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1977 J. Phys. A: Math. Gen. 10 1465

(http://iopscience.iop.org/0305-4470/10/9/008)

J. Phys. A: Math. Gen., Vol. 10, No. 9, 1977. Printed in Great Britain.

Double perturbation theory for the generator coordinate description of collective vibrations

Luc F F Lathouwers† and Richard L Lozes‡

†Dienst Teoretische en Wiskundige Natuurkunde, University of Antwerp (RUCA), Antwerp, Belgium

‡Department of Quantum Chemistry, University of Uppsala, Uppsala, Sweden

Received 5 April 1977

Abstract. A double perturbation theory for generator coordinate integral equations is developed. For the treatment of collective oscillations the well known harmonic approximation turns out to be a suitable unperturbed problem. A test calculation is performed on Lipkin's exactly solvable many body system.

1. Introduction

The generator coordinate method (Griffin and Wheeler 1957, Lathouwers 1975), as suggested by Griffin, Hill and Wheeler (GHW), is a microscopic theory of collective motion in many particle systems. Trial functions for the variational principle are written as superpositions of continuously labelled basis states

$$\psi(x)=\int f(\alpha)\Phi(x|\alpha)\,\mathrm{d}\alpha. \tag{1.1}$$

The intrinsic states $\Phi(x|\alpha)$ depend upon the particle coordinates x and contain a set of parameters or 'generator coordinates'. The variationally optimal weight functions $f(\alpha)$ must satisfy the GHW integral equation

$$\int (H(\alpha,\beta)-E\Delta(\alpha,\beta))f(\beta)\,\mathrm{d}\beta=0. \tag{1.2}$$

This equation does not belong to the classical types studied by Fredholm, Hilbert and Schmidt since it contains two Hermitian kernels

$$H(\alpha,\beta)=\int \Phi^*(x|\alpha)H\Phi(x|\beta)\,\mathrm{d}x, \qquad \Delta(\alpha,\beta)=\int \Phi^*(x|\alpha)\Phi(x|\beta)\,\mathrm{d}x. \tag{1.3}$$

Few equations of the type (1.2) are solvable. An interesting case in which an exact solution is possible occurs for the so called harmonic kernels

$$\begin{aligned}&\Delta(\alpha,\beta)=\mathrm{e}^{-\frac{1}{2}s(\alpha-\beta)^2}\\ &H(\alpha,\beta)=\Delta(\alpha,\beta)[E(0)+\tfrac{1}{2}s(B\alpha^2+2A\alpha\beta+B\beta^2)].\end{aligned} \tag{1.4}$$

The resulting spectrum is that of an harmonic oscillator; the corresponding eigenfunctions are also known

$$E_n = E(0) - \tfrac{1}{2}A + (n+\tfrac{1}{2})\Omega, \qquad \Omega = (A^2 - B^2)^{1/2},$$
$$f_n(\alpha) = N_n \, \mathrm{e}^{-sk\alpha^2/(s-k)} H_n\left[s\left(\frac{2k}{s-k}\right)^{1/2}\alpha\right] \tag{1.5}$$

where $k = 2s[(A+B)/(A-B)]^{1/2}$ and H_n are Hermite polynomials. This provides a good starting point for the description of collective oscillations. For a chosen intrinsic function containing parameters related to the vibrational properties of the system, one can fit the exact kernels to the harmonic ones, thus obtaining a collective excitation frequency Ω. This procedure is commonly referred to as the harmonic approximation (HA).

In order to include anharmonic effects one has to go beyond the HA. Several suggestions in this direction have been made. The most straightforward way is to discretise the GHW equation and reduce it to a matrix eigenvalue problem. There are however several drawbacks such as meshpoint dependence of the results, slow convergence of the eigenvalues and the rapid occurrence of approximate linear dependences due to strong non-orthogonality of the basis functions. Another method, which is a direct extension of the HA, is to expand the kernels to higher orders. The difficulty with this technique is that, whereas the HA is equivalent to a second-order differential equation, including higher powers gives rise to higher-order differential equations. These must then again be solved in an approximate way. In the following we propose to treat anharmonic effects by a generalised perturbation theory (PT) built on the HA as an unperturbed problem. An application and comparison with other methods is made for Lipkin's model.

2. Perturbation theory for generalised eigenvalue problems

We will consider, in general, the diagonalisation of a Hamiltonian in a non-orthogonal basis which leads to eigenvalue problems of the type

$$(H - E\Delta)f = 0. \tag{2.1}$$

These can be matrix equations of finite or infinite order or integral equations as in the GCM. For bound states (2.1) is supplemented with the boundary condition

$$\langle f|\Delta|f\rangle < +\infty \tag{2.2}$$

where the bracket denotes a double summation or integration over the basis state labels. Generalised eigenvalue problems of the type (2.1)+(2.2) also occur in other areas of theoretical physics and applied mathematics, e.g. matrix equations in statistics and differential equations arising from boundary perturbations in membrane theory. Perturbation theory for these problems has been considered by Kato (1966), however, under the restriction that (2.1) can be reduced to the classical form, i.e. only for overlap operators Δ which are invertible or whose negative square root exists. Here we present a straightforward generalisation of Rayleigh–Schrödinger PT both for perturbations in the dynamics (H) and the geometry (Δ) of the eigenvalue problem. We will emphasise the importance of inhomogeneous equations for the eigenfunction corrections and the connection between PT and the variational principle.

2.1. Single and double perturbation series

Assume that (2.1) can be solved in the form

$$(H_0 - E^0\Delta_0)f^0 = 0, \tag{2.3}$$

where H_0 and Δ_0 are unperturbed operators differing from H and Δ by the perturbations V and W

$$V = H - H_0, \qquad W = \Delta - \Delta_0. \tag{2.4}$$

The unperturbed (2.3) and perturbed (2.1) eigenvalue problems can be linked by introducing a coupling constant λ as

$$H(\lambda) = H_0 + \lambda V, \qquad \Delta(\lambda) = \Delta_0 + \lambda W. \tag{2.5}$$

Rayleigh–Schrödinger PT then consists in studying the solutions of the λ dependent eigenvalue problem

$$(H(\lambda) - E(\lambda)\Delta(\lambda))f(\lambda) = 0. \tag{2.6}$$

The classical approach is to expand $E(\lambda)$ and $f(\lambda)$ in power series of the coupling constant

$$\begin{aligned} E(\lambda) &= E^0 + \lambda E^1 + \lambda^2 E^2 + \ldots \\ E(\lambda) &= f^0 + \lambda f^1 + \lambda^2 f^2 + \ldots . \end{aligned} \tag{2.7}$$

In order for (2.7) to be meaningful it will be assumed that these series have a convergence radius of at least unity or can be summed in some other way (Padé approximants, Borel summations, ...). Substitution of the series in (2.1) and identification of λ powers leads to a set of inhomogeneous equations for the eigenfunction corrections

$$(H_0 - E^0\Delta_0)f^n = \sum_{k=1}^{n} (E^k\Delta_0 + E^{k-1}W)f^{n-k} - Vf^{n-1}. \tag{2.8}$$

Introducing the normalisation conventions

$$\langle f^0|\Delta_0|f^0\rangle = \langle f^0|\Delta_0|f\rangle = 1, \tag{2.9}$$

which implies that $\langle f^0|\Delta_0|f^n\rangle = 0$, one can determine the energy corrections by taking the scalar product to the left of (2.8) with f^0. The result reads

$$E^n = \langle f^0|V|f^{n-1}\rangle - \sum_{k=1}^{n} E^{k-1}\langle f^0|W|f^{n-k}\rangle \tag{2.10}$$

which for $n = 1$ gives

$$E^1 = \langle f^0|V|f^0\rangle - E^0\langle f^0|W|f^0\rangle. \tag{2.11}$$

Folklore tells us that the first-order correction equals the average of the perturbation with respect to the unperturbed state. Formula (2.11) confirms this statement for generalised eignevalue problems the perturbation being $V - E^0W$. In the general expression (2.10) the first term, being of pure dynamical nature, is a classical one, for $k = 1$ we have a geometrical contribution while for $k \neq 1$ the terms are of mixed character. One can study the interplay between dynamics and geometry in more detail

by a double PT. This consists in introducing different coupling constants μ and ν, for V and W respectively, and assuming double power series

$$\begin{aligned} E(\mu,\nu) &= E^0 + E^{1,0}\mu + E^{0,1}\nu + E^{2,0}\mu^2 + E^{1,1}\mu\nu + E^{0,2}\nu^2 + \dots \\ f(\mu,\nu) &= f^0 + f^{1,0}\mu + f^{0,1}\nu + f^{2,0}\mu^2 + f^{1,1}\mu\nu + f^{0,2}\nu^2 + \dots . \end{aligned} \tag{2.12}$$

Substitution in (2.1) leads to the inhomogeneous equations

$$(H_0 - E^0\Delta_0) f^{m,n} = \sum_{k=0}^{m}\sum_{l=1}^{n} (E^{k,l}\Delta_0 + E^{k,l-1}W) f^{m-k,n-l} + \sum_{k=1}^{m} E^{k,0}\Delta_0 f^{m-k,n} - V f^{m-1,n} \tag{2.13}$$

which, under the normalisation condition (2.9), give the energy corrections

$$E^{m,n} = \langle f^0 | V | f^{m-1,n} \rangle - \sum_{k=0}^{m}\sum_{l=1}^{n} E^{k,l-1} \langle f^0 | W | f^{m-k,n-l} \rangle . \tag{2.14}$$

Such a general term is of order m in V and n in W. The connection between the single and double PT series is easily established if one arranges the $E^{m,n}$ in the following way:

$$\begin{array}{ccccc} & & & E^{3,0} & \dots \\ & & E^{2,0} & & \\ & E^{1,0} & & E^{2,1} & \dots \\ E^0 & & E^{1,1} & & \\ & E^{0,1} & & E^{1,2} & \dots \\ & & E^{0,2} & & \\ & & & E^{0,3} & \dots \end{array} \tag{2.15}$$

Clearly the corrections arising from the single parameter case are obtained by summing the columns of equation (2.15). Notice, however, that the $E^{m,n}$ do not equal the individual contributions to (2.10). The classification, according to dynamics and geometry, introduced by double PT has definite advantages in cases where V and W are of different magnitude. Indeed if, e.g., $W \gg V$ the $E^{m,0}$ will decrease much more rapidly than the $E^{0,n}$. It will then be sufficient to sum over only part of the above tableau as indicated on figure 1.

3. Solution of inhomogeneous equations

Solving inhomogeneous equations arising from generalised eigenvalue problems is not more difficult than in the classical case. Indeed there exists no such thing as a generalised inhomogeneous equation. Hence, no modification of existing techniques (expansion methods, Green functions, ...) is necessary. For GHW integral equations this means that although the original equation is not of a common type the inhomogeneous equations are classical Fredholm equations of the first kind. The usual way to obtain workable expressions for energy corrections is to expand the eigenfunction corrections in the unperturbed eigenstates. With the normalisation convention (2.9) one obtains directly

$$f_i^n = \sum_{j\neq i} \frac{\langle f_j^0 | g_i^n \rangle f_j^0}{(E_j^0 - E_i^0)} \qquad f_i^{m,n} = \sum_{j\neq i} \frac{\langle f_j^0 | g_i^{m,n} \rangle f_j^0}{(E_j^0 - E_i^0)} \tag{3.1}$$

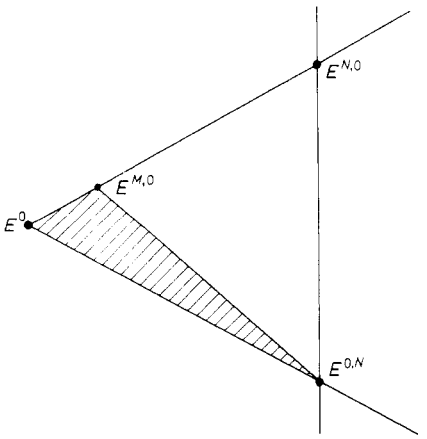

Figure 1. Effective part of the energy corrections $E^{m,n}$ which have to be summed in the case $W \gg V$. $M(N)$ denotes the number of terms after which the pure dynamical (geometrical) parts have converged.

where g_i^n and $g_i^{m,n}$ are the right-hand sides of (2.8) and (2.13). Explicit formulae for the second-order corrections are then easily derived from (2.14)

$$E_i^{2,0} = \sum_{j \neq i} \frac{|V_{ji}|^2}{(E_i^0 - E_j^0)} \tag{3.2}$$

$$E_i^{1,1} = -E_i^0 \sum_{j \neq i} \frac{2\,\mathrm{Re}(V_{ij} W_{ji})}{(E_i^0 - E_j^0)} - V_{ii} W_{ii} \tag{3.3}$$

$$E_i^{0,2} = (E_i^0)^2 \sum_{j \neq i} \frac{|W_{ji}|^2}{(E_i^0 - E_j^0)} + E_i^0 (W_{ii})^2 \tag{3.4}$$

$$E_i^2 = E_i^{2,0} + E_i^{1,1} + E_i^{0,2} \tag{3.5}$$

where

$$V_{ij} = \langle f_i^0 | V | f_j^0 \rangle \qquad W_{ij} = \langle f_i^0 | W | f_j^0 \rangle. \tag{3.6}$$

The derivation of higher-order terms presents no difficulties. The drawback of expansion techniques is the fact that the complete unperturbed spectrum and the corresponding eigenstates have to be known. In many cases this is not feasible. Additional problems can arise due to incompleteness of the basis sets, divergence of the series (3.1)–(3.4) and possible instability of the solutions due to inaccurate data for the inhomogeneous terms. There is therefore a definite need for more direct methods. Techniques for both differential and integral equations have been developed. For details we refer to Hirschfelder *et al* (1964) and Delves and Walsh (1974) respectively.

4. Extension of Wigner's theorem

As early as 1930 Hylleraas (1930) showed that the third-order energy correction in classical Rayleigh–Schrödinger PT can be expressed in terms of the first-order wavefunction correction only. Wigner (1935) extended this result and proved that the

Nth-order eigenfunction correction determines the energy up to and including order $2N+1$. Explicit formulae were derived by Dalgarno and Stewart (1956) and Dupont-Bourdelet *et al* (1960). The basis of Wigner's theorem, is the fact that the energy is a stationary quadratic functional. This is also true for generalised eigenvalue problems since

$$E = E(f) = \frac{\langle f|H|f\rangle}{\langle f|\Delta|f\rangle}. \tag{4.1}$$

If one now partitions the exact solution into a trial function and a corresponding error term

$$f = f_{\text{trial}} + \epsilon f_{\text{error}} \tag{4.2}$$

one has

$$E = E_{\text{trial}} + O(\epsilon^2). \tag{4.3}$$

Setting f_{trial} equal to the perturbation series up to and including the Nth-order term gives

$$\epsilon f_{\text{error}} = \sum_{n=N+1}^{\infty} \lambda^n f^n = \lambda^{N+1}(f^{N+1} + \lambda f^{N+2} + \ldots) \tag{4.4}$$

or $\epsilon = \lambda^{N+1}$. The energy is thus determined up to and including order $2N+1$ such that Wigner's theorem remains valid. The explicit formula can be derived, making repeated use of the inhomogeneous equations, by raising (lowering) the indices on the left- (right-) hand side functions in the scalar products contained in the energy corrections (2.10). The calculation is straightforward but rather tedious. Introducing the proper summations the result reads

$$E^{2n} = \langle f^{n-1}|V|f^n\rangle - \sum_{k=1}^{n-1}\sum_{l=n-k}^{2n-k-1} E^l\langle f^k|\Delta_0|f^{2n-k-l}\rangle - \sum_{k=0}^{n-1}\sum_{l=n-k}^{2n-k} E^{l-1}\langle f^k|W|f^{2n-k-l}\rangle \tag{4.5}$$

$$\begin{aligned} E^{2n+1} = {} & \langle f^n|V|f^n\rangle - \sum_{k=1}^{n}\sum_{l=n-k+1}^{2n-k} E^l\langle f^k|\Delta_0|f^{2n+1-k-l}\rangle \\ & - \sum_{k=0}^{n}\sum_{l=n-k+1}^{2n-k+1} E^{l-1}\langle f^k|W|f^{2n+1-k-l}\rangle. \end{aligned} \tag{4.6}$$

The formulae in the double parameter case can be derived in a similar way. They involve fourfold summations and will not be given here. The expressions (4.5) and (4.6) represent an important shortcut since they reduce the number of inhomogeneous equations to be solved by a factor of two.

5. Application to Lipkin's model

This model has been designed by Lipkin *et al* (1965) to test various types of random phase approximations and perturbation theories as applied to the many particle problem.

It consists of N particles distributed over two N-fold degenerate levels. These levels are distinguished by a label $\sigma = \pm 1$, and the degenerate states by a label p

($p = 1, \ldots, N$). The Hamiltonian of the system is

$$H = \tfrac{1}{2}\epsilon \sum_{p\sigma} \sigma a^{+}_{p\sigma} a_{p\sigma} + \tfrac{1}{2} S \sum_{pq\sigma} a^{+}_{p\sigma} a^{+}_{q\sigma} a_{q-\sigma} a_{p-\sigma}, \tag{5.1}$$

where ϵ is the separation between the two levels and S is the strength of the interaction.

Introducing the quasi-spin operators

$$\begin{aligned} J_{+} &= \sum_{p} a^{+}_{p+1} a_{p-1}, \\ J_{-} &= \sum_{p} a^{+}_{p-1} a_{p+1}, \\ J_{z} &= \tfrac{1}{2} \sum_{p\sigma} \sigma a^{+}_{p\sigma} a_{p\sigma}, \end{aligned} \tag{5.2}$$

the Hamiltonian is expressed as

$$H = \epsilon J_{z} + \tfrac{1}{2} S (J^{2}_{+} + J^{2}_{-}). \tag{5.3}$$

The operators J_{+}, J_{-} and J_{z} satisfy the commutation relations of angular momentum. The Hamiltonian commutes with total quasi-spin J^{2}. For a given number of particles the energy matrix breaks up into submatrices, corresponding to different angular momentum values, the largest one of which has $J = N/2$ and includes the ground state and the collective excited states of interest to this paper. For a full study of the symmetry properties of (5.1) we refer to Lipkin *et al* (1965).

The Hartree–Fock (HF) treatment of Lipkin's model has been studied extensively by Agassi (1966). For small interaction strengths the HF spectrum is equidistant and given by $-N\epsilon/2$, $-(N-1)\epsilon/2$, $-(N-2)\epsilon/2, \ldots$ while the HF ground state $|\mathrm{HF}\rangle$ has all the particles in the lower level. The exact spectrum shows anharmonicities which become more important as the interaction strength increases. The system exhibits collective oscillations in which anharmonicities are caused by correlation effects.

Following da Providencia *et al* (1971) we define the intrinsic states as

$$|\alpha\rangle = \exp(\alpha J_{z}) |\mathrm{HF}\rangle. \tag{5.4}$$

The GC space then includes the states contained in the above mentioned multiplet with $J = N/2$. The GCM, as considered here, is therefore exact and thus provides a good testing ground for approximation schemes. The kernels, for normalised intrinsic states (5.4), can easily be calculated

$$\begin{aligned} \Delta(\alpha, \beta) &= \frac{(1+\alpha\beta)^{N}}{(1+\alpha^{2})^{N/2}(1+\beta^{2})^{N/2}} \\ H(\alpha, \beta) &= \Delta(\alpha, \beta)\left(-\frac{N\epsilon}{2}\frac{(1-\alpha\beta)}{(1+\alpha\beta)} - \frac{N(N-1)S}{2}\frac{(\alpha^{2}+\beta^{2})}{(1+\alpha\beta)^{2}} \right). \end{aligned} \tag{5.5}$$

The minimum of the energy $E(\alpha) = H(\alpha, \alpha)$ occurs for $\alpha = 0$ if $\chi = (N-1)S/\epsilon < 1$. This defines the region of small interaction strengths to which we shall restrict ourselves. Expanding the kernels in Taylor series around $\alpha = 0$ one obtains the following expressions for the quantities appearing in the harmonic kernels (1.4):

$$\begin{aligned} s &= N \qquad & E(0) &= E_{\mathrm{HF}} = -\tfrac{1}{2} N\epsilon \\ A &= \epsilon \qquad & B &= -\epsilon\chi. \end{aligned} \tag{5.6}$$

These data are sufficient to apply the perturbation theory. The expansion formula can be used since the complete unperturbed spectrum and its eigenfunctions are known (1.5). The necessary matrix elements can be evaluated analytically (see Brändas and Laskowski 1975) or by a two-dimensional numerical integration. In the following tables 1–4 we have listed some results for the four lowest states. The values obtained by da Providencia via expansion of the kernels to fourth order are also given (anharmonic approximation) for the ground and first excited state. A dash in the PT results indicates that no numerical convergence was obtained. Both in the anharmonic model and in PT the results are better for a large particle number and worse for larger interaction strengths. The first phenomenon is due to the fact that the Gaussian overlap approxi-

Table 1. Results for the four lowest states using different methods. $N = 8$.

	Harmonic approximation	Anharmonic approximation	1st order PT	2nd order PT	Exact
$NS/\epsilon = 0{\cdot}4$					
E_0	4·032	4·037	4·035	4·035	4·035
E_1	3·095	3·085	3·078	3·078	3·078
E_2	2·158	—	2·087	2·078	2·075
E_3	1·221	—	1·108	—	1·044
$NS/\epsilon = 0{\cdot}6$					
E_0	4·074	4·082	4·080	4·081	4·081
E_1	3·223	3·167	3·173	3·174	3·174
E_2	2·372	—	2·185	—	2·162
E_3	1·521	—	1·226	—	1·093
$NS/\epsilon = 0{\cdot}8$					
E_0	4·143	4·139	4·145	4·146	4·146
E_1	3·429	3·258	3·289	—	3·305
E_2	2·715	—	2·275	—	2·254
E_3	2·001	—	1·337	—	1·126

Table 2. Results for the four lowest states using different methods. $N = 14$.

	Harmonic approximation	Anharmonic approximation	1st order PT	2nd order PT	Exact
$NS/\epsilon = 0{\cdot}4$					
E_0	7·036	7·038	7·038	7·038	7·038
E_1	6·107	6·098	6·096	6·096	6·096
E_2	5·179	—	5·128	5·124	5·123
E_3	4·250	—	4·152	4·131	4·126
$NS/\epsilon = 0{\cdot}6$					
E_0	7·085	7·088	7·088	7·088	7·088
E_1	6·254	6·214	6·218	6·219	6·219
E_2	5·424	—	5·280	5·275	5·273
E_3	4·594	—	4·325	4·289	4·274
$NS/\epsilon = 0{\cdot}8$					
E_0	7·165	7·159	7·162	7·164	7·163
E_1	6·496	6·363	6·376	6·403	6·393
E_2	5·826	—	5·438	5·515	5·475
E_3	5·157	—	4·481	4·571	4·467

Table 3. Results for the four lowest states using different methods. $N = 30$.

	Harmonic approximation	Anharmonic approximation	1st order PT	2nd order PT	Exact
$NS/\epsilon = 0{\cdot}4$					
E_0	15·039	15·040	15·040	15·040	15·040
E_1	14·117	14·111	14·111	14·111	14·111
E_2	13·195	—	13·166	13·165	13·165
E_3	12·272	—	12·211	12·205	12·204
$NS/\epsilon = 0{\cdot}6$					
E_0	15·092	15·094	15·094	15·094	15·094
E_1	14·278	14·256	14·257	14·258	14·258
E_2	13·463	—	13·378	13·378	13·378
E_3	12·649	—	12·472	12·463	12·461
$NS/\epsilon = 0{\cdot}8$					
E_0	15·183	15·178	15·179	15·179	15·179
E_1	14·549	14·468	14·469	14·484	14·480
E_2	13·915	—	13·649	13·701	13·684
E_3	13·281	—	12·767	12·876	12·819

Table 4. Results for the four lowest states using different methods. $N = 50$.

	Harmonic approximation	Anharmonic approximation	1st order PT	2nd order PT	Exact
$NS/\epsilon = 0{\cdot}4$					
E_0	25·040	25·041	25·041	25·041	25·041
E_1	24·120	14·117	24·116	24·116	24·116
E_2	23·200	—	23·182	23·182	23·182
E_3	22·280	—	22·240	22·237	22·237
$NS/\epsilon = 0{\cdot}6$					
E_0	25·096	25·096	25·096	25·096	25·096
E_1	24·287	24·272	24·273	24·273	24·273
E_2	23·478	—	23·422	23·422	23·422
E_3	22·669	—	22·548	22·545	22·545
$NS/\epsilon = 0.8$					
E_0	25·189	25·186	25·186	25·187	25·186
E_1	24·569	24·514	24·514	24·522	24·520
E_2	23·948	—	23·762	23·795	23·785
E_3	23·327	—	22·953	23·025	22·996

mation is better for large N. On the other hand for stronger interactions the anharmonicities in the spectrum increase such that the HA provides a less attractive starting point.

Comparing the quality of the results one can conclude that the anharmonic model gives results which are as good or slightly worse than first-order PT. Second-order PT is in all cases superior to the anharmonic model and removes anharmonicities which are as large as 30% of the average level spacing.

From the economical point of view PT is certainly preferable to higher-order boson expansions. The energy including first-order corrections can be written as

$$E^0 + \langle f^0|H|f^0\rangle - E^0\langle f^0|\Delta|f^0\rangle, \tag{5.7}$$

which necessitates the calculation of two two-dimensional integrals for each level. In the anharmonic model, giving comparable results, one first has to expand the kernels up to fourth order which, for realistic cases, can be rather laborious. In addition one has to solve a fourth-order differential eigenvalue problem, certainly a non-trivial task. Going to higher orders does not present any difficulty in PT since it merely amounts to calculating the double integrals $\langle f_m^0|H|f_n^0\rangle$ and $\langle f_m^0|\Delta|f_n^0\rangle$. In the anharmonic model however higher-order terms lead to higher-order differential equations such that the method becomes more and more difficult to apply. In addition it is clear that the process cannot be continued to infinity.

It is interesting to compare our results with those of PT starting out from the independent particle model. The main body PT in which S is the coupling constant has been carried out by Lipkin *et al* (1965). Their second- and fourth-order energies are comparable with our first- and second-order results. Thus by constructing a collective unperturbed problem via the GCM we have gained a factor of two in the order of the PT.

The fact that first-order PT already gives quite accurate results and that the second-order correction is almost negligible in many cases does not mean that the perturbations involved are small. This becomes clear if one calculates the corrections as given by double PT. In a typical case $N = 30$, $NS/\epsilon = 0{\cdot}6$ one finds the values given in table 5. The individual terms $E^{m,n}$ are thus quite large but if summed vertically in equation (2.15) they become almost negligible. We are thus in a case where both V and W are of the same strength. This is due to the fact that the overlap kernel appears as a multiplicative factor in the Hamiltonian kernel such that the effect of the Gaussian overlap is present in both the geometrical and dynamical perturbations.

Finally we want to discuss the limitation of our treatment. From (5.6) we see that as χ approaches unity B goes to $-A$. The collective excitation frequency will vanish for $\chi = 1$. It is well known that the HA simply breaks down at this point. Indeed for $B = -A$ it is clear that higher-order powers become important. Beyond $\chi = 1$ the energy has a maximum for $\alpha = 0$ and a minimum at $\pm\alpha_0$ with $\alpha_0^2 = (\chi - 1)/(\chi + 1)$. One can still perform the HA around $+\alpha_0$ or $-\alpha_0$, however, parity is then violated and the results are far less accurate (da Providência *et al* 1971). For these large interaction strengths ($\chi > 1$) the exact spectrum is no longer quasi-harmonic but consists of a number of parity doublets. It is therefore impractical (even unwise) to try to apply the HA in this region.

Table 5. Corrections given by double PT for a typical case $N = 30$, $NS/\epsilon = 0{\cdot}6$.

	$E^{2,0}$	$E^{1,1}$	$E^{0,2}$	E^2
E_0	−0·144	0·289	0·145	$-4{\cdot}8\times10^{-7}$
E_1	−0·551	1·120	−0·569	$-4{\cdot}9\times10^{-4}$
E_2	−1·222	2·512	−1·291	$9{\cdot}5\times10^{-5}$
E_3	—	—	—	$8{\cdot}3\times10^{-3}$

6. Discussion

We have developed PT for generalised eigenvalue problems up to a level common to PT for classical eigenvalue problems in most textbooks on quantum mechanics. The extension of Wigner's theorem allows one to calculate the eigenvalues up to and including order $2N+1$ at the expense of solving N inhomogeneous equations for the

eigenfunction corrections. Via double PT one can study the interplay between dynamical and geometrical perturbations. Open problems are the direct solution of inhomogeneous equations and the derivation of convergence theorems.

We have tested the theory as applied to the description of collective vibrations by the GCM. The harmonic approximation then provides a suitable unperturbed problem. The full unperturbed spectrum and its corresponding eigenfunctions are known such that expansion formulae can be applied. A calculation for Lipkin's model has shown that the method is qualitatively and economically superior to da Providência's boson expansions. The advantage of a collective unperturbed problem over PT starting out from the independent particle model seems to be a factor of two in the order of the PT.

One of the interesting aspects of the GCM is that several approximation schemes, such as the random phase approximation (RPA) (Jancovici and Schiff 1964) or the Hermitian operator method (HOM) (Bouten *et al* 1973), can be formulated as harmonic approximations for special choices of intrinsic states containing several generator coordinates. Since there is no problem in extending the above theory to several collective modes all these methods are possible candidates for unperturbed problems. The GCM thus provides a representation in which errors introduced by say RPA or HOM can be removed by PT. Whether the conclusions concerning the quality of our method remain valid for realistic systems is to be studied.

Acknowledgments

One of us (LFFL) would like to thank Professor P O Löwdin for hospitality extended to him at the Department of Quantum Chemistry, University of Uppsala.

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