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SOME STRUCTURAL AND NUMERICAL ASPECTS OF HEISENBERG MATRIX MECHANICS WITH APPLICATIONS TO ONE-DIMENSIONAL SYSTEMS

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The equation of motion method in the form developed originally by Kerman and Klein for the study of nuclear collective motion becomes, when applied to elementary problems in quantum mechanics, a complete alternative to other standard approaches to solving such problems. A discussion of the foundations of the method and fragmentary presentations of a number of applications, exclusively to bound-state problems, illustrate the above contention.

1. Introduction

In 1962, one of the authors (AK), in collaboration with A. Kerman, introduced a new method for the restoration of broken symmetries of mean field descriptions of many-body systems[1]. (For the most recent accounts, see Refs. 2 and 3). During the intervening years, as the result of further development of the theory and a host of applications, many (though not all) of which are reviewed in Ref. 2, it has become apparent that one has a general method of studying quantum systems by means of Heisenberg's matrix mechanics. At various times during the past decade, the authors of the present contribution have toyed with the idea of trying to redo all of elementary quantum mechanics using matrix mechanics. Though this program has hardly progressed as far as we should have liked, we have accumulated a body of unpublished results, of which a fraction will be described in this paper. In addition some fragmentary results have been published. These included a numerical study of the anharmonic oscillator[4], derivation of semiclassical approximations, including new derivations of the WKB approximation[5,6,7], and underlying variational principles[8].

The notes that follow contain a variety of results, formal and numerical. Purely formal results are found, for instance in Secs. 2, 3, 6 and 9. In Sec. 2, we review our proof that the Heisenberg scheme formulated there can be derived from a novel variational principle. Using that variational principle, there follows a proof that in an energy-diagonal representation, off-diagonal matrix elements of the canonical commutation relation are consequences of the equations of motion. The same result is rederived in Sec. 3 directly from the equations of motion. Section 3 also contains a proof that solution of the matrix mechanics scheme according to the proposed algorithm is tantamount to diagonalization of the Hamiltonian. Section 6 describes an extension of the virial theorem. In Sec. 9, we formulate a method for quantizing a system with a coordinate-dependent mass.

Numerical aspects of the approach are discussed in Secs. 4, 5 and 7. In Sec. 4 we formulate an algorithm for studying anharmonic systems that is numerically simpler than that described and carried out in Ref. 4. This is followed in Sec. 5 by a study of some semi-classical aspects of this method. In Sec. 7, we illustrate a completely different numerical method based on the special variational principle (the trace variational principle) underlying the theory. In Sec. 8 the bound spectrum of two well-known exactly solvable models is treated.

2. *Variational principle*

We focus our attention on the system described by the Hamiltonian

$$H = \frac{1}{2} p^2 + V(x). \tag{2.1}$$

The equation of motion

$$[x, H] = \mathrm{i}p, \tag{2.2}$$

$$[\mathrm{i}p, H] = (\mathrm{d}V/\mathrm{d}x) \equiv V', \tag{2.3}$$

are obtained with the help of the commutation relation ($\hbar = 1$)

$$[x, p] = \mathrm{i}. \tag{2.4}$$

We shall be concerned particularly with the matrix elements of (2.2)—(2.4) in the representation in which H is diagonal with eigenvalues E_n, namely,

$$(E_n - E_m)\, x_{mn} = \mathrm{i}p_{mn}, \tag{2.5}$$

$$(E_n - E_m)\,\mathrm{i}p_{mn} = (V')_{mn}, \tag{2.6}$$

and

$$[x, p]_{mn} = \mathrm{i}\delta_{mn}. \tag{2.7}$$

We demonstrate that (2.5), (2.6) and the off-diagonal elements of (2.7) can be derived from a variational principle which is a special case of a more general category of variational principles considered by us previously[8]. The stationary expression is a trace which has three equivalent forms,

$$F \equiv \mathrm{Tr}\,\{»H« - \mathrm{i}H\,[x, p]\} \tag{2.8a}$$

$$= \mathrm{Tr}\,\{»H« - \mathrm{i}p\,[H, x]\} \tag{2.8b}$$

$$= \mathrm{Tr}\,\{»H« + \mathrm{i}x\,[H, p]\}. \tag{2.8c}$$

In these expressions the first occurrance of $H \equiv »H«$ is to be understood as the operator defined by (2.1). In this appearance in the second term of each expression, it is to be understood as an hermitian Lagrange multiplier matrix. We choose to compute the trace in the representation in which this Lagrange multiplier matrix is diagonal (and has precisely the eigenvalues E_n).

Thus, varying (2.8b) with respect to the matrix element p_{mn} for fixed x_{mn} and E_n yields (2.5) and varying (2.8c) with respect to x_{mn} for fixed p_{mn} and E_n yields (2.6).

To derive the off-diagonal elements of (2.7), we make use of the invariance of the trace under an infinitesimal change of basis. In the new basis, the Hamiltonian will not be diagonal, in general, and thus we must allow for a change in the Lagrange multiplier matrix. We calculate

$$0 = \delta F = \mathrm{Tr}\left\{\frac{\partial H}{\partial x}\,\delta x + \frac{\partial H}{\partial p}\,\delta p - \mathrm{i}\delta p\,[H, x] + \mathrm{i}\delta x\,[H, p] - \mathrm{i}\delta H\,[x, p]\right\} = \mathrm{Tr}\,\{-\mathrm{i}\delta H\,[x, p]\}, \tag{2.9}$$

since the first four terms cancel in pairs precisely because of the equations of motion. If we express the infinitesimal change of basis in the standard form

$$\delta\,|n\rangle = -\mathrm{i}\varepsilon\Theta\,|n\rangle, \tag{2.10}$$

where ε is infinitesimal and Θ is Hermitian, we recognize that in a variation about the energy diagonal representation

$$\delta\,\langle n|\,H\,|n\rangle = \mathrm{i}\varepsilon\,\langle n|\,[\Theta, H]\,|n\rangle = 0.$$

On the other hand non-diagonal elements

$$\delta\,\langle m|\,H\,|n\rangle \equiv \langle m|\,\delta H\,|n\rangle \equiv \delta H_{mn} \tag{2.11}$$

can be assigned arbitrary infinitesimal values consistent with hermiticity. From this and (2.9) we can easily conclude that the off-diagonal elements of $[x, p]$ vanish. An extension of the argument to yield the non-vanishing diagonal commutator is not immediately apparent. Indeed the basic kinematical assumption of quantum mechanics can then be understood as a statement about the diagonal elements in the energy representation. This distinction between diagonal and off-diagonal elements will surface again in Sec. 3, where we demonstrate that the vanishing of the off-diagonal (OD) elements is a consequence of the equations of motion.

In place of Hamilton's equations (2.5) and (2.6), we may consider Newton's equation

$$(E_n - E_m)^2 x_{mn} = (V')_{mn}, \tag{2.12}$$

and utilizing (2.5) once more, the commutation relation (2.7) in the form

$$\delta_{mn} = [x, [H, x]]_{mn} = \sum_l (2E_l - E_m - E_n) x_{ml} x_{ln}. \tag{2.13}$$

By using the corresponding substitution in (2.8), we obtain a stationary functional G, which can be used to derive (2.12). The functional is

$$G \equiv \mathrm{Tr}\left\{-\frac{1}{2}[x, H][H, x] + V(x)\right\} \tag{2.14a}$$

$$= \mathrm{Tr}\{H - H[x, [x, H]]\}. \tag{2.14b}$$

Variations with respect to x_{mn} for fixed E_n, using for convenience (2.14a) yields (2.12), whereas a paraphrase of the argument embodied in (2.9) endorses (2.13) for $m \neq n$.

3. *Some consequences of the equations of motion*

a. Vanishing of the off-diagonal matrix elements of the commutator

From (2.12), we have (no sum)

$$(E_l - E_m)^2 x_{ml} x_{ln} = (V')_{ml} x_{ln}, \tag{3.1}$$

$$(E_n - E_l)^2 x_{ml} x_{ln} = x_{ml} (V')_{ln}. \tag{3.2}$$

These equations in various combinations will yield several consequences of interest. For example, from the difference we find

$$\sum_l \{(3.1) - (3.2)\} = (E_n - E_m) \sum_l (2E_l - E_m - E_n) x_{ml} x_{ln} =$$
$$= (V'x)_{mn} - (xV')_{mn} = 0. \tag{3.3}$$

Thus for $m \neq n$, we learn that

$$\sum_{l} (2E_l - E_m - E_n)\, x_{ml} x_{ln} = 0, \tag{3.4}$$

or comparing with (2.13), we conclude that the vanishing of the OD matrix elements of the commutation relations is a consequence of the equations of motion. If was therefore not surprising that we could derive this result as well from the variational principle.

b. Proof that solving the equations of motion diagonalizes the Hamiltonian

We next prove directly that a solution of (2.5) and (2.6) guarantees that the Hamiltonian has been rendered diagonal. From (3.1) and (3.2) we derive for the sum

$$\sum_{l} \{(3.1) + (3.2)\} = \sum_{l} \{(E_l - E_m)^2 + (E_n - E_l)^2\}\, x_{ml} x_{ln} =$$

$$= (xV' + V'x)_{mn} = 2\,(xV')_{mn}. \tag{3.5}$$

From (2.5), we may write

$$(p^2)_{mn} = - \sum_{l} (E_l - E_m)(E_n - E_l)\, x_{ml} x_{ln}. \tag{3.6}$$

Equations (3.5) and (3.6) can be combined in several useful ways: Thus by subtracting twice (3.6) from (3.5) we find

$$(E_n - E_m)^2\, (x^2)_{mn} = -2\,(p^2)_{mn} + 2\,(V'x)_{mn}, \tag{3.7}$$

which is the matrix element of the equation

$$\frac{1}{2}\, [[x^2, H], H] = -p^2 + V'x. \tag{3.8}$$

On the other hand by adding twice (3.6) to (3.5), we find the results

$$\sum_{l} (2E_l - E_m - E_n)^2\, x_{ml} x_{ln} = 2\,(p^2)_{mn} + 2\,(V'x)_{mn}. \tag{3.9}$$

Equation (3.9) will be used to prove that H is diagonal in conjunction with another relation which is a further consequence of (3.1) and (3.2), namely,

$$\sum (2E_l - E_m - E_n)\{(3.1) - (3.2)\} = (E_n - E_m) \sum_{l} (2E_l - E_m - E_n)^2\, x_{ml} x_{ln} =$$

$$= -2i\,(V'p + pV')_{mn} + 2\,(E_n - E_m)\,(V'x)_{mn}, \tag{3.10}$$

after some algebraic rearrangement of the right hand side. Since

$$i(V'p + pV')_{mn} = 2\,[V, H]_{mn} = 2\,(E_n - E_m)\,V_{mn}, \tag{3.11}$$

we have finally, for $m \neq n$, in place of (3.10),

$$\sum_l (2E_l - E_m - E_n)^2\, x_{ml} x_{ln} = -4V_{mn} + 2\,(V'x)_{mn}. \tag{3.12}$$

Comparing (3.9) and (3.12) we conclude that

$$2\,(p^2)_{mn} + 2\,(V'x)_{mn} = -4V_{mn} + 2\,(V'x)_{mn}, \tag{3.13}$$

or

$$H_{mn} = \frac{1}{2}(p^2)_{mn} + V_{mn} = 0, \qquad m \neq n. \tag{3.14}$$

4. *Salient features of a simplified numerical scheme*

In previous work[4], we have described and carried out a numerical procedure for the solution of the matrix equations (2.5)—(2.7). This procedure, completely non-perturbative in the sense that no small parameters is required, was based on the property

$$|x_{n,n+1}| \gg |x_{n,n+3}| \gg |x_{n,n+5}| \gg \dots, \tag{4.1}$$

used to reduce the infinite set of coupled equations to an approximate finite set. (A number of arguments can be adduced for the validity of (4.1). For example, one can reason from the nodal structure of wave functions as a function of the quantum number n. Another argument can be based on the convergence of the sum rule implied by the diagonal matrix elements of (2.13). Finally, a semiclassical argument will be given in Sec. 5a.) By treating as variable all the matrix elements of x and of p within a finite subspace consisting of N states, we were required to solve of the order of N^2 equations to determine these objects. Methods were described for keeping N within bounds even if we wished to describe high-lying states. On the other hand, the previous methods become intractable if we wish to study a non-linear problem with more than one coordinate. This provided incentive for seeking a simplified solution of the one-dimensional problem. This problem has also continued to interest other authors[9-16].

The basis for such a simplification lies in the result established above that the equations of motion and the commutation relations form a redundant set. Since the commutation relations are simpler equations to deal with, we utilize them (or equivalently simple equations) to compute all the »small« matrix elements $x_{n,n\pm 3}$, $x_{n,n\pm 5}$ ..., by a recursive procedure in terms of the large matrix elements. What is of equal importance is that good starting approximations to the large matrix elements require the solution of only a single non-linear algebraic equation for such elements. In this section, we describe the main features of such a scheme.

a. Uncoupled first order calculation

Variants of this method, which we shall describe in a form applicable to any state n, are part of the folklore of the subject, especially in application to the ground state. We shall, nevertheless describe our derivation, first because a detailed form needs to be exhibited for each state, and second, because the approximations needed to derive the appropriate relations are different near $n = 0$ and for large n.

To take a specific case, we choose the oscillator with quartic anharmonicity,

$$H = \frac{1}{2} p^2 + \frac{1}{2} kx^2 + \frac{1}{4} \lambda x^4. \tag{4.2}$$

From the equations of motion and from the commutation relations, we shall first derive an approximate equation that determines $x_{n,n+1}$, namely,

$$-\frac{1}{4}(n+1)^2 + k(x_{n,n+1})^4 + 3\lambda(x_{n,n+1})^6 = 0. \tag{4.3}$$

Toward this goal we apply Eq. (2.12) for $x_{n,n+1}$. With

$$\omega_{ab} \equiv E_a - E_b, \tag{4.4}$$

this becomes

$$\omega^2_{n+1,n} x_{n,n+1} = kx_{n,n+1} + \lambda(x^3)_{n,n+1}. \tag{4.5}$$

Keeping only the largest matrix elements in a sum over intermediate states,

$$(x^3)_{n,n+1} \simeq x_{n,n+1}x_{n+1,n}x_{n,n+1} + x_{n,n+1}x_{n+1,n+2}x_{n+2,n+1} +$$
$$+ x_{n,n-1}x_{n-1,n}x_{n,n+1} = 3(x_{n,n+1})^2 [1 + 0(n^{-2})]. \tag{4.6}$$

That the error is second order in $(1/n)$ is seen by expanding $x_{n-\nu,n+\nu+1}$ in a Taylor series about $\nu = 0$. Here the approximation involved is classical in that the matrix elements are assumed to vary slowly with n. For $n = 0$, the argument proceeds differently, namely

$$(x^3)_{01} \simeq x_{01}x_{10}x_{01} + x_{01}x_{12}x_{21} \simeq 3(x_{01})^3, \tag{4.7}$$

if we make the harmonic approximation $x_{12} = \sqrt{2}x_{01}$, which is truly accurate only for small to moderate λ. No such restriction pertains to (4.6). Thus (4.5) is replaced by

$$\omega^2_{n+1,n} x_{n,n+1} = kx_{n,n+1} + 3\lambda x^2_{n,n+1}. \tag{4.8}$$

Next we utilize the diagonal element of the commutation relation (2.13), again retaining only the dominant terms, to find

$$1 = 2\omega_{n+1,n}(x_{n,n+1})^2 - 2\omega_{n,n-1}(x_{n-1,n})^2. \tag{4.9}$$

TABLE 1.

Element	Exact	Approx.	Energy	Exact	Approx.
x_{01}	0.595	0.591	E_0	0.621	0.624
x_{12}	0.771	0.773	E_1	2.026	2.027
x_{23}	0.894	0.900	E_2	3.698	3.689
x_{34}	0.992	1.000	E_3	5.558	5.536
x_{45}	1.075	1.084	E_4	7.568	7.533
x_{56}	1.147	1.157	E_5	9.709	9.658
x_{67}	1.211	1.223	E_6	11.96	11.90
x_{78}	1.269	1.282	E_7	14.32	14.24
x_{89}	1.323	1.336	E_8	16.78	16.67
$x_{9,10}$	1.372	1.386	E_9	19.32	19.19

First order approximations to energies and dominant matrix elements compared with exact results.

This equation becomes more useful if we sum over n from $0 \to n$, which yields

$$(n+1) = 2\omega_{n+1,n}(x_{n,n+1})^2. \tag{4.10}$$

The combination of (4.8) with (4.10) yields (4.3).

Once $x_{n,n+1}$ is computed from (4.3), which is, of course, exact for $\lambda = 0$, the energy of the state n may be computed with comparable accuracy from a formula based on the virial theorem and the use of (4.10), namely

$$E_n = \langle n|\, H\,|n\rangle = \frac{3}{4}\langle n|\, p^2\,|n\rangle + \frac{k}{4}\langle n|\, x^2\,|n\rangle \cong \frac{3}{16}\left\{\frac{(n+1)^2}{x^2_{n,n+1}} + \right.$$

$$\left. + \frac{n^2}{(x_{n,n-1})^2}\right\} + \frac{k}{4}\{(x_{n,n+1})^2 + (x_{n,n-1})^2\}. \tag{4.11}$$

In Table 1, we list some values for $k = \lambda = 1$ calculated from Eqs. (4.3) and (4.11) and compare with the exact values, the latter obtained in our previous calculations. It is seen that all results shown are accurate to within 1.5%. The error does not exceed 2% for any value of λ.

b. Calculation of small matrix elements

From Eq. (3.4), choosing $m \to n$, $n \to n + 2\nu$, we can derive the following formula for $x_{n,n+2\nu+1}$,

$$x_{n,n+2\nu+1} = [(2E_{n+2\nu+1} - E_n - E_{n+2\nu})\, x_{n+2\nu,n+2\nu+1}]^{-1}$$

TABLE 2.

Element	Exact	Approx.	Element	Exact	Approx.
x_{03}	0.0201	0.0194	x_{05}	7.11×10^{-4}	6.90×10^{-4}
x_{14}	0.0272	0.0268	x_{16}	9.81×10^{-4}	9.70×10^{-4}
x_{25}	0.0326	0.0323	x_{27}	1.192×10^{-4}	1.194×10^{-4}
x_{36}	0.0369	0.0368	x_{07}	2.60×10^{-5}	2.38×10^{-5}
x_{47}	0.0407	0.0407	x_{18}	3.62×10^{-5}	3.52×10^{-5}
x_{58}	0.0440	0.0441	x_{29}	4.46×10^{-5}	4.35×10^{-5}

First order approximations to some matrix elements $x_{n,n+2\nu+1}$ compared with exact values.

$$\Big\{ \sum_{0 \leq \nu' \leq 2\nu} (E_n + E_{n+2\nu} - 2E_{n+\nu'})\, x_{n,n+\nu'} x_{n+\nu',n+2\nu} + (E_n + E_{n+2\nu} - $$
$$ - 2E_{n-1})\, x_{n,n-1} x_{n-1,n+2\nu} + \sum_{|\nu'|>\nu+1} (E_n + E_{n+2\nu} - $$
$$ - 2E_{n+\nu+\nu'})\, x_{n,n+\nu+\nu'} x_{n+\nu+\nu',n+2\nu} \Big\}. \tag{4.12}$$

As will be seen in the next section $(x_{n,n+2\nu+1}/x_{n,n+2\nu-1}) \sim \varepsilon$, where $\varepsilon \sim (1/22)$ for a quartic anharmonicity. If we examine the right-hand side of (4.12), the curly bracket has been written, as a sum of three terms: the first sum involves a sum over larger matrix elements known from a previous approximation. The second involves a matrix element, $x_{n-1,n+2\nu}$, of the same size as that sought, and thus its presence establishes a definite sequence in which formulas (4.12) are to be evaluated for a fixed ν, namely in order of increasing n. Finally, the last sum is $0(\varepsilon^2)$, smaller than previous terms and may be ignored in a first go-round.

In Table 2 we compare some matrix elements $x_{n,n+2\nu+1}$ computed to lowest order by means of (4.12) with exact values obtained previously. For a fixed ν, the results appear to improve with increasing n.

The program described in this section is easy to carry out. It is most efficient for a purely repulsive potential, but can also be applied to a double well potential as long as the tunneling doesn't become too small. In the latter case, we need a new algorithm that recognizes and utilizes the consequences of the doublet structure of the spectrum. These matters will not be pursued here.

5. *Some semiclassical considerations*

a. Study of the truncation hypothesis

The rapid decrease in numerical value of the matrix elements $x_{n,n\pm\nu}$ with increasing ν is the justification for the truncation of the completeness relations or sum rules that form the basis for the methods under study. The corectness of this hypothesis has been amply verified by our numerical results. It is amusing to see, however, that in the simplest cases there is almost a definite convergence factor such that for large n

$$|x_{n,n+3}/x_{n,n+1}| \sim |x_{n,n+5}/x_{n,n+3}| \sim \ldots \sim \varepsilon. \tag{5.1}$$

For the quartic interaction for instance, we shall find below by numerical calculation that $\varepsilon \sim (1/22)$. The verification will be based on a semi-classical approximation to the off-diagonal commutator.

In terms of the definitions

$$x_{n-\nu,n+\nu'} \equiv x_{\nu+\nu'}\left[n + \frac{1}{2}(\nu' - \nu)\right], \tag{5.2}$$

Eq. (3.4), with the replacements $m \to n - \nu$, $n \to n + \nu$ and $l \to n + \nu'$, may be rewritten

$$0 = \sum_{\nu'} (E_{n-\nu} + E_{n+\nu} - 2E_{n+\nu'})\, x_{\nu+\nu'}\left[n + \frac{1}{2}(\nu' - \nu)\right] x_{\nu-\nu'}\left[n + \frac{1}{2}(\nu + \nu')\right]. \tag{5.3}$$

Utilizing the expansions (involving the frequency $\omega(n) = \partial_n E_n$),

$$E_{n+\nu} = E_n + \nu\omega + \frac{1}{2}\nu^2 \partial_n \omega + \ldots, \tag{5.4}$$

$$x_{\nu+\nu'}\left[n + \frac{1}{2}(\nu' - \nu)\right] = x_{\nu+\nu'} + \frac{1}{2}(\nu' - \nu)\, \partial_n x_{\nu+\nu'}, \tag{5.5}$$

we find

$$0 = \sum_{\nu'} \{(\nu'^2 - \nu^2)(\partial_n \omega)\, x_{\nu+\nu'} x_{\nu-\nu'} + \nu'(\nu' - \nu)\, \omega\, (\partial_n x_{\nu+\nu'})\, x_{\nu-\nu'} + \\ + \nu'(\nu' + \nu)\, \omega x_{\nu+\nu'} (\partial_n x_{\nu-\nu'})\} \{1 + O(n^{-2})\}. \tag{5.6}$$

Here we have suppressed the argument n of $\omega(n)$ and $x_\nu(n)$, etc. If $V(x) = \lambda x^{2q}$ then in the large n limit, from the analogues of (4.3) and (4.8), we find

$$x_\nu(n) \sim a_\nu \left(n + \frac{1}{2}\right)^{1/(q+1)}, \tag{5.7}$$

$$\omega(n) \sim \left(n + \frac{1}{2}\right)^{(q-1)/(q+1)}, \tag{5.8}$$

where a_ν is a constant. Eq. (5.6) becomes, in these circumstances, for $\nu \neq 0$

$$\sum_{\nu'} \{(q + 1)\, \nu'^2 - (q - 1)\, \nu^2\}\, x_{\nu-\nu'} x_{\nu+\nu'} = 0. \tag{5.9}$$

As an example consider $q = 2$ (quartic interaction). We have done a simple calculation, solving (5.9) numerically for the ratios $a_{2k+1} = (x_{2k+1}/x_1)$ for $k = 1, 2, 3, 4$ and find

$$\begin{aligned} a_3 &= 0.045077 \equiv \varepsilon \cong (1/22), \\ a_5 &= 1.9481 \times 10^{-3} \cong \varepsilon^2, \\ a_7 &= 8.419 \times 10^{-5} \cong \varepsilon^3, \\ a_9 &= 3.65 \times 10^{-6} \cong \varepsilon^4. \end{aligned} \tag{5.10}$$

b. Approximation to WKB

It is particularly interesting to consider the results of Sec. 4a in the limit of large n. In that limit, the energy (and other physical objects of the theory) should be given correctly by the WKB approximation. Our approximation in this limit is less accurate than WKB: As is well known, the quantities $x_\nu(n)$ defined above correspond to the Fourier coefficients of the classical periodic motion. Of course, the WKB approximation includes the contribution of all Fourier coefficients, whereas the approximation of Sec. 4a includes only the dominant Fourier coefficient. Because of the rapid convergence of the Fourier series, however, this yields a good starting approximation, obtainable together with corrections by purely algebraic processes. For practical purposes this represents a viable alternative to the usual WKB calculations.

As an illustration, Eq. (4.3), which has been derived with the large n approximation for $x_1(n + 1)$, becomes for $x_1 \equiv x_1(n)$

$$0 = 3\lambda x_1^6 + kx_1^4 - \frac{1}{4}\left(n + \frac{1}{2}\right)^2. \tag{5.11}$$

The cubic in x_1^2 can, of course, be solved exactly. The form of the solution depends on the value of the parameter

$$\beta \equiv \frac{81}{4}\frac{\lambda\left(n + \frac{1}{2}\right)}{(3k)^{3/2}}. \tag{5.12}$$

For $\beta \geq 1$ and for $\lambda\left(n + \frac{1}{2}\right) \gg k^{3/2}$, the solution becomes approximately

$$x_1 \cong \left\{\left[\frac{\left(n + \frac{1}{2}\right)^2}{12\lambda}\right]^{1/3} - \frac{k}{9\lambda}\right\}^{1/2} \to \left(n + \frac{1}{2}\right)^{1/3} \Big/ (12\lambda)^{1/6} \quad (\lambda \gg k). \tag{5.13}$$

These approximations are valid to about one percent in their domains of validity.

From (4.11), the energy can be computed from the formula

$$E_n \cong \left[\left(n + \frac{1}{2}\right)^2 / 4x_1^2\right] + kx_1^2 + \frac{3}{2}\lambda x_1^4 = \frac{3}{8}\left(n + \frac{1}{2}\right)^2 \Big/ x_1^2 + \frac{1}{2} kx_1^2, \quad (5.14)$$

using the virial theorem to reach the last form.

Systematic improvement of these results mixes the computation of the contribution of high order Fourier coefficients and of terms which vanish as $n \to \infty$.

6. *Off-diagonal virial theorem*

For many examples of interest, the role played above by the off-diagonal matrix elements of the commutation relations can be taken by a new set of equations derived below which are properly named the off-diagonal virial equations.

We start from the equations of motion (Cf. (3.8))

$$\mathrm{i}\,[\{x, p\}, H] = \frac{1}{2}\,[[x^2, H], H] = -p^2 + xV', \quad (6.1)$$

whose vanishing diagonal elements provide the standard virial theorem. For an off-diagonal matrix element we write

$$\frac{1}{2}(E_{n+\nu} - E_{n-\nu})^2 (x^2)_{n-\nu,n+\nu} = (-p^2 + xV')_{n-\nu,n+\nu}. \quad (6.2)$$

This relation takes on added interest when combined with the matrix statement that the Hamiltonian is diagonal, namely, for $\nu \neq 0$

$$0 = H_{n-\nu,n+\nu} = \left(\frac{1}{2}p^2 + V\right)_{n-\nu,n+\nu}. \quad (6.3)$$

One obvious way of combining (6.2) with (6.3) eliminates the matrix elements of p^2. Of more interest to us is the case where V is a sum of two monomials, e. g. $\frac{1}{2}kx^2 + \frac{1}{4}\lambda x^4$, which we shall use as an illustration in what follows. In such cases, the combination of (6.1) and (6.2) allows us to eliminate the monomial of highest degree. For the example chosen, we then obtain the equation

$$\sum_{\nu'}\left\{\frac{1}{2}(E_{n+\nu} - E_{n-\nu})^2 + k + 3(E_{n+\nu'} - E_{n-\nu})(E_{n+\nu'} - E_{n+\nu})\right\} \times$$
$$\times\, x_{n-\nu,n+\nu'} x_{n+\nu',n+\nu} = 0. \quad (6.4)$$

Equation (6.4) can be used for numerical purposes in place of the corresponding matrix elements of the commutator and gives results of comparable accuracy. In the limit of large n, by use of the WKB forms (5.7) and (5.8), (6.4) becomes

$$\sum_{\nu'} \{(q+1)\,\nu'^2 - (q-1)\,\nu^2 + (k/\omega^2)\}\, x_{\nu-\nu'} x_{\nu+\nu'} = 0, \tag{6.5}$$

for $V(x) = \frac{1}{2} kx^2 + \lambda x^{2q}$. This agrees with (5.9) if $k = 0$.

7. *Application of trace variational principle to anharmonic oscillator*

In Sec. 2 we have shown that the equations of motion can be derived from a special variational principle involving the trace of the Hamiltonian over the space of states under study (in the limit, over the entire Hilbert space). In this section, we shall show how this principle can be applied to the anharmonic oscillator described by the Hamiltonian

$$H = \frac{1}{2} p^2 + \frac{k}{2} x^2 + \frac{\lambda}{4} x^4. \tag{7.1}$$

Taking advantage of the invariance of the trace under a change of basis, we introduce the eigenstates of the harmonic oscillator

$$\widetilde{H} = \frac{1}{2} p^2 + \frac{1}{2} \Omega^2 x^2, \tag{7.2}$$

where Ω is to be fixed by the variational condition

$$(\partial/\partial\Omega)\,\mathrm{Tr}\, H = 0, \tag{7.3}$$

and the trace is to be taken over a suitably selected (see below) subspace of the eigenstates of $\widetilde{H}$, that we shall designate as $|n, \Omega\rangle$. Then

$$\langle n, \Omega|\, H\, |n, \Omega\rangle = \frac{\Omega}{2}\left(n + \frac{1}{2}\right) + \frac{k}{2\Omega} + \frac{3\lambda}{16\Omega^2}(2n^2 + 2n + 1). \tag{7.4}$$

If the subspace is chosen to consist of only the state $|n, \Omega\rangle$, the trace variational principle reduces to the usual variational principle; we thus obtain

$$E_n \cong \langle n, \Omega|\, H\, |n, \Omega\rangle, \tag{7.5}$$

where Ω is determined from the equation $(\partial E_n/\partial\Omega) = 0$ to be the solution of the condition

$$1 - \frac{k}{\Omega^2} - \frac{3\lambda}{2\Omega^3}\left[\frac{2n^2 + 2n + 1}{2n + 1}\right] = 0. \tag{7.6}$$

These results are, of course, exact for $\lambda = 0$, and in the worst case, when $(\lambda/k) \to \to \infty$,

$$E_n \cong \frac{3}{4}\left[\frac{3}{4}\lambda\left(n+\frac{1}{2}\right)^2(2n^2+2n+1)\right]^{1/3}, \tag{7.7}$$

which is accurate to within 2% for all n.

Next we study the two-state approximation for $n = 0$ and $n = 2$. (Because of the inversion symmetry of the Hamiltonian, we do not mix even and odd states.) From Eq. (7.4), we obtain

$$\mathrm{Tr}\, H = \langle 0, \Omega|\, H\, |0, \Omega\rangle + \langle 2, \Omega|\, H\, |2, \Omega\rangle = \frac{3}{2}\left(\Omega + \frac{k}{\Omega}\right) + \frac{21\lambda}{8\Omega^2}, \tag{7.8}$$

and the trace variational principle implies

$$1 - \frac{k}{\Omega^2} - \frac{7\lambda}{2\Omega^3} = 0. \tag{7.9}$$

To find the eigenvalues, we have to diagonalize the 2×2 matrix of H in the space of the first two even harmonic oscillator states with frequency determined by (7.9). We thus find the eigenvalues

$$E_0 = \Omega\left\{\frac{3}{2}\left(1 - \frac{7\lambda}{8\Omega^3}\right) - \sqrt{\left(1 - \frac{5\lambda}{8\Omega^3}\right)^2 + \frac{\lambda^2}{2\Omega^6}}\right\},$$

$$E_2 = \Omega\left\{\frac{3}{2}\left(1 - \frac{7\lambda}{8\Omega^3}\right) + \sqrt{\left(1 - \frac{5\lambda}{8\Omega^3}\right)^2 + \frac{\lambda^2}{2\Omega^6}}\right\}. \tag{7.10}$$

These are also exact for $\lambda = 0$, and in the limit $(\lambda/k) \to \infty$, Eq. (7.10) gives

$$\begin{aligned} E_0 &= 0.4237\lambda^{1/3}, \qquad [E_0\,(\text{exact}) = 0.4208\lambda^{1/3}], \\ E_2 &= 2.992\lambda^{1/3}, \qquad [E_2\,(\text{exact}) = 2.959\lambda^{1/3}]. \end{aligned} \tag{7.11}$$

For the ground state this is better than the one-state trace variational result, $0.4293\lambda^{1/3}$.

A calculation for the three state case gives, for $k = 0$,

$$\begin{aligned} E_0 &= 0.4212\lambda^{1/3} \qquad (\text{error} = 0.095\%), \\ E_2 &= 2.977\lambda^{1/3} \qquad (\text{error} = 0.61\%), \\ E_4 &= 6.531\lambda^{1/3} \qquad (\text{error} = 1.2\%). \end{aligned}$$

These calculations can easily be extended to higher order. Various other ways of improving the calculation suggest themselves. As an example, for a given size of secular determinant, one may replace the trial states $|n, \Omega\rangle$ by perturbatively improved states built upon the latter.

8. *Exactly solvable models*

a. Harmonic oscillator

In this section, we shall illustrate how matrix methods of the type utilized in this paper may also be applied to obtain exact solutions for a few well-known problems. We shall first illustrate the methodology for the harmonic oscillator. In dimensionless form, we study the Hamiltonian

$$H = \frac{1}{2}(p^2 + x^2). \tag{8.1}$$

We study the equations of motion in Lagrangian form,

$$[[x, H], H] = x, \tag{8.2}$$

together with the commutation relation.

$$[x, [H, x]] = 1, \tag{8.3}$$

and an alternate expression for the Hamiltonian,

$$H = \frac{1}{2}\{[x, H]\,[H, x] + x^2\}, \tag{8.4}$$

the latter two equations having benefited from the substitution

$$p = -\mathrm{i}\,[x, H]. \tag{8.5}$$

A matrix element of Eq. (8.2) takes the form

$$\omega_{nm}^2 x_{mn} = x_{mn}. \tag{8.7}$$

A possible solution of this equation is the well-known one that only $x_{n,n\pm 1}$ is nonvanishing, $\omega_{n+1,n} = 1$. The solution is completed by using diagonal matrix elements of (8.3) to solve recursively for the matrix elements

$$x_{n,n+1} = x_{n+1,n} = \sqrt{n+1}. \tag{8.8}$$

The ground state energy is then computed from (8.4) and the total energy recursively by adding the requisite number of energy differences to the ground state energy. A self consistency check on the solution is to calculate the energy difference from (8.4). Finally the momentum matrix is calculated from (8.5). It is obvious that the »success« of the method described above hinges on the *linearity* of the equation of motion (8.2) in the variable x.

In the two examples that are studied below, we shall borrow the technique displayed above, relying on analogues of (8.2)—(8.4). The trick will be to replace the coordinate operator x by a function of x that linearizes the equation of motion. This is possible, of course, only in a limited number of cases.

b. Poschl-Teller potential

We study

$$H = \frac{1}{2} p^2 - \frac{\lambda}{u^2}, \tag{8.9}$$

$$u \equiv \cosh x. \tag{8.10}$$

One now guesses that a suitable operator to study in place of x is

$$v \equiv \sinh x. \tag{8.11}$$

With the help of the relation

$$[v, H] = \frac{i}{2} (pu + up) = \frac{1}{2} (2ipu - v), \tag{8.12}$$

one then verifies the equation of motion

$$[[v, H], H] + vH + Hv + \frac{1}{4} v = 0, \tag{8.13}$$

and the commutation relation

$$[v, [H, v]] = 1 + v^2. \tag{8.14}$$

Multiplying (8.9) from the right by u^2, with the help of (8.12) we can derive

$$Hu^2 = \frac{1}{2} [v, H] [H, v] - \frac{1}{4} \{v [v, H] + 3 [v, H] v\} - \frac{3}{8} v^2 - \lambda. \tag{8.15}$$

The fact that the equation of motion (8.13) is linear in v implies that the only non-vanishing matrix elements of v are those between neighboring exact eigenstates, i. e. $v_{n,n\pm 1}$. Thus, from (8.13) and from ground state diagonal elements for (8.14) and (8.15), we derive, respectively, the three equations

$$\omega_{10}^2 + \omega_{10} + 2E_0 + \frac{1}{4} = 0, \tag{8.13a}$$

$$(2\omega_{10} - 1)\, v_{01}^2 - 1 = 0, \tag{8.14a}$$

$$E_0 (1 + v_{01}^2) + \frac{1}{2} v_{01}^2 \left(\omega_{10}^2 - \omega_{10} - \frac{3}{4}\right) - \lambda = 0. \tag{8.15a}$$

These equations yield the solution

$$\omega_{10} = \left(\sqrt{2\lambda + \frac{1}{4}} - 1\right), \tag{8.16}$$

$$E_0 = -\frac{1}{2}\left(\sqrt{2\lambda + \frac{1}{4}} - \frac{1}{2}\right)^2, \tag{8.17}$$

$$v_{01}^2 = (2\omega_{10} - 1)^{-1}. \tag{8.18}$$

To carry the calculation just a little further, from (8.13) we can derive the recursion relation

$$\omega_{n+1,n} \equiv E_{n+1} - E_n = \sqrt{-2E_n} - \frac{1}{2}. \tag{8.19}$$

Coupled with the previous results (8.17) and (8.18), we can then derive the result

$$E_n = -\frac{1}{2}\left[\sqrt{2\lambda + \frac{1}{4}} - \left(n + \frac{1}{2}\right)\right]^2. \tag{8.20}$$

Matrix elements can also be derived by similar algebraic methods.

c. Morse potential

As a final example, we study the system described by the Hamiltonian

$$H = \frac{1}{2} p^2 + \lambda\, [\exp(-2x) - 2 \exp(-x)]. \tag{8.21}$$

The relevant variable here is

$$v \equiv \exp(x). \tag{8.22}$$

In terms of this quantity, the equations of motion, commutation relations and energy are calculated from the equations

$$[v, H] = \frac{i}{2}(pv + vp) = \frac{1}{2}(2ipv - v), \tag{8.23}$$

$$[[v, H], H] + vH + Hv + \frac{1}{4}v + 2\lambda = 0, \tag{8.24}$$

$$[v, [H, v]] - v^2 = 0, \tag{8.25}$$

$$Hv^2 = \frac{1}{2}[v, H][H, v] + \frac{1}{4}\{v[v, H] - 5[v, H]v\} + \frac{1}{8}v^2 + \lambda(1 - 2v). \tag{8.26}$$

The structure of these equations is quite similar to that studied in the previous subsection. A mild increase in algebraic complexity has its origin in the fact that we are not dealing with an even potential. For the previous example only first off-diagonal elements of the appropriate quantity v were non-vanishing. Here in addition diagonal elements must be included. We shall not give any of the algebraic details that lead to the bound state spectrum

$$E_n = -\frac{1}{2}\left[\sqrt{\lambda/2} - \left(n + \frac{1}{2}\right)\right]^2, \tag{8.27}$$

since these details resemble those already given for the previous example.

9. *Quantization for generalized coordinates*

As the final topic of this compendium of elementary considerations in quantum mechanics, we study the problem of quantization of a classical system with a coordinate-dependent mass. This is a special case of the quantization of a system described by a Lagrangian with kinetic energy defined by a general mass tensor, where any connection with an underlying flat space either has been lost or does not exist. Under such circumstances we must expect on general grounds of the ordering ambiguity for the kinetic energy that a unique quantization procedure does not exist. Our aim will be to describe a convenient, consistent quantization method that can be extended to multidimensional and even infinite dimensional systems.

We therefore consider the classical Lagrangian

$$L_{cl} = \frac{1}{2}M(q)\dot{q}^2 - V(q), \tag{9.1}$$

with the associated momentum

$$p_{cl} = (\partial L_{cl}/\partial \dot{q}) = M\dot{q}. \tag{9.2}$$

To have a quantum theory, we first define three operators, the quantum Lagrangian, momentum, and Hamiltonian, respectively,

$$L \equiv \frac{1}{8}\{\dot{q}, \{\dot{q}, M(q)\}\} - V(q), \tag{9.3}$$

$$p \equiv \frac{1}{2}\{M, \dot{q}\}, \tag{9.4}$$

$$H \equiv \frac{1}{2}\{p, \dot{q}\} - L. \tag{9.5}$$

We then choose the standard formulation of quantum mechanics: if $\mathcal{O}$ is an operator-valued function of q and p, in units in which $\hbar = 1$, the equation of motion and commutation relation, respectively, are

$$\mathrm{i}\dot{\mathcal{O}} = [\mathcal{O}, H], \tag{9.6}$$

$$[q, p] = \mathrm{i}. \tag{9.7}$$

To utilize (9.6) and (9.7), we must eliminate $\dot{q}$ from (9.5) in favour of p. This requires that we invert Eq. (9.4). With the definition

$$B \equiv M^{-1}, \tag{9.8}$$

it is straightforward to prove that

$$\dot{q} = \frac{1}{2}\{p, B\} + \frac{1}{2}[[\dot{q}, M], B] = \{p, B\}, \tag{9.9}$$

provided $\dot{q}$ is linear in p, a consistent assumption. Consequently, the Hamiltonian takes the symmetrical form

$$H = \frac{1}{8}\{p, \{p, B\}\} + V(q). \tag{9.10}$$

Suppose that we wish to apply a Lagrangian scheme of calculation based on sum rules, as exemplified in Secs. 4 and 8. We need suitable expressions for the commutation relation (9.7), for the hamiltonian (9.10), and for the equation of motion (9.6). The first two requirements are satisfied by substituting the relation

$$p = \mathrm{i}\,[H, q], \tag{9.11}$$

thus obtaining

$$[q, [H. q]] = B, \tag{9.12}$$

$$H = \frac{1}{2}\,[q, H]\,[H, q] + V(q). \tag{9.13}$$

at remains only to study the Heisenberg equations of motion and to put them into I form commensurate with (9.12) and (9.13).

We start with the equation

$$\dot{q} = -\mathrm{i}\,[q, H] = \frac{1}{2}\{p, B\}, \tag{9.14}$$

which we thus verify is consistent with our definition of canonical momentum. We further calculate

$$\dot{p} = \frac{1}{2}\{\ddot{q}, M\} + \frac{1}{2}\{\dot{q}, M\} = -\mathrm{i}\,[p, H] = -\frac{\mathrm{d}V(q)}{\mathrm{d}q} + \frac{1}{8}\left\{p, \left\{p, B\frac{\mathrm{d}M}{\mathrm{d}q}B\right\}\right\}. \tag{9.15}$$

The task is now to substitute for p in terms of $\dot{q}$ in the last term of (9.15) and to obtain as symmetrical an expression as possible. The result is

$$\left\{p, \left\{p, B\frac{\mathrm{d}M}{\mathrm{d}q}B\right\}\right\} = \left\{\dot{q}, \left\{\dot{q}, \frac{\mathrm{d}M}{\mathrm{d}q}\right\}\right\} - 8\frac{\mathrm{d}\Phi}{\mathrm{d}q}, \tag{9.16}$$

where Φ, the »quantum potential« (see below for discussion) can be written as

$$\Phi = \int_{q_0}^{q} \mathrm{d}q' \frac{\mathrm{d}B}{\mathrm{d}q'}\frac{\mathrm{d}}{\mathrm{d}q'}\left(B\frac{\mathrm{d}M}{\mathrm{d}q'}\right). \tag{9.17}$$

Combining (9.15) and (9.16), we obtain the Langrangian equation

$$\frac{1}{2}\{\ddot{q}, M\} + \frac{1}{2}\{\dot{q}, M\} - \frac{1}{8}\left\{\dot{q}, \left\{\dot{q}, \frac{\mathrm{d}M}{\mathrm{d}q}\right\}\right\} = -\frac{\mathrm{d}V}{\mathrm{d}q} - \frac{\mathrm{d}\Phi}{\mathrm{d}q}. \tag{9.18}$$

The scheme of calculation is now complete as soon as we make the replacement $\mathrm{i}\dot{q} = [q, H]$ and consequent replacements in (9.18). The reason for the name attached to the quantity Φ is now apparent. As it appears in the result, it is both a potential energy and it is proportional to $\hbar^2$. It is the only quantity that would have been modified if we had chosen a different hermitian quantum form for the kinetic energy. Differences in this extra potential thus measure the ambiguity of quantization. We have, however, presented a possible consistent quantization that has the correct classical limit, the last assertion trivially verifiable by comparing the equation of motion (9.18) with that obtainable from the classical Lagrangian.

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References

1) A. K. Kerman and A. Klein, Phys. Lett. **1** (1962) 185;
2) A. Klein, Prog. in Part. and Nucl. Phys., vol. 10, ed. by D. H. Wilkinson (Pergamon Press, Oxford, 1983) 39;
3) A. Klein, Phys. Rev. **C30** (1984) 1680;
4) C. T. Li, A. Klein and F. Krejs, Phys. Rev. **D17** (1975) 2311;
5) A. Klein, J. Math. Phys. **19** (1978) 292;
6) A. Klein and C. T. Li, J. Math. Phys. **20** (1979) 572;
7) M. G. Vassanji and A. Klein, Phys. Rev. **C19** (1979) 2349;
8) A. Klein, C. T. Li and M. Vassanji, J. Math. Phys. **21** (1980) 2521;
9) F. T. Hioe, D. MacMillen and E. W. Montroll, J. Math. Phys. **17** (1967) 1320;
10) J. Killenbeck, Phys. Lett. **65A** (1978) 87;
11) K. Banerjee and S. P. Bhatnagar, Phys. Rev. **D18** (1978) 4767;
12) W. E. Caswell, Ann. Phys. **123** (1979) 153;
13) J. D. Bronzan and R. L. Sugar, Phys. Rev. **D23** (1981) 1806;
14) R. H. Tipping and J. F. Ogilvie, Phys. Rev. **A27** (1983) 95;
15) K. Yamazaki, Prog. Theor. Phys. **70** (1983) 629;
16) B. R. Clarke, J. Phys. A: Math. Gen. **18** (1985) 2207.

NEKI STRUKTURALNI I NUMERIČKI ASPEKTI HEISENBERGOVE MATRIČNE MEHANIKE S PRIMJENAMA NA JEDNODIMENZIONALNE SISTEME

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Originalni znanstveni rad

Metoda Kermana i Kleina za proučavanje kolektivnog gibanja jezgre predstavlja alternativan pristup rješavanju elementarnih problema kvantne mehanike. Diskutirana je metoda i primijenjena je na nizu problema.