+b$ will be recovered when the commutator is treated.

In order to calculate $[F(x)]_{ab}$ it is useful to introduce the generating function $g(\theta)$,

$$g(\theta)=\sum \alpha_r(e^{ir\theta}+e^{-ir\theta}). \tag{3}$$

If the function $F[g(\theta)]$ is expanded in a Fourier series,

$$F[g(\theta)]=\sum \beta_r(e^{ir\theta}+e^{-ir\theta}),$$

then the coefficients β are functions of the α. If $F(x)=x^e$, then

$$g^e(\theta)=\sum_{r_1\cdots r_e}\alpha_{r_1}\alpha_{r_2}\cdots\alpha_{r_e}(e^{ir_1\theta}+e^{-ir_1\theta})\cdots \times(e^{ir_e\theta}+e^{-ir_e\theta}).$$

Thus the number β_r is given by

$$\beta_r=\sum_{r_1\cdots r_e}\sum \delta_{r,\pm r_1\pm r_2\pm\cdots\pm r_e}\alpha_{r_1}\alpha_{r_2}\cdots\alpha_{r_e},$$

where the inner sum is taken over all of the 2^e possible permutations of the plus and minus signs.

The matrix element $(x^e)_{ab}$ is given by

$$(x^e)_{ab}=\sum_{c_1\cdots c_{e-1}} x_{ac_1}x_{c_1c_2}\cdots x_{c_{e-2}c_{e-1}}x_{c_{e-1}b}.$$

If (2) is used this becomes

$$(x^e)_{ab}=\sum_{c_1\cdots c_{e-1}}\sum_{r_1\cdots r_e}\alpha_{r_1}\cdots\alpha_{r_e}(\delta_{a,c_1+r_1}+\delta_{a,c_1-r_1})(\delta_{c_1,c_2+r_1}+\delta_{c_1,c_2-r_1})\cdots(\delta_{c_{e-1},b+r_e}+\delta_{c_{e-1},b-r_e}).$$

The sums over the indices $c_1,\cdots,c_{e-1}$ may be done to give

$$(x^e)_{ab}=\sum_r(\delta_{a,b+r}+\delta_{a,b-r})\times\sum_{r_1\cdots r_e}\alpha_{r_1}\cdots\alpha_{r_e}\delta_{r,\pm r_1\pm r_2\pm\cdots\pm r_e}.$$

The r sum is over all the r and over the 2^e possible permutation of the signs. This answer may not be correct because the Kronecker δ's may not all have vanishing arguments in the interval of summation. These missing terms are of the type that is consistently neglected in this approximation. For small quantum numbers near the edge of the matrix they will be significant. For powers of x it follows that by comparison with the expression for $g^e(\theta)$ that

$$(x^e)_{ab}=\sum \beta_r(\delta_{a,b+r}+\delta_{a,b-r}).$$

For a function $F(x)$ that has a power-series expansion it is concluded that the matrix element $[F(x)]_{ab}$ is given by

$$[F(x)]_{ab}=\sum \beta_r(\delta_{a,b+r}+\delta_{a,b-r}),$$

while the function $F[g(\theta)]$ is given by

$$F[g(\theta)]=\sum \beta_r(e^{ir\theta}+e^{-ir\theta}).$$

There is one final approximation required before Heisenberg's equation (1) can be reduced to Newton's. The energy difference E_a-E_b is assumed to be proportional to $(a-b)$,

$$(E_a-E_b)=(a-b)\Delta E.$$

The proportionality constant ΔE will have a dependence on $a+b$, but this is temporarily neglected.

The preceding results are substituted into (1) to give

$$-m(a-b)^2(\Delta E/\hbar)^2x_{ab}=[F(x)]_{ab},$$

or if $a\pm b=r$,

$$-mr^2(\Delta E/\hbar)^2\alpha_r=\beta_r. \tag{4}$$

Now multiply by $e^{ir\theta}+e^{-ir\theta}$ and sum over r to rebuild the generating function and the equation becomes

$$m(\Delta E/\hbar)^2\frac{d^2g}{d\theta^2}=F(g).$$

If the substitution

$$\theta=(\Delta E/\hbar)t$$

is made, the equation becomes Newton's equation

$$m\ddot{g}=F(g).$$

If this equation is multiplied by $\dot{g}$ and integrated, the conservation of energy equation

$$\tfrac{1}{2}m\dot{g}^2(t)+V[g(t)]=\tfrac{1}{2}m\dot{g}^2(0)+V[g(0)]=H(0)$$

results. The expansion of the right-hand side in a Fourier series gives

$$H(0)=H(t)=H(0)e^{i0t}.$$

But the Fourier coefficients to be interpreted as matrix elements so that

$$H_{ab}=H(0)\delta_{ab}.$$

The diagonalization of the Hamiltonian is equivalent to classical conservation of energy.

Having determined the function $g(\theta)$ it must be expanded in the Fourier series

$$g(\theta)=\sum \alpha_r(e^{ir\theta}+e^{-ir\theta})$$

to determine the matrix elements of x. But the α_r are still functions of ΔE besides the mass and the parameters required to specify the potential. This is because the relation between θ and t contains the as yet undetermined ΔE, and while $g(t)$ satisfies Newton's equation it is the Fourier coefficients of $g(\theta)$ that determine the α. To determine ΔE it is necessary to use the commutation relation.

III. EXTENSION TO SEVERAL DEGREES OF FREEDOM

For a problem with d degrees of freedom there are d coordinates, $x^{(1)}, x^{(2)}, \ldots, x^{(d)}$. The matrix elements of an operator $x^{(i)}$ will have $2d$ indices, $x^{(i)}_{a_1,a_2,\ldots,a_d,b_1,b_2,\ldots,b_d}$. In general the indices will be represented by a vector $\vec{a} = (a_1, \ldots, a_d)$ where the a_i are integers. Using these conventions the Heisenberg equations become the collection

$$m_i[(E_{\vec{a}} - E_{\vec{b}})/\hbar]^2 x^{i}_{\vec{a}\,\vec{b}} = [F(x^{(i)}, x^{(2)}, \ldots, x^{(d)}]_{\vec{a}\,\vec{b}}.$$

The energy difference $E_{\vec{a}} - E_{\vec{b}}$ is given by

$$E_{\vec{a}} - E_{\vec{b}} = (\vec{a} - \vec{b}) \cdot \vec{\Delta} E,$$

where the vector $\vec{\Delta} E$ has components $\Delta E_1, \ldots, \Delta E_d$.

Each of the coordinates matrices is approximated by

$$(x^{(i)})_{\vec{a}\,\vec{b}} = \sum_{\vec{r}} \alpha^{(i)}_{\vec{r}} (\delta_{\vec{a},\vec{b}+\vec{r}} + \delta_{\vec{a},\vec{b}-\vec{r}}), \tag{5}$$

where $\vec{r}$ is a vector with integer components $r_1, \ldots, r_d$. For each $x^{(i)}$ the generating function $g^{(i)}$ given by

$$g^{(i)}(t) = \sum_{\vec{r}} \alpha^{(i)}_{\vec{r}} \{\exp(i[\vec{r} \cdot \vec{\Delta} E)/\hbar]t) + \text{c.c.}\} \tag{6}$$

is introduced. The entire discussion of Sec. II can be repeated to show that the generating functions satisfy the Newtonian equation of motion

$$m_i \frac{d^2 g^{(i)}}{dt^2} = F^{(i)}[g^{(1)}, \ldots, g^{(\alpha)}].$$

The clumsy theorem required to relate the Heisenberg and Newtonian equations is for monomials in the x^i: If the matrix element

$$[x^{(1)e_1} x^{(2)e_2} \cdots x^{(d)e_d}]_{\vec{a}\,\vec{b}} = \sum \beta_{\vec{r}} (\delta_{\vec{a},\vec{b}+\vec{r}} + \delta_{\vec{a},\vec{b}-\vec{r}}),$$

and if the product of generating functions $g^{(i)}$

$$g^{(1)e_1} g^{(2)e_2} \cdots g^{(d)e_d} = \sum \bar{\beta}_{\vec{r}} \{\exp(i[(\vec{r} \cdot \vec{\Delta} E)/\hbar]t) + \text{c.c.}\},$$

then

$$\beta_{\vec{r}} = \bar{\beta}_{\vec{r}}.$$

The proof proceeds as in the single-degree-of-freedom case provided that the components of $\vec{\Delta} E$ are irrational with respect to each other. Once this result is established, the passage from the approximate Heisenberg equation to the Newtonian equation is straightforward and energy conservation is equivalent to the diagonalization of H.

IV. COMMUTATION RULES

It is not possible to calculate the commutator by the methods of the preceding two sections. If these methods were employed the result would be to calculate the Fourier coefficients of $(m\dot{g})g - g(m\dot{g})$. But since g is an ordinary function the result would be zero. The reason that quantum and classical mechanics are interchangeable so far is that the matrices (2) and the generating functions have the same multiplication rules.

A commutator has minus signs and the numerical values are the small differences of large numbers. A method to remove the minus signs is necessary before the type of approximation used above can be introduced. A satisfactory approach is to sum parallel to the diagonal to produce sums in which each term is positive. It is possible to make approximations in these formulas without the danger of making the type of errors associated with approximations in sums that contain both positive and negative numbers. The commutator formula is given first for a single-degree-of-freedom system where everything can be carried out explicitly. For a system with more than one degree of freedom the ordering of the energy levels is a mysterious phenomenon[3] and implicit results are derived.

The momentum p is given by

$$(\hbar/mi)p = [H, x],$$

so that the commutator relation is

$$[H, [H, x]] = (\hbar/mi)[p, x] = -(\hbar^2/m).$$

The diagonal matrix element of this relation is

$$\sum_b (E_b - E_a) x_{ab}^2 = \hbar^2/2m.$$

If the system is one-dimensional, a and b are just non-negative integers and the sum can be changed by setting $b = a + r$,

$$\sum_{r \geq -a} (E_{a+r} - E_a)(x_{a,b+r})^2 = \hbar^2/2m.$$

Now the terms with positive values of r are all positive while those with negative values of r are negative. If the above equation is summed on a from $a = 0$ to $a = A$ it turns out that the negative terms will all be cancelled by a subset of the positive terms. To see this divide the sum into two parts,

$$S_1 = \sum_{a=0}^{A} \sum_{r=1}^{\infty} (E_{a+r} - E_a)(x_{a,a+r})^2 > 0,$$

$$S_2 = \sum_{a=0}^{A} \sum_{r=-a}^{0} (E_{a+r} - E_a)(x_{a,a+r})^2 < 0,$$

so that

$$S_1 + S_2 = (\hbar^2/2m) \sum_{a=0}^{A} 1$$
$$= (\hbar^2/2m)(A+1).$$

Consider the term S_2 and change the sign of r,

$$S_2 = \sum_{a=0}^{A} \sum_{r=0}^{a} (E_{a-r} - E_a)(x_{a,a-r})^2.$$

Interchange the a and r sums and use the symmetry of x to give

$$S_2 = -\sum_{r=0}^{A} \sum_{a=r}^{A} (E_a - E_{a-r})(x_{a-r,a})^2.$$

Next let the a sum run from $a=0$ to $A-r$ to give

$$S_2 = -\sum_{r=0}^{A} \sum_{a=0}^{A-r} (E_{a+r} - E_a)(x_{a,a+r})^2.$$

Finally, interchange the order of the a and r sums again to give

$$S_2 = -\sum_{a=0}^{A} \sum_{r=0}^{A-a} (E_{a+r} - E_a)(x_{a,a+r})^2.$$

The two sums S_1 and S_2 may be combined and the result is

$$S_1 + S_2 = \sum_{a=0}^{A} \sum_{r=A-a+1}^{\infty} (E_{a+r} - E_a)(x_{a,a+r})^2$$
$$= (\hbar^2/2m)(A+1).$$

Each term in the sum is positive since $E_{a+r} > E_a$ and $x_{a,a+r}$ is real. The approximations of the preceding sections may be introduced into this formula with impunity to give

$$\sum_{a=0}^{A} \sum_{r=A-a+1}^{\infty} r \Delta E \alpha_r^2 = (\hbar^2/2m)(A+1).$$

Again invert the order of summation to yield

$$\sum_{r=0}^{\infty} r \Delta E \alpha_r^2 \sum_{a=A-r+1}^{A} 1 = (\hbar^2/2m)(A+1).$$

The a sum can be done and the final formula is

$$(\Delta E) \sum r^2 \alpha_r^2 = (\hbar^2/2m)(A+1).$$

As a consequence of this formula (ΔE) becomes a function of A, the index parallel to the diagonal.

The result for ΔE is not as explicit as it appears since the α's are dependent on ΔE. Because of this dependence the α's also pick up the previously neglected dependence on the matrix index parallel to the diagonal.

In a problem with d degrees of freedom almost the same derivation can be given, but because the matrix indices are now d-component vectors the order relations are confused. Two types of order will be distinguished. If each of the components of $\vec{a}$, a_i, is smaller than the corresponding component b_i of $\vec{b}$ then $\vec{a}$ will be said to be less than $\vec{b}$. It is not necessary with this definition of greater and lesser than for each pair of vectors one is greater than the other. To each index $\vec{a}$ there corresponds an energy $E_{\vec{a}}$. An index $\vec{b}$ is in the set $D_{\vec{a}}^{-}$ if $E_{\vec{b}} \leq E_{\vec{a}}$ and the index $\vec{b}$ is in the set $D_{\vec{a}}^{+}$ if $E_{\vec{a}} < E_{\vec{b}}$. If $a \in D_b^-$ then $b \in D_a^+$ unless $E_{\vec{b}} = E_{\vec{a}}$.

The commutator equation is

$$\sum_{\vec{b}} (E_{\vec{b}} - E_{\vec{a}}) x_{\vec{a},\vec{b}}^2 = \hbar^2/2m.$$

Replace $\vec{b}$ by $\vec{a}+\vec{r}$ which gives

$$\sum_{\vec{a}+\vec{r} \geq 0} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2 = \hbar^2/2m.$$

Instead of summing over a from $a=0$ to $a=A$ the appropriate domain of summation is $\vec{a} \in D_{\vec{A}}^{-}$. The commutator equation summed over this region is

$$\sum_{\vec{a} \in D_{\vec{A}}^{-}} \sum_{\vec{a}+\vec{r} \geq 0} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2 = (\hbar^2/2m) \sum_{\vec{a} \in D_{\vec{A}}^{-}} 1.$$

The sum on the right-hand side cannot be done at this stage since the distribution of energy levels is not known. The left-hand side can be separated as before into a positive portion S_1 and a negative portion S_2:

$$S_1 = \sum_{\vec{a} \in D_{\vec{A}}^{-}} \sum_{\vec{a}+\vec{r} \in D_{\vec{a}}^{+}} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2,$$

$$S_2 = \sum_{\vec{a} \in D_{\vec{A}}^{-}} \sum_{0 \leq \vec{a}+\vec{r} \in D_{\vec{a}}^{-}} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2.$$

As before, the sum S_2 will be manipulated until it cancels a portion of the positive sum S_1. The first step is to replace $\vec{r}$ by $-\vec{r}$,

$$S_2 = -\sum_{\vec{a} \in D_{\vec{A}}^{-}} \sum_{\vec{0} \leq \vec{a}-\vec{r} \in D_{\vec{a}}^{+}} (E_{\vec{a}} - E_{\vec{a}-\vec{r}})(x_{\vec{a}-\vec{r},\vec{a}})^2.$$

The interchange of the $\vec{a}$ and $\vec{r}$ sums gives

$$S_2 = -\sum_{\vec{r} \in D_{\vec{A}}^{+}} \sum_{\vec{r} \leq \vec{a} \in D_{\vec{A}}^{-}} (E_{\vec{a}} - E_{\vec{a}-\vec{r}})(x_{\vec{a}-\vec{r},\vec{a}})^2.$$

This is symbolically the same result as in the one-dimensional case. That $\vec{r}$ can vary over all of

$D^{-}_{\vec{A}}$ follows since if $\vec{a}$ is any point in $D^{-}_{\vec{A}}$ choose $\vec{r} = \vec{a}$ so that $\vec{r} - \vec{a} = \vec{0}$ and $\vec{0}$ exists in $D^{-}_{\vec{A}}$, so that $\vec{r}$ takes on each value in $D^{-}_{\vec{A}}$. Conversely if $\vec{r} \in D^{+}_{\vec{A}}$ then since $\vec{a} \in D^{-}_{\vec{A}}$, $\vec{a} - \vec{r}$ cannot be positive, at best it can be undefined with respect to zero. The limits on $\vec{a}$ reproduce the limits in the previous sum.

As before the next step is to replace $\vec{a} - \vec{r}$ by $\vec{a}$ to give

$$S_2 = -\sum_{\vec{r} \in D^{\mp}_{\vec{A}}} \sum_{0 \le \vec{a}, \vec{a}+\vec{r} \in D^{\mp}_{\vec{A}}} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2 .$$

As in the one-dimensional case the sums are again exchanged to give

$$S_2 = -\sum_{\vec{a} \in D^{\mp}_{\vec{A}}} \sum_{0 \le \vec{r}, \vec{a}+\vec{r} \in D^{\mp}_{\vec{A}}} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2 .$$

This sum can be combined with S_1 to give the expression

$$\sum_{\vec{a} \in D^{\mp}_{\vec{A}}} \sum_{\vec{a}+\vec{r} \in (D^{+}_{\vec{a}} - D^{\mp}_{\vec{A}}) = D^{+}_{\vec{A}}} (E_{\vec{a}+\vec{r}} - E_{\vec{a}})(x_{\vec{a},\vec{a}+\vec{r}})^2 = (\hbar^2/2m) \sum_{D^{\mp}_{\vec{A}}} 1 .$$

As before the summands are all positive and it is safe to use the approximation to give

$$\sum_{\vec{a} \in D^{\mp}_{\vec{A}}} \sum_{\vec{a}+\vec{r} \in D^{\pm}_{\vec{A}}} (r \cdot \vec{\Delta} E) \alpha_{\vec{r}}^{\,2} = (\hbar^2/2m) \sum_{D^{\mp}_{\vec{A}}} 1 .$$

Further simplification can be achieved by inverting the order of the sums to give

$$\sum_{\vec{r} \ge 0} (\vec{r} \cdot \vec{\Delta} E) \alpha_{\vec{r}}^{\,2} \sum_{\vec{a} \in D^{-}_{\vec{A}},\ \vec{a}+\vec{r} \in D^{+}_{\vec{A}}} 1 = (\hbar^2/2m) \sum_{D^{-}_{\vec{A}}} 1 . \tag{7}$$

The same remarks apply here and further emphasis must be placed on the necessity of knowing the energy spectrum before the formula is useful. There are d canonical pairs in a d-degree-of-freedom problem so that there are d equations to determine the d unknowns $\vec{\Delta} E$.

V. EXAMPLES

A number of simple examples are treated to show how these techniques work out in practice. The first three are in one dimension: The simple harmonic oscillator, the particle in a box, and the $x^2 + x^4$ oscillator. The last example is a particle in a central potential in two dimensions and in particular to a particle in a circular box.

Example 1: The harmonic oscillator

The equation of motion is

$$\ddot{x} + \omega^2 x = 0 .$$

The solution for the generating function is

$$g(t) = \alpha_1 (e^{i\omega t} + e^{-i\omega t}) .$$

In terms of θ this becomes

$$g(\theta) = \alpha_1 [\exp(i\hbar\theta\omega/\Delta E) + \text{c.c.}] .$$

There is only one nonvanishing matrix element, $\alpha = x_{a,a+1} = x_{a+1,a}$. The commutation condition is

$$\alpha_1^{\,2} = \frac{\hbar^2}{m(\Delta E)} \frac{a+1}{2} .$$

Since the generating function must be of the form

$$g(\theta) = \alpha_1 (e^{i\theta} + e^{-i\theta}) ,$$

it follows that

$$\Delta E = \hbar\omega ,$$

and thus α_1 becomes

$$\alpha_1^{\,2} = \frac{\hbar}{2m\omega} (a+1) .$$

These are the well-known results.

Example 2: The particle in a box in one dimension

A particle of mass m is confined to move between $x = 0$ and $x = l$. Its velocity is v. The generating function $g(\theta)$ has a nonvanishing value for $\theta = t = 0$ while $\dot{g}(t)$ and $g'(\theta)$ are zero for $t = \theta = 0$. The correct solution for $g(t)$ is then the cosine-type solution

$$g(t) = \frac{l}{2} + \begin{cases} \left(\frac{l}{2} - vt\right), & 0 \le t \le \frac{l}{v} \\ -\frac{3l}{2} + vt, & \frac{l}{v} \le t \le \frac{2l}{v} . \end{cases}$$

The Fourier expansion of $g(\theta)$ is given by

$$g(\theta) = \frac{2l}{\pi^2} \sum_{r=0}^{\infty} \frac{1}{(2r+1)^2} \left[\exp\left((2r+1) \frac{rv\hbar}{l\Delta E} i\theta\right) + \text{c.c.} \right] .$$

Because of the nature of the potential, the solution for α is given without use of the commutator,

$$\alpha_r = \frac{1}{(2r+1)^2} \frac{2l}{\pi^2} .$$

The commutator condition is

$$\sum (2r+1)^2 \left[\frac{2l}{\pi^2} \frac{1}{(2r+1)^2} \right]^2 = \frac{\hbar^2}{m\Delta E} \left(\frac{a+1}{2} \right) .$$

If the sum is done this becomes

$$\left(\frac{2l}{\pi^2} \right)^2 \frac{\pi^2}{8} = \frac{\hbar^2}{m\Delta E} \left(\frac{a+1}{2} \right) ,$$

so that $\Delta E=(\pi^2/4)(\hbar^2/ml^2)(a+1)$.

Thus the solutions for x_{ab} and p_{ab} are given by

$$x_{a,a+2r}=p_{a,a+2r}=0,$$

$$x_{a,a+2r+1}=\frac{1}{(2r+1)^2}\frac{2l}{\pi^2},$$

$$p_{a,a+2r+1}=\frac{2i\hbar}{l}\frac{a+1}{2r+1}.$$

These can be compared with the exact answers which give for the nonvanishing matrix elements

$$x_{a,a+2r+1}=\frac{1}{(2r+1)^2}-\frac{1}{(2a+2r+1)^2}\frac{2l}{\pi^2},$$

$$p_{a,a+2r+1}=\frac{4i\hbar}{l}\frac{a(a+2r+1)}{(2a+2r+1)(2r+1)}.$$

These agree in both cases for the leading terms.

Example 3: The quartic anharmonic oscillator

The Newtonian equation of motion is

$$m\ddot{x}+m\omega^2x+4\lambda x^3=0.$$

The solution with the cosine behavior is

$$g(\theta)=G\,\mathrm{cn}(\eta\theta,k),$$

where cn is a Jacobi elliptic function.[4] The constants G, η, and k are related to the parameters m, ω, and λ by the relations

$$m\hbar^2\omega^2+2\lambda\hbar^2G^2=\eta^2(1-k^2)(\Delta E)^2$$

$$\hbar^2\omega^2=(1-2k^2)\eta^2(\Delta E)^2,$$

$$2\lambda\hbar^2G^2=mk^2\eta^2(\Delta E)^2.$$

Only two of these three relations are independent. These can be used to calculate G and η^2 which are given by

$$G^2=\frac{k^2}{1-k^2}\frac{m\omega^2}{2\lambda},$$

$$\eta^2=\frac{1}{1-2k^2}\left(\frac{\hbar\omega}{\Delta E}\right)^2.$$

Since $g(\theta)$ must be periodic in θ with period 2π, the period of the elliptic function cn must be adjusted to satisfy this condition. The period of $\mathrm{cn}(\eta\theta,k)$ is given by $4K$ where

$$K=\int_0^{\pi/2}(1-k^2\sin^2\phi)^{-1/2}d\phi.$$

Thus since $2\pi\eta=4K$, it follows that

$$\eta=\left(\frac{1}{1-2k^2}\right)^{1/2}\left(\frac{\hbar\omega}{\Delta E}\right)=\frac{2K}{\pi},$$

so that

$$\frac{\pi}{2}\left(\frac{\hbar\omega}{\Delta E}\right)(1-2k^2)^{-1/2}=\int_0^{\pi/2}(1-k^2\sin^2\phi)^{-1/2}d\phi$$

is the third equation that permits the calculation of the parameters of the elliptic function G, η, and k in terms of the parameters m, ω, and λ of the problem and ΔE. Notice that if $k=0$, the elliptic function becomes an ordinary cosine and the problem reduces to the simple harmonic oscillator.

The elliptic function cn may be expanded in a Fourier series,

$$G\,\mathrm{cn}(\eta\theta,k)=\frac{2\pi G}{Kk}\sum\frac{q^{r+1/2}}{1+q^{2r+1}}\cos[(2r+1)\theta].$$

The new parameter q is related to k by

$$1-k^2=\prod_n\left(\frac{1-q^{2n-1}}{1+q^{2n-1}}\right)^8.$$

The quantities α_r are given by

$$\alpha_r=\frac{2\pi G}{Kk}\frac{q^{r+1/2}}{1+q^{2r-1}}$$

From the earlier formula it can be seen that k must be quite large before q differs appreciably from zero so the α_r are very rapidly decreasing functions of r.

The commutator relation is

$$\left(\frac{2\pi G}{Kk}\right)^2\sum(2r+1)^2\frac{q^{2r+1}}{(1+q^{2r-1})^2}=\frac{\hbar^2}{m(\Delta E)}\frac{a+1}{2}.$$

This equation provides a fourth relation which permits the determination of the elliptic function parameters G, η, k, K, and q and the energy difference ΔE in terms of the problem parameters m, ω, and λ and the quantum number a. The matrix elements α_r are then readily determined. The solution of these four coupled equations is a nontrivial numerical problem and it has not yet been carried out.

Example 4: Particle in a central force in two dimensions

The equations of motion in classical mechanics are

$$m\ddot{r}-L^2/mr^3+\frac{\partial V}{\partial r}=0,$$

$$\dot{\theta}=L/mr^2.$$

The solutions give r as a periodic function of the time with a period T_1. Since the angular velocity $\dot{\theta}$ is determined by r it has the same period T_1. However, θ which is found by integrating $\dot{\theta}$ will have a periodic part but in addition may have a portion of the type ct where c is a constant if $\dot{\theta}$ has a nonvanishing average value c. The ct part of θ introduces a second periodicity into $\sin\theta$ and $\cos\theta$ with a period $T_2=2\pi/c$. The coordinates x and y will have terms of the form $e^{\pm i\omega_2 t}$ where $\omega_2=2\pi/T_2$ and no other T_2 dependence. Thus the selection rule that x and y have nonvanishing ma-

trix elements only between states of adjacent angular momenta is derived in the present formalism. The radial portion of the matrix element depends of course on the explicit form of the potential.

VI. CONCLUSION

The approximation that the matrix elements of the coordinates x_{ab} may be treated as independent of $a+b$ leads to a reduced problem. The matrices in the reduced problem (5) have the same multiplication rules as a set of generating functions (6). The generating functions satisfy the Newtonian equations of motion so that the reduced problem may be solved if the corresponding classical problem is soluble. To recover the full quantum-mechanical problem from the reduced problem the commutation relations are introduced by means of (7).

The technique is a development of earlier efforts to solve the matrix equations of anharmonic-oscillator problems as sets of coupled algebraic equations.[1] The results are relatively independent of the size of the anharmonic term for one-degree-of-freedom systems. In the single-degree-of-freedom systems the r^2 in (4) suggests a rapid falloff in α with r. This expectation is borne out by numerical calculations and the examples. The analogous equation for a coupled system would involve $(\vec{r}\cdot\vec{\Delta}E)^2$, and $\vec{r}\cdot\vec{\Delta}E$ is not necessarily an increasing function of $\vec{r}$ as $\vec{r}$ gets far from the origin. This suggests that there are resonance phenomena that allow energy to be shifted between different modes. Numerical calculations for a system of two coupled anharmonic oscillators show that the matrix elements $x_{aba+1b-2}$ and $y_{aba-2b+1}$ can become quite large, approximately equal to x_{aba+1b} and $y_{ababb+1}$ while $x_{aba+1b+2}$ and $y_{aba+2b+1}$ are small. No general insights into this resonance phenomenon have been available from the numerical studies. Presumably the Fourier coefficients in the classical solution to a coupled problem will show similar resonance phenomena. The identification and classification of large matrix elements and the equivalent Fourier coefficients which should make the understanding of the behavior of coupled systems possible.

If the Newtonian equation of motion is solved and this solution is expanded in a Fourier series as is done in the examples, approximate expressions for the coordinate and momentum operators can be produced. To achieve more accurate numerical results these can be used as the starting point for a perturbation procedure based on the requirements the operators satisfy, the canonical commutation relations, and that the Hamiltonian is diagonal. My very limited experience is that this perturbation procedure is always rapidly convergent.

ACKNOWLEDGMENTS

This work was supported in part by the U. S. Department of Energy.

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