INIS-mf--8954

Quantum Theory of Anharmonic Oscillators

- Some Exact Relations between Matrix Elements and their Use for Various Approximation Methods -

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Abstract:

This is an investigation of an anharmonic oscillator characterized by the potential $\frac{\omega_0^2}{2}q^2+\lambda' q^4$. By using the equations of motion and the relations obtained by evaluating $\langle i|\{H,O\}_+|j\rangle$ where O is an arbitrary operator, H is our total Hamiltonian and $|i\rangle$ and $|j\rangle$ are exact eigenstates of H, we derive an exact recurrence formula. This formula allows us to express τ-functions with a higher power of the variables through τ-functions with a lower power of the variables and energy eigenvalues. In this way we derive several exact relations, which are, in a sense, generalizations of the virial theorem and sum rules (eq. (4.5), (4.6) and (5.4)). These exact relations are the central equations of this paper. On the basis of these exact relations we propose our "nearest neighbour level" (N.N.L) approximation, which seems to provide a good approximation scheme. We can also use our exact relations to test the validity of various approximation methods, and as an example, we discuss the "New-Tamm-Dancoff" (N.T.D)-type of approximation in detail.

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§ 1. Introduction and Summary

Anharmonic oscillator models have played a very important role in various branches of physics ranging from particle physics to solid state physics. The virtue of this model lies in its simplicity, but nevertheless non-trivial nonlinearity; in particular one may obtain any quantity exactly by numerically solving the Schrödinger equation. So we can test any approximation method by comparing the approximate values with these exact values. The Montroll group[1),2)] elaborated these exact numerical values by using big computer facilities, so that we can use their results as standard references.

In an another investigation by the present author[3)], we have recently developed a systematical approximation method, whose lowest order approximation corresponds to a generalization of Ritz's variation method. The numerical results obtained are in excellent agreement with the exact results and higher approximations seem to converge very quickly for all ranges of λ (coupling constant) and i (the quantum number of the energy level).

In this paper we adopt a completely different approach to this problem. We first derive several exact relations between matrix elements, which are in some sense generalizations of the virial theorem and sum rules. These exact relations allow us to express practically any observables of our system by a small number of "input" quantities. This input itself must be calculated approximately. On the other hand if we use the exact values as input, we can evaluate any quantity of interest exactly, so that we can use these exact values to test the validity of an approximation method. This last point will be

discussed in § 10 for the "New-Tamm Dancoff" (N.T.D.) type of approximation as an example.

In § 2 we will define our notation and the τ-functions, which are the main mathematical tools in our analysis, and the related important mathematical relations for handling these τ-functions. In § 3 we derive the equation of motion for τ-functions (3.1), and use it to reduce $\tau(k|\ell)$ to a (exact) sum of $\tau(n|0)$, as shown in (3.3) where k, n $(\ell,0)$ are the powers of the variables q(p). In the usual treatment, as e.g. in the N.T.D. type, people usually use (3.1) to express τ-functions with a smaller number of variables by τ-functions with larger number of variables, and in this case one has to make some approximations in order to obtain a finite solvable system. But our use of (3.1) is quite different. In § 4, with the aid of a quantity written in eq. (4.2), which is the <u>anti</u>commutator of H with the dynamical variables, we can derive an exact recurrence formula (4.4), which allows us to express $\tau(n|0)$ with larger n as a sum of those with smaller n. In this way we can finally express any $\tau(k|\ell)$ in terms of $\Delta_{ij}(=\langle i|q^2|j\rangle)$ and $\Gamma_{ij}(=\langle i|p^2|j\rangle)$. Thus we obtain several <u>exact</u> relations, as given in (4.5) and (4.6). These are, in a sense, a generalization of the virial theorem. The advantage of our approach lies in the fact that we can start from functions $\tau(k|\ell)$ with small k and ℓ, which form a closed set, and do not have to relate them to those with larger k and ℓ. By adopting this opposite direction of approach, we can obtain an <u>exact</u> reduction formula, and arrive at exact relations after <u>finite</u> steps of algebra. § 5 gives a spectral representation and the related <u>exact</u> relationships, as given in (5.4), which are in some sense a generalization of the sum rules. In § 6 we give

the definitions of the normal product functions ϕ, used in the N.T.D. type of approximation. In § 7 we will show that any sensible approximation method, like the Hartree-Fock self consistent method, Ritz's variation method, N.T.D. method and the nearest neighbour level (N.N.L.) approximation, which is the one proposed in this paper, gives the same results for the ground state and the first excitation energy in the lowest approximation. In § 8 we present an approximation method, which consists of the use of exact relations derived above, and combines them with our N.N.L. approximation. The numerical results are satisfactory, as one can see also from Table 1. In § 9 we carry out our 2nd N.N.L. approximation which improves the lowest order results considerably. In § 10 we will evaluate the neglected quantities in the N.T.D. method, using our exact relations. In Appendix A we give the proof of eq. (2.4) ommitted in the text. Appendix B contains the main results of an extension of our approach to more general types of potentials in the form $V(q) = \sum_s \frac{\lambda_s}{s} q^s$.

§ 2. Notations and the Symmetrized Product Function τ.

The Hamiltonian of our anharmonic oscillator is given by

$$H = \frac{1}{2}(p^2 + \omega_0^2 q^2) + \lambda q^4 , \qquad [p, q] = -i \tag{2.1}$$

We have chosen units in which $\hbar = m = 1$. We define the normalized exact eigenstate $|i\rangle$ of our total Hamiltonian H, with the eigen-

value E_i, by

$$H|i\rangle = E_i|i\rangle \quad , \qquad \langle i|j\rangle = \delta_{ij} \tag{2.2}$$

We also use the following notations

$$\left.\begin{aligned} &\omega_{ij} \equiv E_i - E_j \quad , \quad \overline{W_{ij}} \equiv \tfrac{1}{2}(E_i + E_j) \\ &\Delta_{ij} \equiv \langle i|q^2|j\rangle, \quad \Gamma_{ij} \equiv \langle i|p^2|j\rangle \end{aligned}\right\} \tag{2.3}$$

Now we want to define a symmetrized product of q and p. For example: $Sy(qp) = \frac{1}{2}(qp+pq)$, $Sy(q^2p) = \frac{1}{3}(q^2p+qpq+pq^2)$ etc. But the general form of $Sy(q^kp^\ell)$ is not so easily found by inspection. It is most conveniently obtained by the generating function:

$$Sy(q^k p^\ell) = \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\; e^{xq+yp}\right]_{x=y=0} \tag{2.4}$$

(x,y are c-number parameters)

For the symmetrized product $Sy(q^kp^\ell)$ we can prove the following relations (the proof is given in Appendix A):

$$q^n Sy(q^k p^\ell) = \sum_{r=0}^{(\mathrm{Min}\, n,\ell)} \binom{n}{r}\binom{\ell}{r} r!\left(+\tfrac{i}{2}\right)^r Sy(q^{k+n-r}p^{\ell-r}) \tag{2.4a}$$

$$Sy(q^k p^\ell)\, q^n = \sum \quad " \quad " \quad " \left(-\tfrac{i}{2}\right)^r Sy(\quad " \quad) \tag{2.4b}$$

$$p^m Sy(q^k p^\ell) = \sum_{r=0}^{(\mathrm{Min}\, m,k)} \binom{m}{r}\binom{k}{r} r!\left(-\tfrac{i}{2}\right)^r Sy(q^{k-r}p^{m+\ell-r}) \tag{2.4c}$$

$$Sy(q^k p^\ell)\, p^m = \sum \quad " \quad " \quad " \left(+\tfrac{i}{2}\right)^r Sy(\quad " \quad) \tag{2.4d}$$

Now we define the symmetrized product function τ_{ij} by

$$\tau_{ij}(k|\ell) \equiv \langle i | S_y (q^k p^\ell) | j \rangle \tag{2.5}$$

This function is the central tool in our treatment of anharmonic oscillators, and, in the case of a time dependent formulation, is obtained by putting all times equal in the time ordered product function.

§ 3. The Equations of Motion for τ, and its Use to Express $\tau(k|\ell)$ as a Sum of $\tau(n|0)$.

With the aid of eqs. (2.4) we can calculate easily the right hand side of

$$i\omega_{ij}\,\tau_{ij}(k|\ell) = i\langle i | [H, S_y(q^k p^\ell)] | j \rangle ,$$

and we get

$$\begin{aligned} i\omega_{ij}\,\tau_{ij}(k|\ell) &= k\,\tau_{ij}(k-1|\ell+1) - \ell\,\omega_0^2\,\tau_{ij}(k+1|\ell-1) \\ &\quad -4\lambda'\ell\,\tau_{ij}(k+3|\ell-1) + \lambda'\ell(\ell-1)(\ell-2)\,\tau_{ij}(k+1|\ell-3). \end{aligned} \tag{3.1}$$

This is the equation of motion for the system of τ-functions and represents the usual starting point for the New-Tamm-Dancoff (N.T.D.) approach[4]. We use this to express the τ-functions with the largest ℓ value through τ-functions with lower ℓ values:

$$\tau_{ij}(k|\ell) = \frac{1}{k+1}\Big\{ i\omega_{ij}\,\tau_{ij}(k+1|\ell-1) + (\ell-1)\omega_0^2\,\tau_{ij}(k+2|\ell-2)$$

$$+4(\ell-1)\lambda'\,\tau_{ij}(k+4|\ell-2) - (\ell-1)(\ell-2)(\ell-3)\lambda'\,\tau_{ij}(k+2|\ell-4)\Big\} \quad (3.2)$$

This is a recurrence formula, which allows us to write $\tau_{ij}(k|\ell)$ as a sum of τ's with smaller ℓ. So, after a finite number of algebraic steps, we can express $\tau_{ij}(k|\ell)$ in the form:

$$\tau_{ij}(k|\ell) = \sum_{n=N_1}^{N_2} C_{k\ell}(\omega_{ij}, n)\,\tau_{ij}(n|0) \quad (3.3)$$

where $\sum$ is a finite sum, ranging from N_1 to N_2, where $N_1 \geq k+\frac{\ell}{2}$, $N_2 \leq k+2\ell$. This means that a general $\tau_{ij}(k|\ell)$ can be expressed (exactly) by a finite sum of $\tau_{ij}(n|0)$. So, if we were able to express a general $\tau_{ij}(n|0)$ by some $\tau_{ij}(n'|0)$ with n' smaller than n, then a general $\tau_{ij}(k|\ell)$ could be expressed through these. This is our program to be performed in the next section.

At this point two remarks may be added concerning the general structure of eq. (3.3):

First, as can be seen from eq. (3.2), τ-functions with $k+\ell$ = even (odd) are always connected with τ-functions with $k+\ell$ = even (odd). This is due to the parity property of our Hamiltonian (H is an even function of p and q). So eqs. (3.3) are completely separated for $k+\ell$ = even and odd.

Secondly, the coefficients $C_{k\ell}(\omega_{ij},n)$ depend on the states i and j only through ω_{ij}. The functional structure of $C_{k\ell}(\omega_{ij},n)$ is independent of i and j, and thus they all are the same functions for any i and j.

§ 4. Exact Relations to Express $\tau(n|0)$

We will drop hereafter the state suffices i and j, if there is no ambiguity, and use $\lambda' \equiv \frac{\lambda}{4}$.

As a special case of (3.1) we have

$$\left.\begin{aligned} i\omega\,\tau(k|1) &= k\,\tau(k-1|2) - \omega_0^2\,\tau(k+1|0) - \lambda\,\tau(k+3|0) \\ i\omega\,\tau(k+1|0) &= (k+1)\,\tau(k|1) \end{aligned}\right\}$$

Eliminating $\tau(k|1)$ from these two equations, we get

$$\left(\omega_0^2 - \frac{\omega^2}{k+1}\right)\tau(k+1|0) = k\,\tau(k-1|2) - \lambda\,\tau(k+3|0) \qquad (4.1)$$

Up to this point, all relations are obtained from our fundamental equation of motion (3.1). Now in order to eliminate $\tau(k-1|2)$ from (4.1), in order to get relations containing only the type of $\tau(n|0)$, we need new independent equations, not contained in (3.1). We can obtain such an (exact) equation by calculating the right hand side of

$$W_{ij}\,\tau_{ij}(k|l) = \frac{1}{2}\langle i|\,\{H, S_y(q^k p^l)\}_+\,|j\rangle . \qquad (4.2)$$

Let us consider the special case $k \to k-1$, $l=0$; then with the help of eq. (2.4) we have

$$W\,\tau(k-1|0) = \frac{1}{2}\tau(k-1|2) - \frac{(k-1)(k-2)}{8}\tau(k-2|0) + \frac{\omega_0^2}{2}\tau(k+1|0) + \frac{\lambda}{4}\tau(k+3|0) \qquad (4.3)$$

Eliminating $\tau(k-1|2)$ from (4.1) and (4.3), we finally get

$$\lambda\tau(k+3|0) = \frac{2}{(k+1)(k+2)}\left\{\omega^2 - (k+1)^2\omega_0^2\right\}\tau(k+1|0) \tag{4.4}$$

$$+ \frac{4k\,W}{(k+2)}\tau(k-1|0) + \frac{k(k-1)(k-2)}{2(k+2)}\tau(k-3|0).$$

This is a recurrence formula for $\tau(n|0)$, allowing us to express a τ-function with larger n in terms of τ-functions with smaller n, which can be solved successively. We can prove that the equations (4.2) with $\ell\neq 0$ provide no independent information other than (4.3). They are already contained in the combinations of eq. (3.1) and (4.3).

The remarks at the end of § 3 apply also here, i.e. (4.4) connects the functions $\tau(n|0)$ with only even or odd n, respectively. By using eq. (4.4) we can express $\tau(2n+1|0)$ in terms of a function of ω and W times $\tau(1|0)$. Together with eq. (3.2), we can write down the first few $\tau(2n-\ell+1|\ell)$ explicitly (these are exact relations):

$$\tau(0|1) = i\omega\,\tau(1|0) \tag{4.5a}$$

$$\lambda\tau(3|0) = (\omega^2 - \omega_0^2)\,\tau(1|0) \tag{4.5b}$$

$$\lambda\tau(2|1) = \frac{i\omega}{3}(\omega^2 - \omega_0^2)\,\tau(1|0) \tag{4.5c}$$

$$\lambda\tau(1|2) = \left\{-\frac{1}{12}(\omega^2+3\omega_0^2)(\omega^2-\omega_0^2) + \lambda W\right\}\tau(1|0) \tag{4.5d}$$

$$\lambda\tau(0|3) = \left\{-\frac{1}{60}(\omega^2+11\omega_0^2)(\omega^2-\omega_0^2) + \frac{9\lambda}{5}W\right\} i\omega\,\tau(1|0) \tag{4.5e}$$

$$\lambda^2 \tau(5|0) = \left\{ \frac{1}{6}(\omega^2 - 9\omega_0^2)(\omega^2 - \omega_0^2) + 2\lambda W \right\} \tau(1|0) \qquad (4.5f)$$

$$\lambda^2 \tau(4|1) = \left\{ \frac{1}{6}(\omega^2 - 9\omega_0^2)(\omega^2 - \omega_0^2) + 2\lambda W \right\} \frac{i\omega}{5} \tau(1|0) \qquad (4.5g)$$

$$\lambda^2 \tau(3|2) = \left\{ -\frac{1}{180}(\omega^2 + 5\omega_0^2)(\omega^2 - 9\omega_0^2)(\omega^2 - \omega_0^2) \right. \qquad (4.5h)$$

$$\left. + \frac{\lambda}{5}(3\omega^2 - 5\omega_0^2) W + \frac{\lambda^2}{2} \right\} \tau(1|0)$$

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In general they have the following structure

$$\lambda^n \tau_{ij}(k|2n+1-k) = T_{nk}(\omega_{ij}, W_{ij})\, \tau_{ij}(1|0) = T'_{nk}(E_i, E_j)\, \tau_{ij}(1|0) \qquad (4.5)$$

The special case i=j is trivial, because in this case both sides of eq. (4.5) are identically zero, due to parity.

Next, let us treat $\tau(2n|0)$ in a similar manner. We can also write down the first few $\tau(2n-\ell|\ell)$; by remarking that $\tau_{ij}(0|0) = \langle i|j\rangle = \delta_{ij} = \delta$, if we use the notation of dropping i and j, and using the notations Δ_{ij} and Γ_{ij} as defined by eq. (2.3), we get

$$W\delta = \frac{3}{4}\Gamma + \frac{\omega_0^2}{4}\Delta + \frac{\omega^2}{8}\Delta \qquad (4.6a)$$

$$\tau(1|1) = \frac{i\omega}{2}\Delta \qquad (4.6b)$$

$$\tau(3|1) = \frac{i\omega}{4}\tau(4|0) \qquad (4.6c)$$

$$\lambda\,\tau(4|0) = \Gamma - \omega_0^2\,\Delta + \frac{\omega^2}{2}\,\Delta \tag{4.6d}$$

$$\tau(1|3) = \frac{i\omega}{2}\left\{\tau(2|2) + \frac{\omega_0^2}{2}\,\tau(4|0) + \frac{\lambda}{3}\,\tau(6|0)\right\} \tag{4.6e}$$

$$\tau(5|1) = \frac{i\omega}{6}\,\tau(6|0) \tag{4.6f}$$

$$\lambda\,\tau(3|3) = \frac{-i\omega}{4}\left\{\tau(0|4) + 2\,\omega_0^2\,\tau(2|2) + \omega_0^2\,\tau(4|0) + \frac{2\lambda}{3}\,\omega_0^2\,\tau(6|0) - 3\lambda\,\Delta\right\} \tag{4.6g}$$

$$5\lambda\,\tau(2|2) = 4\lambda W\Delta + \lambda\,\delta - \left(\omega_0^2 + \frac{\omega^2}{4}\right)\lambda\,\tau(4|0) \tag{4.6h}$$

$$7\lambda\,\tau(0|4) = 12\lambda W\Gamma + 3\lambda\,\omega_0^2\,\delta + \frac{15}{2}\lambda^2\Delta - \frac{\lambda(3\omega_0^2+\omega^2)}{5}(4W\Delta+\delta) \tag{4.6i}$$

$$+\frac{1}{120}(72\,\omega_0^4 + 32\,\omega_0^2\omega^2 + \omega^4)\,\lambda\,\tau(4|0)$$

$$7\lambda^2\,\tau(4|2) = 4\lambda W\Gamma + \lambda\,\omega_0^2\,\delta + 6\lambda^2\Delta - \frac{2\lambda(4\omega_0^2-\omega^2)}{5}(4W\Delta+\delta) \tag{4.6j}$$

$$+\frac{1}{60}(96\,\omega_0^4 + 10\,\omega_0^2\,\omega^2 - \omega^4)\,\lambda\,\tau(4|0)$$

$$5\lambda^2\,\tau(6|0) = 12\lambda W\Delta + 3\lambda\,\delta + \left(-8\,\omega_0^2 + \frac{\omega^2}{2}\right)\lambda\,\tau(4|0) \tag{4.6k}$$

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In general these relations have the following structure

$$\lambda^n\,\tau_{ij}(k|2n+2-k) = S_{n,k}(\omega_{ij}, W_{ij}, \Gamma_{ij}, \Delta_{ij}) \tag{4.6'}$$

But (4.6a) allows us to express Γ_{ij} by Δ_{ij} (for the case of

$i \neq j$), or to express Γ_{ii} in terms of $W_{ii}=E_i$ and Δ_{ii} (for the case of i=j). So we get

$$\lambda^n \tau_{ij}(k|2n+2-k) = S_{n,k}(\omega_{ij}, W_{ij}, \Delta_{ij}) \tag{4.6}$$

The special case i=j gives ($\omega_{ii}=0$, $W_{ii}=E_i$)

$$\lambda^n \tau_{ii}(k|2n+2-k) = S_{n,k}(E_i, \Delta_{ii}) = S'_{n,k}(\Gamma_{ii}, \Delta_{ii}) \tag{4.6s}$$

As we have written explicitly in (4.5) and (4.6), one of the interesting structural features of these equations is the fact that $\tau(k|2n+1-k)$ and $\tau(k|2n+2-k)$ are always multiplied by λ^n, so that we can easily apply a perturbation theory for small λ.

But the most important feature of these equations is the fact that they are exact relations, like a virial theorem. In fact our eqs. (4.5) and (4.6) are in some sense a generalization of virial equations. (4.6d) is nothing else than the virial equation for our Hamiltonian, if we put i=j there.

§ 5. The Green's Function and the Spectral Representation

Of course, all dynamical information on our anharmonic oscillator will be obtained, if we know the two point function in a time dependent formulation. Let us consider

$$\Delta_{ii}(t) \equiv \langle i|q(t)\,q(0)|i\rangle = \langle i|\,q\,e^{-i(H-E_i)t}\,q\,|i\rangle$$

$$= \sum_k e^{-i\omega_{ki}t}\,\rho_{ki} = \sum_{k,n} \frac{(-i\omega_{ki}t)^n}{n!}\,\rho_{ki} \qquad (5.1)$$

where

$$\rho_{ki} = |\langle i|q|k\rangle|^2 = \rho_{ik} \qquad (5.2)$$

With the help of (4.5) and (4.6) we can exactly express the right hand side of the equation

$$\left[\left(i\frac{\partial}{\partial t}\right)^n \Delta_{ii}(t)\right]_{t=0} = \sum_k \omega_{ki}^n\,\rho_{ki} = \langle i|\,q(H-E_i)^n q\,|i\rangle \qquad (5.3)$$

in terms of Δ_{ii} and Γ_{ii}

As an example let us calculate the case n=3. Then by using the equation of motion and the commutation relations, we have

$$\langle i|\,q(H-E_i)^3 q\,|i\rangle = \langle i|\,p(H-E_i)\,p\,|i\rangle$$

$$= -\frac{i}{2}\langle i|(\omega_0^2 q + \lambda q^3)p - p(\omega_0^2 q + \lambda q^3)|i\rangle$$

$$= \frac{1}{2}\langle i|\,\omega_0^2 + 3\lambda q^2|i\rangle = \frac{3}{2}\lambda\Delta_{ii} + \frac{\omega_0^2}{2}$$

In this manner, with the aid of eq. (4.6) for i=j, we obtain the following formulae, which are also exact:

$$\sum_k \rho_{ki} = \Delta \tag{5.4a}$$

$$i\dot{\Delta} = \sum_k \omega_{ki} \rho_{ki} = \frac{1}{2} \tag{5.4b}$$

$$i^2 \ddot{\Delta} = \sum_k \omega_{ki}^2 \rho_{ki} = \Gamma \tag{5.4c}$$

$$i^3 \dddot{\Delta} = \sum_k \omega_{ki}^3 \rho_{ki} = \frac{3}{2}\lambda\Delta + \frac{\omega_0^2}{2} \tag{5.4d}$$

$$i^4 \overset{(4)}{\Delta} = \sum_k \omega_{ki}^4 \rho_{ki} = \frac{3\lambda}{5}(1 + 3\Delta\Gamma + \omega_0^2\Delta^2) + \frac{\omega_0^2}{5}(2\Gamma + 3\omega_0^2\Delta) \tag{5.4e}$$

$$i^5 \overset{(5)}{\Delta} = \sum_k \omega_{ki}^5 \rho_{ki} = \frac{9\lambda}{2}\Gamma - \frac{3}{2}\lambda\omega_0^2\Delta + \frac{\omega_0^4}{2} \tag{5.4f}$$

Eq. (5.4b) is the famous sum rule. The other equations of (5.4) are in some sense generalizations of the sum rule. We remark that the spectral functions ρ_{ki} are zero for k-i = even, because of parity. As we have remarked above, the important point of (5.4) is the fact that these relations are exact, and that on the right hand side of these equations there appear only Δ_{ii} and Γ_{ii}, and nothing else. But the sums over k in $\sum_k$ on the left hand sides are <u>infinite</u> sums in general.

Up to here we have derived a number of exact relations, which allow us to evaluate in general any observable in our dynamical system if we know a small number of input data. This means if we fix the states of interest i and j, then any matrix element $F_{ij} = \langle i|F(p,q)|j\rangle$, where F(p,q) is an arbitrary function of p and q, i.e. an arbitrary observable of our system, can, in principle, be exactly expressed by ω_{ij}, W_{ij} (or E_i and E_j) and $\tau_{ij}(1|0)$ or $\Delta_{ij}(=\tau_{ij}(2|0))$. If we want to determine the "input" data themselves, then we must use some approximation, but in this case also our exact relations help us. In the usual approximation treatment one already has to use an approximation, where we can still proceed exactly in our approach. So, for the case of a specific approximation, our exact relations allow us to judge whether the approximations are good or not. These points will become clearer in the discussion of approximation methods in § 10.

§ 6. The Normal Product Function ϕ.

One of the usual approximation methods is the New Tamm-Dancoff type, where one chooses appropriate combinations of τ to define the normal product function ϕ. Then the approximation is made by setting the higher ϕ's equal to zero, with the hope that they become smaller in proceeding to higher ϕ. We will see below that this is generally not true. The ϕ-functions can be most conveniently defined by their generating

functions, as in the case of τ-functions. There are some variants in the definition of ϕ-functions, which lead to somewhat different N.T.D. approximations:

(a) Define[4]

$$\phi^{a}_{ij}(k|\ell) = \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\left\{e^{-\frac{1}{2}x^2\langle 0|q^2|0\rangle - \frac{1}{2}y^2\langle 0|p^2|0\rangle}\langle i|e^{xq+yp}|j\rangle\right\}\right]_{x=y=0} \quad (6.1)$$

Through definition

$$\phi^{a}_{oo}(2|0) = \phi^{a}_{oo}(0|2) = 0$$

exactly, i.e., the 2-point contractions are subtracted by this definition of ϕ^a, but the other ϕ^a_{oo} functions are not zero in general.

(b) Define[5]

$$\phi^{b}_{ij}(k|\ell) = \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\left\{e^{-\frac{1}{4}x^2-\frac{1}{4}y^2}\langle i|e^{xq+yp}|j\rangle\right\}\right]_{x=y=0} \quad (6.2)$$

This one is obtained by setting $\langle 0|q^2|0\rangle = \langle 0|p^2|0\rangle = 1/2$ in (6.1), and corresponds to the use of the free propagator for the 2-point contraction function. This definition is the simplest one, but in this case all ϕ^b_{oo} functions are not zero in general.

(c) Define[6]

$$\phi^{c}_{ij}(k|\ell) = \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\left\{\frac{\langle i|e^{xq+yp}|j\rangle}{\langle 0|e^{xq+yp}|0\rangle}\right\}\right]_{x=y=0} \quad (6.3)$$

In this case

$$\phi^{c}_{oo}(k|\ell) = 0 \quad \text{for all } k \text{ and } \ell, \text{ except for } k=\ell=0,$$

by definition. All the vacuum contraction functions are subtracted here, not only the two point functions like in (a). Theoretically this would be the best definition for the ϕ-functions, but it is much more complicated for practical purposes than the other ones.

§ 7. The Lowest Order Approximation.

In this section we want to show that, in the lowest order approximation, any sensible approximation like the Hartree-Fock method, Ritz's variation method with Gaussian trial functions, Heisenberg's N.T.D. method, and our nearest neighbour level (N.N.L.) approximation method give exactly the same results.

§ 7a. The Hartree-Fock Self Consistent Method.

In this treatment, we substitute the nonlinear term $\frac{\lambda}{4} q^4$ by the approximate effective quadratic expression

$$\frac{\lambda}{4} q^4 \longrightarrow \frac{\lambda}{4} (6 c q^2 - 3 c^2)$$

where the parameter c is to be determined selfconsistently. The Hartree-Fock Hamiltonian is thus given by

$$H_{H.F} = \frac{1}{2}\left\{ p^2 + (\omega_0^2 + 3\lambda c) q^2 \right\} - \frac{3\lambda}{4} c^2 \qquad (7.1)$$

For this quadratic Hamiltonian $H_{H.F.}$, everything can be explicity found, namely

$$\left.\begin{aligned} H_{H.F}|0_{H.F.}\rangle &= E_0(c)|0_{H.F.}\rangle \\ E_0(c) &= \tfrac{1}{2}\sqrt{\omega_0^2+3\lambda c} - \frac{3\lambda}{4}c^2 \\ \omega_{10} &= E_1 - E_0 = \sqrt{\omega_0^2+3\lambda c} \end{aligned}\right\} \qquad (7.2)$$

The parameter c can be determined by the self consistency requirement:

$$c = \langle 0_{H.F}|q^2|0_{H.F.}\rangle = \frac{1}{2\sqrt{\omega_0^2+3\lambda c}} \qquad (7.3)$$

The same value for c can be also found by minimizing $E_0(c)$ with respect to c

$$\partial E_0(c)/\partial c = 0$$

Equation (7.2), with c determined from (7.3), is the main result of the Hartree-Fock method. Solving for ω_{10} we find a cubic equation for ω_{10}

$$\omega_{10}^2 = \omega_0^2 + \frac{3\lambda}{2\omega_{10}} \qquad (7.4)$$

§ 7b. Ritz's Variation Method with a Gaussian Trial Function.

Choose a Gaussian trial function:

$$\psi_0(q) = \langle q|\psi_0\rangle = \left(\frac{1}{2\pi a}\right)^{\frac{1}{4}} e^{-\frac{q^2}{4a}} \tag{7.4a}$$

The ground state energy becomes now

$$E_0(a) = \langle\psi_0|H|\psi_0\rangle = \frac{1}{8a} + \frac{\omega_0^2 a}{2} + \frac{3\lambda a^2}{4} \tag{7.5}$$

The parameter a is determined by the variation method, which is

$$\frac{\partial E_0}{\partial a} = 0 \longrightarrow a = \frac{1}{2\sqrt{\omega_0^2 + 3\lambda a}} \tag{7.6}$$

The value of a determined in this way is the same as the self consistency parameter c of eq. (7.3). With this value for a, the expression for the ground state energy (7.5) becomes identical to the Hartree-Fock result (7.2).

§ 7c. The N.T.D. method

Using eq. (3.1) and the lowest N.T.D. approximation $\phi(3|0) = \tau(3|0) - 3\Delta\tau(1|0) \simeq 0$, we find[4]

$$\omega = \omega_{10} = E_1 - E_0 = \sqrt{\omega_0^2 + 3\lambda\Delta} \tag{7.7}$$

But in order to determine the value of Δ, usually[4] the nearest neighbour level (N.N.L) approximation is used which will be discussed in § 7d, where $\rho_{k0}=0$ for $k\geq 2$ in (5.4a), (5.4b) and

(5.4c) with i=0, so that

$$\Delta = \rho_{10}, \quad \omega_{10}\rho_{10} = \frac{1}{2}, \qquad \Gamma = \omega_{10}^2\rho_{10}. \tag{7.8}$$

Now (4.ba) with i=j=0 gives us

$$E_o = \frac{3}{4}\Gamma + \frac{\omega_o^2}{4}\Delta \tag{7.9}$$

Together with (7.7) and (7.8), (7.9) gives us exactly the same results as found above in § 7a and § 7b (Δ=a=c).

As we have seen, (7.8) is not contained in the N.T.D. approximation*). If we want to perform everything in the framework of N.T.D., then we should determine Δ and Γ in this frame. We can obtain the necessary two equations by setting, for example, $\phi(4|0)=\phi(2|2)=0$. But we can equally well use $\phi(2|2)=\phi(0|4)=0$. They provide different equations. So, this way of determining Δ and Γ seems quite arbitrary, and above all, the so obtained results are of poorer numerical quality than the results obtained above by the other methods. Nevertheless it is possible to do everything in the framework of N.T.D. method defined in the sense of the footnote but the results seems to be worst.

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*) We call in this paper the "N.T.D. method" as the approximation method which uses $\phi(k|\ell)=0$ for $k+\ell \geq N$, for some properly defined ϕ functions of § 6. In this sense the usual N.T.D. method[4),5),6)] is a mixture of the N.T.D. method defined here, plus some other approximations.

§ 7d. The Nearest Neighbour Level (N.N.L.) Approximation.

This approximation is defined by setting

$$\rho_{ko} = 0 \quad \text{for} \quad k \geq 2 \tag{7.10}$$

If we use this condition in (5.4a) to (5.4d) we get four equations

$$\Delta = \rho_{10}, \quad \omega_{10}\rho_{10} = \frac{1}{2}, \quad \omega_{10}^2\rho_{10} = \Gamma, \quad \omega_{10}^3\rho_{10} = \frac{3}{2}\lambda\Delta + \frac{\omega_o^2}{2} \tag{7.11}$$

From these four equations we can deterime the four unknowns ω_{10}, ρ_{10}, Δ and Γ. We easily find

$$\Delta = \frac{1}{2\sqrt{\omega_o^2+3\lambda\Delta}}, \quad \omega_{10}^2 = \omega_o^2 + \frac{3\lambda}{2\omega_{10}}$$

This is nothing else than (7.3) and (7.4). In this way we get the same results as obtained by the other methods described above.

For $\frac{\lambda}{\omega_o^3} \equiv g \ll 1$ we get

$$\left.\begin{aligned} \Gamma &= \frac{\omega_o}{2}\left(1+\frac{3}{4}g+\cdots\right), \quad \Delta = \frac{1}{2\omega_o}\left(1-\frac{3}{4}g+\cdots\right) \\ \omega_{10} &= \omega_o\left(1+\frac{3}{4}g+\cdots\right), \quad E_o = \frac{\omega_o}{2}\left(1+\frac{3}{8}g+\cdots\right) \end{aligned}\right\} \tag{7.12}$$

These results agree with the correct perturbation theory results to order g. We cannot obtain the correct coefficients for g^2, as we have obviously neglected some g^2 terms in our approximation.

For the case $\lambda/\omega_0^3 \equiv g >> 1$ we obtain

$$\left.\begin{aligned}
\Delta = \rho_{10} &= \frac{1}{2\omega_{10}} = \frac{1}{2}\left(\frac{3}{2}g\right)^{-\frac{1}{3}} + \cdots\cdots = 0.4368\, g^{-\frac{1}{3}} + \cdots \\
\Gamma &= \frac{\omega_{10}}{2} = \frac{1}{2}\left(\frac{3}{2}g\right)^{+\frac{1}{3}} + \cdots\cdots = 0.5724\, g^{\frac{1}{3}} + \cdots \\
\omega_{10} &= \left(\frac{3}{2}g\right)^{\frac{1}{3}} + \cdots\cdots = 1.1447\, g^{\frac{1}{3}} + \cdots \\
E_0 &= \frac{3}{4}\Gamma + \frac{\omega_0^2}{4}\Delta = \frac{3}{8}\left(\frac{3}{2}g\right)^{\frac{1}{3}} + \cdots = 0.4293\, g^{\frac{1}{3}} + \cdots \\
\Gamma &= 3\Delta^2 g + \cdots\cdots
\end{aligned}\right\} \quad (7.13)$$

The corresponding exact values are

$$\left.\begin{aligned}
\Delta^{(e)} &= 0.4561\, g^{-\frac{1}{3}} + \cdots, \quad \Gamma^{(e)} = 0.5611\, g^{\frac{1}{3}} + \cdots \\
\omega_{10}^{(e)} &= 1.0871\, g^{\frac{1}{3}} + \cdots, \quad E_0^{(e)} = \frac{3}{4}\Gamma^{(e)} + \cdots = 0.4208\, g^{\frac{1}{3}} + \cdots \\
\Gamma^{(e)} &= 2.6972\,(\Delta^{(e)})^2 g + \cdots
\end{aligned}\right\} \quad (7.14)$$

The agreement is rather satisfactory in view of the fact that we used only the lowest approximation.

§ 8. The Excited Levels in the N.N.L. Approximation.

With the help of our exact relations (4.5), (4.6) and (5.4), we can calculate within the framework of our N.N.L. approximation even the higher energy levels and arbitrary matrix elements between higher levels. We will show this, as an example, for the energy levels.

Let us consider eqs. (5.4) with fixed i. We use the N.N.L. approximation defined by:

$$\rho_{ki} = 0 \qquad \text{except for} \quad k = i \pm 1 \tag{8.1}$$

From (5.4a), (5.4b) and (5.4c) we obtain

$$\begin{aligned} &\Delta_{ii} = \rho_{i+1,i} + \rho_{i-1,i} \\ &\omega_{i+1,i}\,\rho_{i+1,i} = \tfrac{1}{2} + \omega_{i,i-1}\,\rho_{i,i-1} = \tfrac{3}{2} + \omega_{i-1,i-2}\,\rho_{i-1,i-2} \\ &\qquad = \cdots\cdots = \tfrac{1}{2}(i+1) \qquad (\because\ \omega_{10}\rho_{10} = \tfrac{1}{2}) \\ &\Gamma_{ii} = \omega_{i+1,i}^2\,\rho_{i+1,i} + \omega_{i,i-1}^2\,\rho_{i,i-1} = \tfrac{1}{2}\left\{(i+1)\,\omega_{i+1,i} + i\,\omega_{i,i-1}\right\} \end{aligned} \tag{8.2}$$

Substituting these into the expression for E_i, obtained by setting i=j in eq. (4.6a), we have

$$E_i = \frac{3}{4}\Gamma_{ii} + \frac{\omega_0^2}{4}\Delta_{ii}$$

$$= \frac{3}{8}\left\{(i+1)\,\omega_{i+1,i} + i\,\omega_{i,i-1}\right\} + \frac{\omega_0^2}{8}\left\{\frac{i+1}{\omega_{i+1,i}} + \frac{i}{\omega_{i,i-1}}\right\}$$

$$E_{i-1} = \frac{3}{4}\Gamma_{i-1,i-1} + \frac{\omega_0^2}{4}\Delta_{i-1,i-1}$$

$$= \frac{3}{8}\left\{i\,\omega_{i,i-1} + (i-1)\,\omega_{i-1,i-2}\right\} + \frac{\omega_0^2}{8}\left\{\frac{i}{\omega_{i,i-1}} + \frac{i-1}{\omega_{i-1,i-2}}\right\}$$

Subtracting the two we obtain

$$\omega_{i,i-1} = \frac{3}{8}\left\{(i+1)\,\omega_{i+1,i} - (i-1)\,\omega_{i-1,i-2}\right\} + \frac{\omega_0^2}{8}\left\{\frac{i+1}{\omega_{i+1,i}} - \frac{i-1}{\omega_{i-1,i-2}}\right\}$$

or (8.3)

$$\frac{i+1}{8}\left(3\,\omega_{i+1,i} + \frac{\omega_0^2}{\omega_{i+1,i}}\right) = \omega_{i,i-1} + \frac{i-1}{8}\left(3\,\omega_{i-1,i-2} + \frac{\omega_0^2}{\omega_{i-1,i-2}}\right)$$

This is a recurrence formula expressing $\omega_{i+1,i}$ in terms of the lower $\omega_{i,i-1}$, $\omega_{i-1,i-2}$. Since ω_{10} is already given in § 7d, in the frame of our N.N.L. approximation, we get in this way $\omega_{i+1,i}$. The results agree with the correct perturbation results up to order g for weak coupling, while for strong coupling g>>1, if we put

$$A_n \equiv \frac{\omega_{n+1,n}}{\omega_{n,n-1}} \qquad (8.4)$$

we have

$$A_n = \frac{1}{n+1}\left\{\frac{8}{3} + (n-1)\frac{1}{A_{n-1}}\right\} \tag{8.5}$$

We can determine successively A_n:

$$A_1 = \frac{4}{3}\ ,\ A_2 = \frac{41}{36}\ ,\ A_3 = \frac{136}{123}\ ,\ A_4 = \frac{439}{408}\ ,\ A_5 = \frac{4204}{3951}\ ,\ \ldots\ldots$$

We give the first nine A_n with the corresponding exact values[1] in Table 1. We see that $\left|\frac{A_n - A_n^{(e)}}{A_n^{(e)}}\right| < 0.001$ for $n>5$, and the agreement is satisfactory in spite of the fact that this is only our lowest order N.N.L. approximation.

As a second example for showing the usefulness of our N.N.L. approximation for excited levels, we will give a direct way of calculating the higher energy levels without relying on such a successive procedure. As an example we will calculate here ω_{20} in the strong coupling limit($\lambda/\omega_o^3 >> 1$, or $\omega_o=0, \lambda=1$). Let us start from (4.6d) with i=j=0

$$\Gamma = \langle 0|q^4|0\rangle = \Delta^2 + \sum_{k=2}^{\infty} |\langle 0|q^2|k\rangle|^2 \tag{8.6}$$

Then (4.6h) and (4.6a) give us

$$\begin{aligned} 5\,\tau_{00}(2|2) &= 4E_0\Delta + 1 = 3\Gamma\Delta + 1 \\ &= 5\langle 0|\frac{p^2q^2+q^2p^2+1}{2}|0\rangle \\ &= \frac{5}{2} + 5\Delta\Gamma + 5\sum_{k=2}^{\infty}\langle 0|p^2|k\rangle\langle k|q^2|0\rangle \end{aligned} \tag{8.7}$$

Now eq. (4.6a) with i=0, j=k gives us

$$\langle 0|P^2|k\rangle = -\frac{1}{6}\omega_{k0}^2 \langle 0|q^2|k\rangle \tag{8.8}$$

By substituting this expression into eq. (8.7), we obtain

$$\frac{3}{2} + 2\Delta\Gamma = \frac{5}{6}\sum_{k=2}^{\infty} |\langle 0|q^2|k\rangle|^2 \omega_{k0}^2 \ . \tag{8.9}$$

As long as we take the infinite sum in (8.9), this is still an exact relation. We now use our N.N.L. approximation, which in this case is defined by

$$|\langle 0|q^2|k\rangle|^2 \equiv \rho'_{k0}=0 \qquad \text{for} \quad k\geq 4^{*)} \tag{8.10}$$

If we use (8.10), our eqs. (8.7) and (8.9) become now

$$\left.\begin{aligned} \Gamma &= \Delta^2 + \rho'_{20} \\ \frac{3}{2} + 2\Delta\Gamma &= \frac{5}{6}\omega_{20}^2 \rho'_{20} \end{aligned}\right\}$$

which gives us

$$\omega_{20}^2 = \frac{9 + 12\Delta\Gamma}{5(\Gamma - \Delta^2)} \ ,$$

and if we use the values (7.13) for Δ and Γ obtained in our N.N.L. approximation, we get

$$\omega_{20} = \sqrt{\frac{72}{5}}\,\Delta = 2.508$$

The corresponding exact value is

$$\omega_{20}^{(e)} = 2.538$$

---

*) $\rho'_{k0}=0$ for odd k, due to the parity property.

We have explicity shown these calculations as an illustration of the usefulness of our exact relations obtained in § 4, § 5 and the validity of our N.N.L. approximation. In such a way, we can calculate rather easily the energy levels and arbitrary matrix elements of the anharmonic oscillator by just algebraic manipulations.

§ 9. The 2nd N.N.L. Approximation.

Our secound N.N.L. approximation amounts to setting

$$\rho_{k0}=0 \qquad \text{except for} \quad k = 1,3 \quad . \tag{9.1}$$

in eq. (5.4) with i=0. From the six eq's. (5.4a)∿ (5.4f) [write $\omega_1 = \omega_{10}$, $\omega_3 = \omega_{30}$, $\rho_{10} = \rho_1$, $\rho_{30} = \rho_3$] we get

$$\left.\begin{aligned}
&\Delta = \rho_1 + \rho_3 \,, \quad \frac{1}{2} = \omega_1 \rho_1 + \omega_3 \rho_3 \\
&\Gamma = \omega_1^2 \rho_1 + \omega_3^2 \rho_3 \,, \quad \frac{3}{2}\lambda\Delta + \frac{\omega_0^2}{2} = \omega_1^3 \rho_1 + \omega_3^3 \rho_3 \\
&\frac{3}{5}\lambda\left(1 + 3\Delta\Gamma + \omega_0^2\Delta^2\right) + \frac{\omega_0^2}{5}\left(2\Gamma + 3\omega_0^2\Delta\right) \\
&\qquad = \omega_1^4 \rho_1 + \omega_3^4 \rho_3 \\
&\frac{9}{2}\lambda\Gamma - \frac{3}{2}\lambda\omega_0^2\Delta + \frac{\omega_0^4}{2} = \omega_1^5 \rho_1 + \omega_3^5 \rho_3
\end{aligned}\right\} \tag{9.2}$$

We can determine the six unknowns ω_1, ω_3, ρ_1 ρ_3, Δ and Γ from these six equations:

For weak coupling, $\lambda/\omega_o^3 \equiv g \ll 1$, we get

$$\left.\begin{aligned}
&\omega_{10} = \omega_0\left(1+\frac{3}{4}g+\cdots\right), \quad \omega_{30} = 3\omega_0+\cdots \\
&\rho_{10} = \frac{1}{2\omega_0}\left(1-\frac{3}{4}g+\frac{207}{128}g^2+\cdots\right), \quad \rho_{30} = \frac{3}{256}g^2+\cdots \\
&\Delta = \frac{1}{2\omega_0}\left(1-\frac{3}{4}g+\frac{105}{64}g^2+\cdots\right) \\
&\Gamma = \frac{\omega_0}{2}\left(1+\frac{3}{4}g-\frac{63}{64}g^2+\cdots\right) \\
&E_0 = \frac{3}{4}\Gamma+\frac{\omega_0^2}{4}\Delta = \frac{\omega_0}{2}\left(1+\frac{3}{8}g-\frac{21}{64}g^2+\cdots\right)
\end{aligned}\right\} \quad (9.3)$$

These results agree with the correct perturbation results up to order g^2.

For the strong coupling limit, $\lambda/\omega_o^3 = g \gg 1$, we obtain

$$\left.\begin{aligned}
&\Delta = 0.456\, g^{-\frac{1}{3}}+\cdots && (0.4561) \\
&\Gamma = 0.561\, g^{\frac{1}{3}}+\cdots && (0.5611) \\
&\omega_{10} = 1.09\, g^{\frac{1}{3}}+\cdots && (1.0871) \\
&\omega_{30} = 4.22\, g^{\frac{1}{3}}+\cdots && (4.2002) \\
&\sqrt{\Gamma_{30}} = \langle 0|q|3\rangle = 0.0367\, g^{-\frac{1}{3}}+\cdots && (0.0364)
\end{aligned}\right\} \quad (9.4)$$

Here we give the corresponding exact numerical coefficients in parentheses. Obviously the agreement is excellent.

§ 10. The Exact Evaluation of the Neglected Quantities in the Various Approximation Methods.

As we have frequently emphasized above, the exact relations (4.5), (4.6) and (5.4) allow us to calculate almost everything in our system, if we know the exact values of Δ and Γ. For the case of i=j=0, ($\lambda=1, \omega_0=0$) we know the exact values $\Delta^e=0.4561$, $\Gamma^e=0.5611$, obtained by solving numerically the Schrödinger equation[1),2),4)]. Accordingly, for i=j=0 we can calculate the exact expectation values of any function of p and q, and can calculate the values of the neglected quantities in the various approximations. In this way we can judge the validity of the specific approximation method, at least for this simple one dimensional nonlinear problem. In the following, as an illustration, we will do that for the N.T.D. type of approximation. We will concentrate on the strong coupling limit ($\lambda=1, \omega_0=0$), as this case is the most interesting one. Inserting the exact values Δ^e and Γ^e into the exact relations (4.6) we easily get the exact values ($\omega=0$)

$$\Gamma^e=\tau^e(410)=0.5611,\quad \tau^e(212)=0.3535,\quad \tau^e(014)=0.9954$$
$$\tau^e(610)=1.0606,\quad \tau^e(412)=0.5259,\ \text{etc.} \tag{10.1}$$

i) Usual N.T.D. method[4)]

Now we can calculate the magnitude of the ϕ-functions neglected in the usual N.T.D. approximation. [Use definition (6.1)]

$$\phi^e(4|0) \equiv \tau^e(4|0) - 3\,(\Delta^e)^2 = -\,0.0629$$

$$\phi^e(2|2) \equiv \tau^e(2|2) - \Delta^e \Gamma^e = +\,0.0976$$

$$\phi^e(0|4) \equiv \tau^e(0|4) - 3\,(\Gamma^e)^2 = +0.0510 \qquad (10.2)$$

$$\phi^e(6|0) \equiv \tau^e(6|0) - 15\,\Delta^e \tau^e(4|0) + 30\,(\Delta^e)^3 = +\,0.0694$$

$$\phi^e(4|2) \equiv \tau^e(4|2) - 6\,\Delta^e \tau^e(2|2) + 6\,(\Delta^e)^2 \Gamma^e - \Gamma^e \tau^e(4|0) = +0.0562$$

These values are exact, (we used only exact relations and the definition of ϕ). So we get

$$\frac{\phi^e(4|0)}{\tau^e(4|0)} = 0.1121, \quad \frac{\phi^e(2|2)}{\tau^e(2|2)} = 0.2761, \quad \frac{\phi^e(0|4)}{\tau^e(0|4)} = 0.0512 \qquad (10.3a)$$

$$\frac{\phi^e(6|0)}{\tau^e(6|0)} = 0.0647, \quad \frac{\phi^e(4|2)}{\tau^e(4|2)} = 0.1069 \qquad (10.3b)$$

The N.T.D. approximation rests on the hope that these numbers are small; expecially, the numbers in (10.3b) should be smaller than the numbers in (10.3a), since (10.3b) are the results of higher N.T.D. approximations than those of (10.3a). We see that the improvement is not significant.

ii) Heisenberg's[4] simplified version of the N.T.D. method.

This approximation consisted in expressing τ-functions in terms of ϕ-functions and neglecting all ϕ-functions except the non-vanishing lowest one. In our case, the lowest configurations $\phi(4|0)$, $\phi(2|2)$, $\phi(0|4)$ are the same as in i). For

the next lowest configuration, this amounts to approximate

$$\tau(6|0) \doteq 15\,\Delta^3 \quad , \quad \tau(4|2) \doteq 3\Delta^2\Gamma$$

We can evaluate the errors by calculating exactly the numbers

$$\frac{\tau^e(6|0) - 15(\Delta^e)^3}{15(\Delta^e)^3} = -0.255, \quad \frac{\tau^e(4|2) - 3(\Delta^e)^2\Gamma^e}{3(\Delta^e)^2\Gamma^e} = +0.502$$

These numbers are by no means small.

iii) Maki's[6] N.T.D. method.

This is an approximation method which takes into account all the connected diagrams, and theoretically would be the best one but it is rather complicated (cf. (6.3)). Using eq. (4.6h) we find for the connected diagram contributions

$$\Delta_c(4|0) = \Gamma - 3\Delta^2 = 0.013$$

$$\Delta_c(2|2) = \frac{1}{5}(1 - 2\Delta\Gamma) = 0.217$$

The numbers are Maki's estimate. The corresponding exact numbers are, however,

$$\Delta_c^e(4|0) = -0.0630, \qquad \Delta_c^e(2|2) = 0.0976$$

Which shows that Maki's numbers are also far from being correct. We can also check the validity of Maki's eq. (4.9) by using (4.5)

$$\tau^e(5|0) - 10\,\Delta^e\tau^e(3|0) + 15(\Delta^e)^2\tau^e(1|0) - 5\Delta_c^e(4|0)\,\tau^e(1|0)$$

$$= \left\{\frac{1}{6}\omega^4 + 2W - 10\,\Delta^e\omega^2 + 15(\Delta^e)^2 - 5\Delta_c^e(4|0)\right\}\tau^e(1|0)$$

For the case of j=1, i=0, substituting the exact values $\omega=\omega_{10}=1.0871$, $W=\frac{1}{2}(E_o+E_1)=0.9644$, $\Delta=\Delta^e=0.4561$, we can evaluate the factor of $\tau^e(1\,0)$ on the right hand side of the above expression, and get for the right hand side

$$0.2764\ \tau^{(e)}(1|0)$$

Similarly we get

$$\tau^e(4|1) - 6\,\Delta^e\,\tau^e(2|1) + 3(\Delta^e)^2\tau(0|1) - 4\,\Delta_c^e(3|1)\,\tau^e(1|0)$$

$$= (-\lambda)\,(0.1359)\,\tau^e(1|0)$$

$$\tau^e(3|2) - 3\,\Delta^e\,\tau^e(1|2) - \Gamma^e\tau^e(3|0) + 3\,(\Delta_c^e(2|2) - \Delta^e\,\Gamma^e)\,\tau^e(1|0)$$

$$= -(0.1739)\,\tau^e(1|0)\,,$$

these numbers, which are put equal to zero by Maki, are not so small as one might have hoped, thus the complicated Maki's N.T.D. method does not improve the numerical results of the usual N.T.D. Summarizing, we may conclude that for the strong coupling limit the 2nd N.T.D. approximation <u>does not improve</u> the lowest approximation essentially. We have chosen, as a concrete example, the N.T.D. method, but we can in principle test any approximation method in a similar fashion. We already saw in § 9 that our N.N.L. approximation, combined with our exact relations, gives us very satisfactory results.

It is a great pleasure for the author to thank H.Mitter, H.Latal and the members of Theoretical Physics Institute of the University of Graz, where the author was a visiting professor for 1982/83, for their warm hospitality, interest and encouragement. The financial support of the Austrian Ministry of Science and Research, which made his stay there possible, is appreciated.

Note added

After the completion of this preprint, the author became aware of the existence of a paper by R.H.Tipping and T.F.Ogilivie[7] in the newest Phys.Rev.A (Jan 1983 issue). Their intention and the main results, such as the hypervirial theorem and generalized sum rules have many common features to our paper (of course the method of derivation is somewhat different). But as they worked only with the matrix elements of q^ℓ, while the general dynamical variables of our dynamical system are $Sy(q^k p^\ell)$, and we derived many relations valid for these general dynamical variables and also worked out many points concerning the approximation methods, which are not contained in ref.7. we decided to publish this paper in its original form. Ref.7. contains many valuable references to earlier works.

Appendix A. Proof of eq. (2.4).

We will prove only (2.4a); (2.4b) is the Hermitian conjugate of (2.4a) and (2.4c) can be proved quite similarly.

$$q^n S_y(q^k p^\ell) = \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\, q^n e^{xq+yp}\right]_{x=y=0}$$

$$= \left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\left\{\left(q-\tfrac{iy}{2}\right)+\tfrac{iy}{2}\right\}^n e^{xq}\, e^{yp}\, e^{-\frac{ixy}{2}}\right]_{x=y=0}$$

$$= \sum_{r=0}^{n}\binom{n}{r}\left[\frac{\partial^k}{\partial x^k}\frac{\partial^\ell}{\partial y^\ell}\left(\tfrac{iy}{2}\right)^r\left(q-\tfrac{iy}{2}\right)^{n-r} e^{x\left(q-\frac{iy}{2}\right)} e^{yp}\right]_{x=y=0}$$

$$= \sum_{r=0}^{(\mathrm{Min}\, n,\ell)}\binom{n}{r}\left(\tfrac{i}{2}\right)^r\binom{\ell}{r} r!\left[\frac{\partial^k}{\partial x^k}\frac{\partial^{\ell-r}}{\partial y^{\ell-r}}\left(q-\tfrac{iy}{2}\right)^{n-r} e^{x\left(q-\frac{iy}{2}\right)} e^{yp}\right]_{x=y=0}$$

$$= \sum_{r=0}\binom{n}{r}\binom{\ell}{r} r!\left(\tfrac{i}{2}\right)^r\left[\frac{\partial^{k+n-r}}{\partial x^{k+n-r}}\cdot\frac{\partial^{\ell-r}}{\partial y^{\ell-r}} e^{x\left(q-\frac{iy}{2}\right)} e^{yp}\right]_{x=y=0}$$

$$= \sum_{r=0}^{(\mathrm{Min}\, n,\ell)}\binom{n}{r}\binom{\ell}{r} r!\left(\tfrac{i}{2}\right)^r S_y\left(q^{k+n-r} p^{\ell-r}\right)$$

Appendix B. Extension to the Case of a General Potential V(q).

We have discussed the quartic potential λq^4 as a concrete example. But our considerations are equally valid for a more general potential V(q), which can be written as $\sum_s \frac{\lambda_s}{s} q^s$,. We will only state the corresponding most important equations, without giving the calculations.

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

$$i\left[H, S_\gamma(q^k p^\ell)\right] = S_\gamma\left(p^{\ell+1}\frac{\partial}{\partial q} q^k\right) - \sum_{r=0} \left(-\frac{1}{4}\right)^r \frac{1}{(2r+1)!} S_\gamma\left(\frac{\partial^{2r+1}}{\partial p^{2r+1}} p^\ell q^k \frac{\partial^{2r+1}}{\partial q^{2r+1}} V(q)\right)$$

Taking the <i| |j> matrix element, we get for $V(q) = \sum_s \frac{\lambda_s}{s} q^s$

$$i\omega\tau(k|\ell) = k\tau(k-1|\ell+1) - \sum_s \lambda_s \sum_{r=0} \left(-\frac{1}{4}\right)^r \binom{\ell}{2r+1} s(s-1)\cdots(s-2r)\,\tau(k+s-2r+1|\ell-2r-1) \tag{3.1G}$$

The steps leading to (3.3) are similar here, and, in place of (4.4), we now have

$$\left.\begin{aligned} &\sum_s \left(1+\frac{2k}{s}\right)\lambda_s \tau(k+s-1|0) \\ &= \frac{\omega^2}{k+1}\tau(k+1|0) + 2k\,\overline{w}\cdot\tau(k-1|0) + \frac{k(k-1)(k-2)}{4}\tau(k-3|0) \end{aligned}\right\} \tag{4.4G}$$

For these general cases there appears one different feature which was not seen clearly in the case of λq^4. We will describe this, as an example, for the q^6 case. We obtain for this case, in place of (4.5) and (4.6) a form as

$$\tau(2n-1|0) = f_n^{(1)}(\omega,\overline{w})\,\tau(1|0) + f_n^{(3)}(\omega,\overline{w})\,\tau(3|0)\,, \quad n\geq 3$$

$$\tau(2n|0) = f_n^{(0)}(\omega,\overline{w})\,\delta_{ij} + f_n^{(2)}(\omega,\overline{w})\,\tau(2|0) + f_n^{(4)}(\omega,\overline{w})\,\tau(4|0), \quad n\geq 3$$

These five functions f are, so to say, input data and we have no equation to determine these within our framework. In the q^4 case we have relations to express $\tau(3|0)$ and $\tau(4|0)$, so that we have only 3 input functions $f^{(0)}$, $f^{(1)}$, $f^{(2)}$ there.

The Hartree-Fock self consistency method discussed in § 7a becomes, in case of $V(q) = \frac{\lambda}{2n} q^{2n}$,

$$H_{H.F.} = \frac{1}{2}\left\{p^2 + \left(\omega_0^2 + \frac{(2n)!}{2^n(n-1)!}\lambda\langle q^2\rangle^{n-1}\right)q^2\right\} - \left(\frac{n-1}{2n}\right)\frac{(2n)!}{2^n n!}\lambda\langle q^2\rangle^{2n} \qquad (7.1G)$$

The self consitency requirement is

$$\langle q^2\rangle = \langle 0_{H.F.}|q^2|0_{H.F.}\rangle = \frac{1}{2\sqrt{\omega_0^2 + \lambda\langle q^2\rangle^{n-1}\frac{(2n)!}{2^n n!}}} \qquad (7.3G)$$

and

$$E_{0,H.F.} = \frac{1}{8\langle q^2\rangle}\left(\frac{n+1}{n}\right) + \frac{\omega_0^2\langle q^2\rangle}{2}\left(\frac{n-1}{n}\right) \qquad (7.2G)$$

For the same Hamiltonian, Ritz's variation method with the same Gaussian trial function (7.4') gives us

$$E_0(a) = \frac{1}{8a} + \frac{\omega_0^2 a}{2} + \frac{\lambda}{2n}\frac{(2n)!}{2^n n!}\, a^n$$

$$E_0'(a) = 0 \longrightarrow \quad a_0 = 1/2\sqrt{\omega_0^2 + \lambda a_0^{n-1}\frac{(2n)!}{2^n n!}}$$

$$E_0(a_0) = \frac{1}{8a_0}\left(\frac{n+1}{n}\right) + \frac{\omega_0^2 a_0}{2}\left(\frac{n-1}{n}\right)$$

These expressions are, also in this case, identical with the Hartree-Fock method, since $\langle q^2 \rangle = a_0$

Now (5.4a), (5.4b), (5.4c) are independent of dynamics, namely valid for any V(q). They are just the sum rules. From (5.4a) on, however, they contain the specific dynamics of the system.

Now for $V(q) = \sum_s \frac{\lambda_s}{s}\, q^s$, the virial equation gives us

$$\Gamma_{ii} = \langle i | p^2 | i \rangle = \sum_s \lambda_s \langle i | q^s | i \rangle$$

$$\therefore \quad E_i = \frac{1}{2}\Gamma_{ii} + \sum_s \frac{\lambda_s}{s}\langle i | q^s | i \rangle = \left(\frac{1}{2} + \sum_s \frac{1}{s}\right)\Gamma_{ii} \equiv f\,\Gamma_{ii}$$

where we have put

$$f \equiv \frac{1}{2} + \sum_s \frac{1}{s} \,. \qquad (f = \tfrac{3}{4} \quad \text{for the quartic case})$$

The formulation leading to (8.3) can be repeated here and we arrive at

$$(i+1)\,\omega_{i+1,i} = \frac{2}{f}\,\omega_{i,i-1} + (i-1)\,\omega_{i-1,i-2}$$

or

$$A_n = \frac{1}{n+1}\left\{\frac{2}{f} + (n-1)\,\frac{1}{A_{n-1}}\right\} \qquad (8.3G)$$

where

$$A_n = \omega_{n+1,n} / \omega_{n,n-1}$$

Table 1. $A_n = \omega_{n+1,n}/\omega_{n,n-1}$ $(\lambda/\omega_o^3 >> 1)$

n	A_n	$A_n^{(e)}$	$A_n/A_n^{(e)}-1$
1	1.333333	1.334651	-0.000969
2	1.138889	1.145793	-0.006062
3	1.105691	1.102179	+0.003187
4	1.075980	1.077856	-0.001743
5	1.064034	1.063006	+0.000968
6	1.052252	1.052934	-0.000649
7	1.046090	1.045650	+0.000421
8	1.039805	1.040134	-0.000315
9	1.036041	1.035809	+0.000224

Comparison of our calculated A_n and the exact $A_n^{(e)}$. A_n are our calculated results from (8.5), which are obtained from our N.N.L. approximation eq. (8.2). $A_n^{(e)}$ is taken from the exact numerical results of reference 1.

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