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Quantum theory of anharmonic oscillators—a variational and systematic general approximation method

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Abstract. This is an investigation of the energy levels and wavefunctions of an anharmonic oscillator characterised by the potential $\frac{1}{2}\omega^2 q^2 + \lambda q^4$. As a lowest-order approximation an extremely simple formula for energy levels, $E_i^{(0)} = (i+\frac{1}{2})\frac{1}{4}(3/\alpha_i + \alpha_i)$, is derived ($i$ being the quantum number of the energy level), which covers any (λ, i). α_i is the real positive root of a cubic equation: $y_i\alpha_i^3 + \alpha_i^2 - 1 = 0$, with $y_i = 6\lambda(2i^2+2i+1)/(2i+1)$. This formula reproduces the exact energy levels within an error of about 1% for any (λ, i) (the worst case is 2% for $i = 0, \lambda \to \infty$). Systematically higher orders of 'our' perturbation theory are developed, which contains the 'usual' perturbation theory for the limiting case of small λ, but 'our' perturbation theory is valid for any (i, λ). 'Our' second-order perturbation theory reduces the errors of our lowest-order results by a factor of about $\frac{1}{5}$ in general. Various ranges (large, intermediate, small) of (i, λ) are investigated and compared with the exact values obtained by the Montroll group. For $i = 0, 1$, even 'our' fourth-order perturbation calculation can be elaborated explicitly, which reduces the error to about 0.01% for any λ. For small λ it gives correct numerical coefficients up to λ^4 terms, as it should.

1. Introduction and summary

The anharmonic oscillator model has played a tremendous role, because it is a most simple but nontrivial nonlinear problem. It occurs in the evolution of many branches of physics ranging from particle physics to molecular dynamics. For the relevance of this model to the various branches of physics we would like to refer to Hioe *et al* (1978, to be referred to as HMM). For this reason the Montroll group elaborated the detailed papers, Hioe *et al* (1978), Hioe and Montroll (1975), using a big computer facility. We will use these papers as a standard reference for comparison with our work, and will refer to their results as e.g. (HMM (1.18*b*)), meaning Hioe *et al* (1978), equation (1.18*b*) etc.

Our approach to the problem consists of some kind of variational approximation; the 'variational' parameter α_i is adjusted for each value of i and λ with a special combination $y_i = 6\lambda(2i^2+2i+1)/(2i+1)$. α_i is a root of (2.10). y_i is essentially 6Λ in the notation of HMM. In order to be applicable to more realistic problems, the method should be as simple as possible. Our method is simple enough, amounting to performing an appropriate scale transformation (or Bogoliubov transformation) corresponding to each given (λ, i). We decompose the canonical variables q and p into

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creation and annihilation operators by $q=(\alpha_i/2\omega)^{1/2}(b_i+b_i^+)$, $p=i^{-1}(\omega/2\alpha_i)^{1/2}(b_i-b_i^+)$. $\alpha_i=1$ corresponds to the 'usual' treatment. Expressing our total Hamiltonian through b_i and b_i^+, then after the performance of Wick ordering, the diagonal term with respect to $n_i=b_i^+b_i$ is defined as $H_i^{(0)}$ and the remaining nondiagonal term as $H_i^{(I)}$. The single 'variational' parameter α_i is determined such as to make $E_i^{(0)}$ obtained from $H_i^{(0)}$ an optimum, which will make $H_i^{(I)}$ small. $E_i^{(0)}$, obtained in this way, is given by the formula in the abstract, which covers fairly well *all ranges* of (i,λ). If we plot a graph of the energy levels using this formula, we get almost the same graph as given by (HMM figure 1). We cannot see any difference at this scale of the graphs. In order to see more clearly the accuracy of our results, we draw a graph of $R_i^{(0)}=E_i^{(0)}/E_i^{(e)}$ in figure 4, where i is the level number, (0) means our zeroth approximation results, and (e) means the exact values of HMM. In figure 4 we also draw $R_i^{(2)}=(E_i^{(0)}+E_i^{(2)})/E_i^{(e)}$, where (2) means 'our' second-order approximation results, which improves $R_i^{(0)}$ considerably.

Our $H_i^{(0)}$ is diagonal but nonlinear (containing n_i^2), and through our choice of α_i we extract out of the total Hamiltonian in a subtle way optimally nonlinear effects corresponding to each (i,λ). Our splitting into $H_i^{(0)}$ and $H_i^{(I)}$ is so differently and nicely done for each (i,λ) that, although our $H_i^{(I)}$ contains no small fixed parameter, its effects are always small for any range of (i,λ). Incidentally, through our choice of α_i, our $H_i^{(I)}$ have vanishing matrix elements $\langle 2|H_0^{(I)}|0\rangle$ and $\langle 3|H_1^{(I)}|1\rangle$, for any λ as will be shown in (5.2) and (5.4), which makes 'our' perturbation calculation especially simple for $i=0$ and $i=1$.

In § 2 we will explain our method of approximation sketched above, and § 3 contains the results for 'our' lowest-order approximation. From § 4 on, we will develop in a systematic way 'our' higher-order perturbation theory, treating $H_i^{(I)}$ as perturbation, which can be done, in principle, to any order. As we have emphasised above, $H_i^{(I)}$ does *not* contain any small fixed numerical coefficient, still effectively it is always small, as will be seen below. Section 4 contains 'our' second-order perturbation results $E_i^{(2)}$ †, which reduce to the 'usual' second-order perturbation theory in the special limiting case of small λ, while our formula (4.4) covers all ranges of (i,λ), including very large λ. It is fairly accurate also for the intermediate values of i or λ, as will be most clearly seen in figure 4 or table 4.

The cases $i=0$ and $i=1$ are especially simple, so we can even go to the fourth order of 'our' perturbation calculation. We do that in § 5 and it reduces the error to within 0.01% for any λ, so that in figure 4 $R_0^{(4)}$ and $R_1^{(4)}$ lie almost on the abscissa on this scale of graphs. For small λ, as shown in (5.16), they contain the well known usual perturbation coefficients up to the λ^4 term correctly. But our general formulae (5.12) and (5.17) are valid for any λ, including $\lambda\to\infty$.

In § 6 we discuss the small λ regime, based on 'our' second-order perturbation results (4.4) and arrive at (6.4), and, for large i with $(i\lambda)=\beta$ finite, at (6.5) which is equally good for small $\beta=\lambda i$ as the result of (HMM (1.18b)). (HMM (1.18b)) is not good for $\beta\geqslant 0.5$, while our (4.4) is good also for any β, as will be clearly seen in figure 5.

Section 7 contains a discussion of (4.4) for the large λ regime for $i\geqslant 2$ ($i=0,1$ have already been discussed in § 5). The results are (7.2), (7.3) and (7.4), whose

† We use the notational convention $E_i^{(j)}$, where i is the number of the energy level, and (j) is the order of 'our' perturbation theory. Thus, e.g., $E_0^{(4)}$ is the fourth-order correction of the zeroth state. We also use the convention $\bar{E}_i^{(2)}=E_i^{(0)}+E_i^{(2)}$, $\bar{E}_i^{(4)}=E_i^{(0)}+E_i^{(2)}+E_i^{(4)}$, $R_i^{(j)}=\bar{E}_i^{(j)}/E_i^{(e)}$, where $E_i^{(e)}$ are the exact values of HMM.

numerical accuracies are discussed in § 9. Section 8 contains a discussion of (4.4) for $i \to \infty$, with finite large and small $\beta = i\lambda$, and the results are our equation (8.3), which covers any β values quite well, contrary to (HMM (1.18b)) which is valid only for small β. Section 9 gives some numerical results. For the states $i = 0, 1$, our fourth approximation results based on (5.12) and (5.17) are summarised in tables 1 and 2, for various intermediate λ. We see that our formulae give excellent results also for such an intermediate regime of λ. For states $i \geqslant 2$, our numerical estimate for intermediate values of λ is based on our second approximation formula (4.4). The errors, as compared with the exact values, can be most clearly seen in figure 4. We summarise for $i = 2, 3, 8$ the numerical results in table 4. The $i = 8$ state is chosen as an example, for an intermediate i. As we will see below, almost all our calculations are algebraic; we never used integrations here, and only once differentiated in equation (2.7a). We reduced a difficult nonlinear differential equation's eigenvalue problem to an algebraic manipulation. Our most difficult task here is to solve the cubic equation (2.10). The calculations are really elementary, although for higher approximations the arithmetic becomes somewhat complicated. The numerical calculations are also very simple and almost all the numerical computation was done by the author on a desk computer.

Next we should mention something about the symmetry properties. As our total Hamiltonian has even parity (even function of p and q), any sensible approximation should not destroy this parity property. This means, in our case, that the state with $i =$ even (odd) should be an even (odd) state. Our approximation retains, of course, this symmetry property. So the $i = 1$ state is the lowest state of the $i =$ odd states, which is guaranteed to be orthogonal to the $i = 0$ state with even parity. This means that it is guaranteed that $E_0^{(0)} \geqslant E_0^{(e)}$ and $E_1^{(0)} \geqslant E_1^{(e)}$ due to the variational character of our zeroth-order approximation, but for other i and for higher approximations we have no guarantee whether our calculated values are larger or smaller than the exact values. (We will encounter this problem, for example, for $i = 8$. We see from figure 4 that $R_8^{(0)} < 1$ and $R_8^{(2)} > 1$.)

Lastly we want to discuss our wavefunctions. The lowest-order wavefunction corresponding to the eigenvalue $E_i^{(0)}$ is given by (3.3). It is just the usual Hermite function, only scaled appropriately by our α_i. We have not given the corresponding wavefunction for $E_i^{(2)}$, but it is quite easily constructed explicitly, if necessary, by a standard perturbation procedure using $H_i^{(I)}$ as perturbation. Our states are not orthogonal to each other, because they are based on differently scaled Hermite functions.

2. The method of approximation

Our anharmonic oscillator is characterised by the Hamiltonian

$$H = \tfrac{1}{2}(p^2 + \omega^2 q^2) + \lambda' q^4. \tag{2.1}$$

We have chosen units in which $\hbar = m = 1$. Let us substitute p and q by

$$q = (\alpha/2\omega)^{1/2}(b + b^+), \qquad p = i^{-1}(\omega/2\alpha)^{1/2}(b - b^+), \qquad [b, b^+] = 1, \tag{2.2}$$

where α is our characteristic variational parameter, which will play the central role in our approximation method and will be defined below. $\alpha = 1$ leads to the well known creation and annihilation operators a and a^+ of the simple harmonic oscillator. Inserting (2.2) into our Hamiltonian (2.1) and expressing H in terms of b and b^+, we

then arrange this into Wick's normal product ordering to obtain easily $H = H^{(0)} + H^{(I)}$,

$$\begin{aligned} H^{(0)}/\omega &= (1/4\alpha + \tfrac{1}{4}\alpha + \tfrac{3}{4}\lambda\alpha^2)(2n+1) + \tfrac{3}{2}\lambda\alpha^2 n^2, \\ H^{(I)}/\omega &= (-1/4\alpha + \tfrac{1}{4}\alpha + \tfrac{3}{2}\lambda\alpha^2)(b^2 + b^{+2}) + \tfrac{1}{4}\lambda\alpha^2(b^4 + 4nb^2 + 4b^{+2}n + b^{+4}), \end{aligned} \tag{2.3}$$

where

$$n \equiv b^+ b, \qquad \lambda \equiv \lambda'/\omega^3, \tag{2.4}$$

$H^{(0)}$ is the diagonal part and $H^{(I)}$ is the nondiagonal part of the total H, with respect to n. We define as usual

$$|i\rangle \equiv (1/\sqrt{i!})(b^+)^i|0\rangle \qquad (i = 1, 2, \ldots) \qquad b|0\rangle = 0 \tag{2.5}$$

and get

$$H^{(0)}|i\rangle = E_i^{(0)}(\alpha)|i\rangle \qquad \text{and} \qquad \langle i|H^{(I)}|i\rangle = 0 \tag{2.6}$$

where

$$E_i^{(0)}(\alpha)/\omega = (1/4\alpha + \tfrac{1}{4}\alpha + \tfrac{3}{4}\lambda\alpha^2)(2i+1) + \tfrac{3}{2}\lambda\alpha^2 i^2 \tag{2.7}$$†

and then

$$\partial E_i^{(0)}(\alpha)/\partial\alpha = (-1/4\alpha^2 + \tfrac{1}{4} + \tfrac{3}{2}\lambda\alpha)(2i+1) + 3\lambda\alpha i^2. \tag{2.7a}$$

Now we choose our α to optimise $E_i^{(0)}(\alpha)$, namely we define our α_i by

$$\partial E_i^{(0)}(\alpha)/\partial\alpha = 0 \to \alpha = \alpha_i$$

so

$$\alpha_i^3[6\lambda(2i^2 + 2i + 1)/(2i+1)] + \alpha_i^2 - 1 = 0. \tag{2.8}$$

For states $i \geqslant 2$ this type of variational determination of α_i may be questionable. We can justify our choice of α_i in the following way. For our Hamiltonian H, the virial theorem requires

$$\langle \tfrac{1}{2}p^2 \rangle = \langle \tfrac{1}{2}q^2 + 2\lambda q^4 \rangle$$

for any eigenstate of H. If we require this to be valid also for our approximate eigenstates $|i\rangle$, the above equation becomes

$$(1/4\alpha)(2i+1) = \tfrac{1}{4}\alpha(2i+1) + \tfrac{3}{2}\lambda\alpha^2(2i^2 + 2i + 1)$$

which is nothing else than (2.8).

Now define

$$\begin{aligned} y_i &\equiv 6\lambda(2i^2 + 2i + 1)/(2i+1) \equiv 6\bar{\Lambda}_i, \\ \bar{\Lambda}_i &\equiv \lambda(2i^2 + 2i + 1)/(2i+1) = (i + \tfrac{1}{2})\lambda[1 + \tfrac{1}{4}(i + \tfrac{1}{2})^{-2}] \\ &= \Lambda_i[1 + \tfrac{1}{4}(i + \tfrac{1}{2})^{-2}], \\ \Lambda_i &\equiv (i + \tfrac{1}{2})\lambda. \end{aligned} \tag{2.9}$$

Λ_i is the notation used in HMM. With this y_i our α_i is given by a solution of

$$y_i\alpha_i^3 + \alpha_i^2 - 1 = 0. \tag{2.10}$$

† From here on we put $\omega = 1$, without loss of generality.

This equation determines our variational parameter α_i in terms of y_i, which is a special combination of λ and i (the level number). y_i is essentially $6\Lambda_i$ of HMM, except for the factor $1+\frac{1}{4}(i+\frac{1}{2})^{-2}$, which plays some role for small i, but is practically one for large i. *In our approximation we choose α_i for each level i differently.* For fixed i we have only one special expansion parameter y_i, which can be small or large, corresponding to small or large λ, and our lowest approximation result $E_i^{(0)}$ depends only on α_i (equation (2.11), see below) which covers all ranges of λ.

With this α_i our $E_i^{(0)}$ becomes

$$E_i^{(0)}(\alpha_i) = \tfrac{1}{8}(2i+1)(3/\alpha_i + \alpha_i)$$

or (2.11)

$$\varepsilon_i^{(0)} \equiv E_i^{(0)}(\alpha)/(i+\tfrac{1}{2}) = \tfrac{1}{4}(3/\alpha_i + \alpha_i)$$

where α_i is defined as a real positive solution of the cubic equation (2.10). Equation (2.10) has three real solutions for $27y_i^2 < 4$. In this case we choose the positive root, which leads to $\alpha_i \to 1$ for $\lambda \to 0$, the correct usual perturbation calculation.

In summarising up to here, we have split our total H into a nonperturbed part $H_i^{(0)}$ and a perturbed part $H_i^{(I)}$, which are given by

$$\begin{aligned} H_i^{(0)} &= (1/4\alpha_i + \tfrac{1}{4}\alpha_i + \tfrac{3}{4}\lambda\alpha_i^2)(2n_i+1) + \tfrac{3}{2}\lambda\alpha_i^2 n_i^2, \\ H_i^{(I)} &= (-1/4\alpha_i + \tfrac{1}{4}\alpha_i + \tfrac{3}{2}\lambda\alpha_i^2)(b_i^2 + b_i^{+2}) + \lambda\alpha_i^2(n_i b_i^2 + b_i^{+2} n_i) + \tfrac{1}{4}\lambda\alpha_i^2(b_i^4 + b_i^{+4}) \end{aligned} \tag{2.12}$$

where $n_i = b_i^+ b_i$ is still *an operator*. Our $H_i^{(0)}$ is diagonal but nonlinear (containing n_i^2). We separate our total H into different parts $H_i^{(0)}$ and $H_i^{(I)}$ for each level i. (α_i is different for different i, defined by (2.10).)

Our b_i and b_i^+ are different for each level, and are given by

$$b_i = (\omega/2\alpha_i)^{1/2} q + i(\alpha_i/2\omega)^{1/2} p = \tfrac{1}{2}[(\alpha_i^{-1/2} + \alpha_i^{1/2})a + (\alpha_i^{-1/2} - \alpha_i^{1/2})a^+] \tag{2.13}$$

where a and a^+ are the usual creation and annihilation operators for the free harmonic oscillator. b_i^+ is the Hermitian conjugate of b_i. Thus $[b_i, b_j] \neq 0$ for $i \neq j$. Looking at (2.13), our method amounts to performing different Bogoliubov transformations for each i and λ †.

In our approximation method we attack each level separately. For fixed i, α_i is still adjusted for different λ. Thus choosing our best α_i as a solution of (2.10), our method amounts to performing a perturbation procedure by treating $H_i^{(0)}$ as the unperturbed part and $H_i^{(I)}$ as perturbation. As we will see below, $H_i^{(I)}$ is always small compared with $H_i^{(0)}$, but does *not* contain any small parameter of fixed value, so that our method is valid for all ranges of $0 < \lambda < \infty$ and $0 \leq i < \infty$, with one *simple analytic formula.*

3. The lowest-order approximation for arbitrary λ and i

The lowest-order approximation is to neglect $H_i^{(I)}$ and retain only $H_i^{(0)}$. Then the results are already given in § 2, namely

$$\varepsilon_i^{(0)} \equiv E_i^{(0)}/(i+\tfrac{1}{2}) = \tfrac{1}{4}(3/\alpha_i + \alpha_i) \tag{3.1}$$

† I am indebted to H Mitter for pointing out this fact.

where α_i is the positive real root of

$$y_i\alpha_i^3 + \alpha_i^2 - 1 = 0 \tag{3.2}$$

where

$$y_i = 6\lambda[(2i^2+2i+1)/(2i+1)].$$

We give $\varepsilon_i^{(0)}$ and α_i as a function of y_i in figures 1, 2 and 3. Figure 2 demonstrates the accuracy of our lowest-order result $\varepsilon_i^{(0)}$ for the small y_i region.

If we calculate energy levels for $i = 0, 1, 2, \ldots, 8$ as functions of λ from (3.1), and plot a curve, then we obtain quite a similar graph to that in (HMM, figure 1), and we cannot see any difference at this scale of graphs. In order to see the errors of our approximation we give a graph of the ratio $R_i^{(0)} = E_i^{(0)}/E_i^{(e)}$ ($i = 0, 1, 2, 3$ and 8) as a function of λ in figure 4, where $E_i^{(0)}$ are our calculated values obtained from (3.1), and $E_i^{(e)}$ are the exact values given by Hioe and Montroll (1975). The superscript (0) means the lowest approximation values. In figure 4 we also give the values obtained by our second approximation shown by a dotted curve $R_i^{(2)}$ with superscript (2). As we will see from figure 4, our $R_i^{(0)}$ has at most an error of 2% (for $i = 0, 1$; $\lambda \gg 1$)

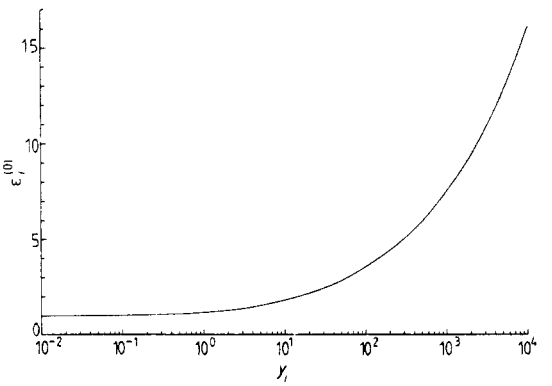

Figure 1. Our lowest-order energy value $\varepsilon_i^{(0)} = E_i^{(0)}/(i+\frac{1}{2})$ of (3.1) as a function of $y_i = 6\lambda(2i^2+2i+1)/(2i+1)$ on a logarithmic scale.

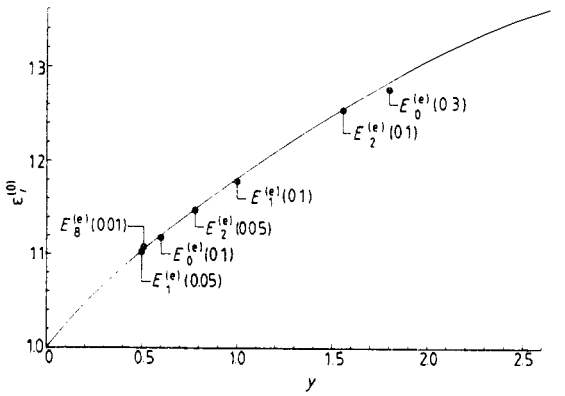

Figure 2. Our $\varepsilon_i^{(0)}$ of (3.1) for small y_i and some exact values; $E_i^{(e)}$ (0.1) means $E_i^{(e)}$ for $\lambda = 0.1$, for example.

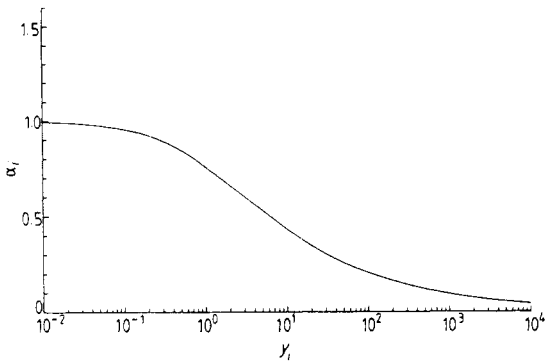

Figure 3. Our characteristic variational parameter α_i as a function of $y_i = 6\lambda(2i^2+2i+1)/(2i+1)$ on a logarithmic scale.

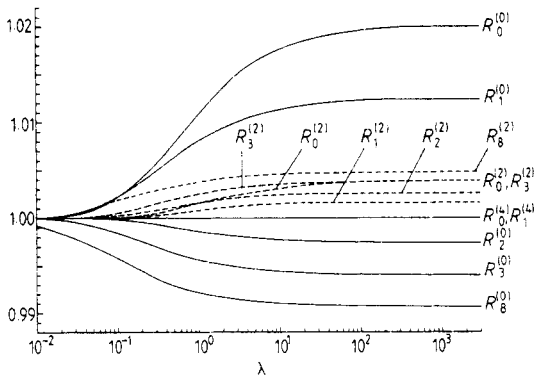

Figure 4. Ratio $R_i^{(j)} = \bar{E}_i^{(j)}/E_i^{(e)}$ as function of λ, where (j) represents the order of our approximation, and $E_i^{(e)}$ are the exact values, taken from Hioe and Montroll (1975).

and the error is usually less than 1% ($0.99 < R_i^{(0)} < 1.01$) for almost every value of i and λ. (As we will see in § 8, this is true even for $i \gg 1$, namely in the WKB region.)

As our approach is variational, it is guaranteed that $R_0^{(0)}$ and $R_1^{(0)}$ are larger than 1, while the $R_i^{(0)}$ ($i \geq 2$) are not necessarily larger than 1, because our excited levels are not orthogonal to the lower levels. The fact that $R_1^{(0)}$ is larger than 1 comes from the symmetry property of our total H: since H is an even function of q and p, the ground state is an even function while the first excited state is an odd function, and our approximation does not destroy this symmetry.

The corresponding states are given by

$$|i^{(0)}\rangle = (1/\sqrt{i!})(b_i^+)^i|0\rangle.$$

Thus the wavefunctions in the q-representation are the usual Hermite polynomials, but appropriately scaled by α_i:

$$\psi_i^{(0)}(q) \equiv \langle q|i^{(0)}\rangle = \left(\frac{\omega}{\pi\alpha_i}\right)^{1/4} \frac{1}{(2^i i!)^{1/2}} H_i\left(\left(\frac{\omega}{\alpha_i}\right)^{1/2} q\right) \exp\left(-\frac{\omega}{2\alpha_i} q^2\right). \tag{3.3}$$

4. The second-order perturbation due to $H_i^{(I)}$ for arbitrary λ and i

The first-order perturbation due to $H_i^{(I)}$ is zero, as was shown in (2.6): $\langle i|H_i^{(I)}|i\rangle = 0$.

The second-order perturbation is given by

$$\begin{aligned}
E_i^{(2)} &= \langle i|H_i^{(I)}(E_i^{(0)} - H_i^{(0)}(n))^{-1}H_i^{(I)}|i\rangle \\
&= (1/i!)(\tfrac{1}{4}\lambda\alpha_i^2)^2[\langle 0|b^{i+4}(E_i^{(0)} - H_i^{(0)}(n=i+4))^{-1}(b^+)^{i+4}|0\rangle \\
&\quad + \langle 0|b^i(b^+)^4(E_i^{(0)} - H_i^{(0)}(n=i-4))^{-1}b^4(b^+)^i|0\rangle] \\
&\quad + (1/i!)(-(4\alpha_i)^{-1} + \tfrac{1}{4}\alpha_i + \tfrac{3}{2}\lambda\alpha_i^2 + i\lambda\alpha_i^2)^2 \\
&\quad \times \langle 0|b^{i+2}(E_i^{(0)} - H_i^{(0)}(n=i+2))^{-1}(b^+)^{i+2}|0\rangle \\
&\quad + (1/i!)(-(4\alpha_i)^{-1} + \tfrac{1}{4}\alpha_i + \tfrac{3}{2}\lambda\alpha_i^2 + (i-2)\lambda\alpha_i^2)^2 \\
&\quad \times \langle 0|b^i(b^+)^2(E_i^{(0)} - H_i^{(0)}(n=i-2))^{-1}b^2(b^+)^i|0\rangle \\
&= \left(\frac{\lambda\alpha_i^2}{4}\right)^2\left(\frac{(i+4)(i+3)(i+2)(i+1)}{E_i^{(0)} - H_i^{(0)}(n=i+4)} + \frac{i(i-1)(i-2)(i-3)}{E_i^{(0)} - H_i^{(0)}(n=i-4)}\right) + (4\alpha_i)^{-2} \\
&\quad \times\{(i+2)(i+1)[-1+\alpha_i^2+2\lambda\alpha_i^3(2i+3)]^2(E_i^{(0)} - H_i^{(0)}(n=i+2))^{-1} \\
&\quad + i(i-1)[-1+\alpha_i^2+2\lambda\alpha_i^3(2i-1)]^2(E_i^{(0)} - H_i^{(0)}(n=i-2))^{-1}\}. \qquad (4.1)
\end{aligned}$$

Using the relation for α_i given by (2.10), and y_i given in (2.9), we obtain after some elementary algebra

$$\begin{aligned}
E_i^{(2)} &= \left(\frac{1-\alpha_i^2}{\alpha_i}\frac{1}{6(2i^2+2i+1)}\right)^2 \\
&\quad \times\left[\left(\frac{2i+1}{4}\right)^2\left(\frac{(i+4)(i+3)(i+2)(i+1)}{E_i^{(0)} - H_i^{(0)}(n=i+4)} + \frac{i(i-1)(i-2)(i-3)}{E_i^{(0)} - H_i^{(0)}(n=i-4)}\right)\right. \\
&\quad \left. + (i+2)(i+1)i(i-1)\left(\frac{i(i-1)}{E_i^{(0)} - H_i^{(0)}(n=i+2)} + \frac{(i+2)(i+1)}{E_i^{(0)} - H_i^{(0)}(n=i-2)}\right)\right] \qquad (4.2)
\end{aligned}$$

while

$$\begin{aligned}
V_i(k) &\equiv E_i^{(0)} - H_i^{(0)}(n=i+k) \\
&= -\left(\frac{1}{4\alpha_i} + \frac{\alpha_i}{4} + \frac{3\lambda\alpha_i^2}{4}\right)(2k) - \frac{3\lambda\alpha_i^2}{2}[(i+k)^2 - i^2] \\
&= -\frac{k}{4\alpha_i}\frac{1}{(2i^2+2i+1)}[8i^2+2i(k+4)+(k+3)-(2ki+k-1)\alpha_i^2] \qquad (4.3)
\end{aligned}$$

(k can be negative also) and we finally get

$$\begin{aligned}
E_i^{(2)} &= \left(\frac{1-\alpha_i^2}{6}\right)^2\frac{1}{\alpha_i(2i^2+2i+1)} \\
&\quad \times\left[\left(\frac{2i+1}{4}\right)^2\left(-\frac{(i+4)(i+3)(i+2)(i+1)}{8i^2+16i+7-\alpha_i^2(8i+3)} + \frac{i(i-1)(i-2)(i-3)}{8i^2-1+\alpha_i^2(8i+5)}\right)\right.
\end{aligned}$$

$$+2(i+2)(i+1)i(i-1)$$
$$\times\left(-\frac{i(i-1)}{8i^2+12i+5-\alpha_i^2(4i+1)}+\frac{(i+2)(i+1)}{8i^2+4i+1+\alpha_i^2(4i+3)}\right)\Bigg]. \tag{4.4}$$

Thus our second-order perturbation results are given by $\bar{E}_i^{(2)}=E_i^{(0)}+E_i^{(2)}$, where $E_i^{(0)}$ is given by (3.1). This expression has some resemblance to (HMM (1.17)), because they are related by a similar calculational way. But they are not the same, and above all (HMM (1.17)) is valid only for small λ, while our results are valid for arbitrary λ. The two expressions deviate at about $\beta\sim 1$, as will be clearly seen from the graph of figure 5.

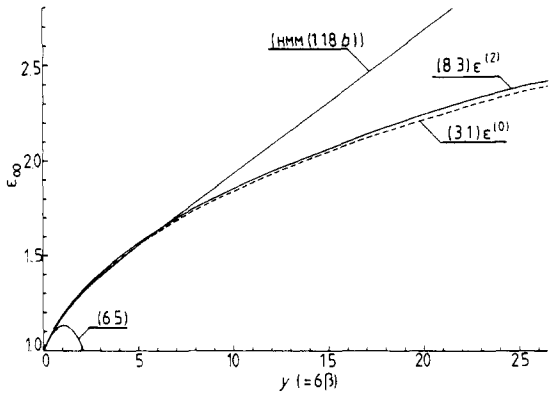

Figure 5. Comparison of various $\varepsilon_i=E_i/(i+\frac{1}{2})$ for very large i, finite $\beta=i\lambda$. Equation (6.3) is good only for small β; (HMM, (1.18b)) is better, but it becomes proportional to $y(\equiv 6\beta)$ for large β. Our formulae for $\varepsilon_i^{(0)}$ ((3.1)) and $\varepsilon_i^{(2)}$ ((8.3)) deviate at about $\beta=1$ ($y=6$) from (HMM (1.18b)) and are valid for intermediate *and* large β.

As we see from the graphs of figure 4, $|(\bar{E}_i^{(2)}-E_i^{(e)})/E_i^{(e)}|$ are usually less than 0.01 for all ranges of λ and i, and furthermore $E_i^{(2)}$ has the correct sign and magnitude to reduce the error of $E_i^{(0)}$ by a factor of about $\frac{1}{5}$.

As we have already remarked in § 3, we always have $R_0^{(0)}\geqslant 1$ and $R_1^{(0)}\geqslant 1$, while, as we may easily see from (4.4), if we put $i=0$ or $i=1$ there, $E_0^{(2)}<0$ and $E_1^{(2)}<0$, so our second approximation gives $R_i^{(0)}\equiv E_i^{(0)}/E_i^{(e)}>\bar{E}_i^{(2)}/E_i^{(e)}\equiv R_i^{(2)}$ for $i=0,1$. But from the beginning it is not guaranteed that $R_i^{(2)}\geqslant 1$ for $i=0,1$; only after numerical calculations did we find this to be the case.

Similarly for $i\geqslant 2$, generally speaking we are not sure whether $R_i^{(0)}$ is larger or smaller than 1, and $R_i^{(2)}$ is nearer to 1 than $R_i^{(0)}$. Only after numerical calculations do we see that this is really the case for all ranges of λ and i (even for $i\to\infty$).

5. The fourth-order perturbation due to $H_i^{(I)}$, for the ground ($i=0$) and first excited ($i=1$) states for arbitrary λ

We may continue 'our' perturbation calculation due to $H_i^{(I)}$ systematically to higher orders, but in full generality this would become much more complicated and the numerical improvements are expected to be quite small, which will be shown below

to be true. So we will concentrate in this section only on the ground and the first excited states ($i=0, 1$), but still leave λ arbitrary.

The calculations of states with $i=0, 1$ are especially simple, as can be seen in formula (4.4) of § 4. In (4.4), for $i=0, 1$, only the first term of the four terms in [. . .] survives, which originates from b^4 and b^{+4} in $H_0^{(I)}$ and $H_1^{(I)}$. This is due to our choice of α_0 and α_1, namely

$$[-(4\alpha_0)^{-1}+\tfrac{1}{4}\alpha_0+\tfrac{3}{2}\lambda\alpha_0^2]=0 \qquad \text{for any } \lambda,$$

since $y_0=6\lambda$ (see (2.9)). Then the coefficient of the $(b_0^2+b_0^{+2})$ term of $H_0^{(I)}$ is zero. Hence our $H_0^{(I)}$ becomes simply

$$\begin{aligned} H_0^{(I)} &= \tfrac{1}{4}\lambda\alpha_0^2(b_0^4+4n_0b_0^2+4b_0^{+2}n_0+b_0^{+4}) \\ &= [(1-\alpha_0^2)/(24\alpha_0)](b_0^4+4n_0b_0^2+4b_0^{+2}+b_0^{+4}). \end{aligned} \tag{5.1}$$

Hence clearly

$$\left.\begin{aligned} &H_0^{(I)}|0\rangle=\tfrac{1}{4}\lambda\alpha_0^2b_0^{+4}|0\rangle\sim|4\rangle, \\ \text{i.e.}\quad &\\ &\langle 2|H_0^{(I)}|0\rangle=\langle 0|H_0^{(I)}|2\rangle=0 \qquad \text{for any } \lambda \end{aligned}\right\} \tag{5.2}$$

identically. This makes our calculation for the ground state ($i=0$) especially simple.

For the $i=1$ state we have $y_1=10\lambda$ so we have

$$[-(4\alpha_1)^{-1}+\tfrac{1}{4}\alpha_1+\tfrac{3}{2}\lambda\alpha_1^2]=-\lambda\alpha_1^2$$

and

$$H_1^{(I)}=-\lambda\alpha_1^2(b_1^2+b_1^{+2})+\tfrac{1}{4}\lambda\alpha_1^2(b_1^4+4n_1b_1^2+4b_1^{+2}n_1+b_1^{+4}).$$

This time the coefficient of $(b_1^2+b_1^{+2})$ does not vanish, but we can write

$$\begin{aligned} H_1^{(I)} &= (\lambda\alpha_1^2/4)[b_1^4+(b_1^+)^4+4(n_1-1)b_1^2+4b_1^{+2}(n_1-1)] \\ &= [(1-\alpha_1^2)/40\alpha_1][b_1^4+(b_1^+)^4+4(n_1-1)b_1^2+4b_1^{+2}(n_1-1)] \end{aligned} \tag{5.3}$$

and we see

$$b_1^{+2}(n_1-1)|1\rangle=0$$

so that

$$\left.\begin{aligned} &H_1^{(I)}|1\rangle=(\lambda\alpha_1^2/4)(b_1^+)^4|1\rangle\sim|5\rangle, \\ \text{and therefore}\quad &\\ &\langle 3|H_1^{(I)}|1\rangle=\langle 1|H_1^{(I)}|3\rangle=0 \qquad \text{for any } \lambda. \end{aligned}\right\} \tag{5.4}$$

The first excited state, $i=1$, is also simple, which is the lowest state with odd parity.

For states $i\geqslant 2$, the situation is much more complicated as can be seen already from the second-order calculation of § 4 and formula (4.4).

The properties (5.2) and (5.4) guarantee that the third-order perturbations are zero, since

$$\langle 0|H_0^{(I)}H_0^{(I)}H_0^{(I)}|0\rangle\sim\langle 4|H_0^{(I)}|4\rangle=0, \qquad \langle 1|H_1^{(I)}H_1^{(I)}H_1^{(I)}|1\rangle\sim\langle 5|H_1^{(I)}|5\rangle=0. \tag{5.5}$$

On the other hand this is generally not the case for $i\geqslant 2$, as for example

$$\langle 2|H_2^{(I)}H_2^{(I)}H_2^{(I)}|2\rangle\sim\langle 2|H_2^{(I)}H_2^{(I)}|0\rangle\sim\langle 2|H_2^{(I)}|4\rangle\neq 0. \tag{5.6}$$

By the same reasoning, for the states $i=0, 1$ the fifth-order perturbations are not zero, as for example

$$\langle 0|H_0^{(I)}H_0^{(I)}H_0^{(I)}H_0^{(I)}H_0^{(I)}|0\rangle \sim \langle 4|H_0^{(I)}H_0^{(I)}H_0^{(I)}|4\rangle \sim \langle 8|H_0^{(I)}|6\rangle \neq 0$$

since $H_0^{(I)}$ contains $b_0^{+2}n_0$, which brings $|4\rangle \to |6\rangle$.

With these preliminary remarks let us now begin our fourth-order perturbation calculation for $i=0$ and $i=1$. For $i=0, 1$ we have

$$H_0^{(0)}(n_0) = (4\alpha_0)^{-1}[(3+\alpha_0^2)(n_0+\tfrac{1}{2})+(1-\alpha_0^2)n_0^2], \tag{5.7}$$

$$H_1^{(0)}(n_1) = (20\alpha_1)^{-1}[(13+7\alpha_1^2)(n_1+\tfrac{1}{2})+3(1-\alpha_1^2)n_1^2], \tag{5.8}$$

and, as in (4.3),

$$V_i(k) \equiv E_i^{(0)} - H_i^{(0)}(n=i+k) = H_i^{(0)}(n=i) - H_i^{(0)}(n=i+k),$$

$$V_0(k) = -(k/4\alpha_0)[3+k-\alpha_0^2(k-1)], \tag{5.9}$$

$$V_1(k) = -(k/20\alpha_1)[19+3k-\alpha_1^2(3k-1)]. \tag{5.10}$$

We will explicitly carry out the calculation for $i=0$, but for $i=1$ we will state only the results.

The standard perturbation theory gives us

$$E_0^{(4)} = \langle 0|H_0^{(I)}(E_0^{(0)}-H_0^{(0)})^{-1}[H_0^{(I)}P(E_0^{(0)}-H_0^{(0)})^{-1}H_0^{(I)} - \langle 0|H_0^{(I)}(E_0^{(0)}-H_0^{(0)})^{-1}H_0^{(I)}|0\rangle](E_0^{(0)}-H_0^{(0)})^{-1}H_0^{(I)}|0\rangle$$

where

$$P \equiv 1 - |0\rangle\langle 0|$$

is the projection operator onto the non $|0\rangle$ states. From (5.2) we get

$$\begin{aligned} E_0^{(4)} &= |\langle 0|H_0^{(I)}|4\rangle|^2(V_0(4))^{-2}[\langle 4|H_0^{(I)}P(E_0^{(0)}-H_0^{(0)})^{-1}H_0^{(I)}|4\rangle - E_0^{(2)}) \\ &= |\langle 0|H_0^{(I)}|4\rangle|^2(V_0(4))^{-2}\left(\sum_{k=2,6,8}|\langle 4|H_0^{(I)}|k\rangle|^2(V_0(k))^{-1} - E_0^{(2)}\right) \end{aligned} \tag{5.11}$$

where $E_0^{(2)}$ is given by (4.4) with $i=0$, namely

$$E_0^{(2)} = |\langle 0|H_0^{(I)}|4\rangle|^2(V_0(4))^{-1},$$

in this notation. $V_0(k)$ is given in (5.9) and

$$\langle 0|H_0^{(I)}|4\rangle = (1/\sqrt{4!})[(1-\alpha_0^2)/24\alpha_0]\langle 0|b_0^4 b_0^{+4}|0\rangle = \sqrt{4!}[(1-\alpha_0^2)/24\alpha_0]$$

etc. So after some calculation we arrive at

$$E_0^{(4)} = -\frac{(1-\alpha_0^2)^4}{72\alpha_0}\frac{1}{(7-3\alpha_0^2)^2}\left(\frac{8}{5-\alpha_0^2}+\frac{80}{3(9-5\alpha_0^2)}+\frac{35}{8(11-7\alpha_0^2)}-\frac{1}{8(7-3\alpha_0^2)}\right). \tag{5.11a}$$

So our fourth-order final result for $i=0$ and arbitrary λ is given by

$$\left.\begin{aligned} &\bar{E}_0^{(4)} = E_0^{(0)} + E_0^{(2)} + E_0^{(4)} \\ &\text{where } E_0^{(4)} \text{ is given by (5.11}a\text{) and} \\ &E_0^{(0)} = \tfrac{1}{8}(3/\alpha_0+\alpha_0), \\ &E_0^{(2)} = -[(1-\alpha_0^2)^2/24\alpha_0](7-3\alpha_0^2)^{-1} \end{aligned}\right\} \tag{5.12}$$

and α_0 is the positive real root of

$$6\lambda\alpha_0^3+\alpha_0^2-1=0.$$

This formula covers all ranges of λ, and the worst case $\lambda\to\infty$ gives only a 0.01% error compared with the exact numerical results obtained in Hioe and Montroll (1975). As can be seen from our figure 4, if we tolerated a maximum error of 0.4%, then the much simpler formula $E_0^{(0)}+E_0^{(2)}$ of § 4 is sufficient for our purposes. And even our extremely simple formula $E_0^{(0)}$ covers all ranges of λ within a maximum error of 2%, as we can clearly see from figure 4. A more detailed numerical comparison in the intermediate λ region will be given in table 1.

Let us first discuss the case $\lambda\gg 1$. We get for the leading terms

$$\bar{E}_4^{(0)}=E_0^{(0)}+E_0^{(2)}+E_0^{(4)}=0.668\,0582\lambda^{1/3}+0.143\,468\lambda^{-1/3}+\ldots. \tag{5.13}$$

This should be compared with the exact values (cf HMM, table 1)

$$E_0^{(e)}=0.667\,9826\lambda^{1/3}+0.143\,67\lambda^{-1/3}+\ldots.$$

Next let us discuss the case of λ being small. For λ small our α_0 is given by

$$\alpha_0=1-3\lambda+\tfrac{5}{2}(3\lambda)^2-8(3\lambda)^3+\tfrac{231}{8}(3\lambda)^4+\ldots \tag{5.14}$$

and our $H_0^{(I)}$ contains as a factor $\lambda\alpha_0^2$ (see (5.1)). If we perform the lth order of 'our' perturbation theory, we neglect only terms of order λ^{l+1} so that our formula should give the correct usual perturbation result up to order λ^l. This means, our $E_0^{(0)}$ gives the correct λ^0 and λ^1 coefficients (because $E_0^{(1)}=0$), $E_0^{(0)}+E_0^{(2)}$ goes up to λ^3 (because $E_0^{(3)}=0$), $E_0^{(0)}+E_0^{(2)}+E_0^{(4)}$ gives the correct coefficients up to λ^4 (because $E_0^{(5)}\neq 0$). We will show that this is really the case, and this fact will also guarantee that we are on the right track. If we systematically expand our formulae for small λ, using (5.14), we get

$$\begin{aligned}
E_0^{(0)}&=\tfrac{1}{2}+\tfrac{1}{4}(3\lambda)-\tfrac{1}{4}(3\lambda)^2+\tfrac{1}{2}(3\lambda)^3-\tfrac{21}{16}(3\lambda)^4+\ldots,\\
E_0^{(2)}&=-\tfrac{1}{24}(3\lambda)^2+\tfrac{13}{48}(3\lambda)^3-\tfrac{49}{32}(3\lambda)^4+\ldots, \qquad (5.15)\\
E_0^{(4)}&=-\tfrac{467}{3456}(3\lambda)^4+\ldots,
\end{aligned}$$

$$\bar{E}_0^{(4)}=\tfrac{1}{2}+\tfrac{3}{4}\lambda-\tfrac{21}{8}\lambda^2+\tfrac{333}{16}\lambda^3-\tfrac{30885}{128}\lambda^4+\ldots, \tag{5.16}$$

which reproduce the well known correct numerical coefficients given for example by Bender and Wu (1969, 1973) up to λ, λ^3 and λ^4, respectively, for $E_0^{(0)}$, $\bar{E}_0^{(2)}$ and $\bar{E}_0^{(4)}$, as was argued above. This means that our formulae cover also the weak coupling ($\lambda\ll 1$) region quite satisfactorily, as they should. But our formula (5.12) covers *all ranges of* λ with quite small error. As was already remarked above, since $E_0^{(5)}$ is not zero, we cannot get the correct λ^5 coefficient if we expand (5.12). The fact that our $E_0^{(0)}+E_0^{(2)}$ gives the correct λ^3 coefficient is due to the special circumstance that $E_0^{(3)}=0$.

Now, for the first excited state ($i=1$), we have instead of (5.12):

$$\bar{E}_1^{(4)}=E_1^{(0)}+E_1^{(2)}+E_1^{(4)} \tag{5.17}$$

where

$$\left.\begin{aligned} E_1^{(0)} &= \tfrac{3}{8}(3/\alpha_1+\alpha_1), \\ E_1^{(2)} &= -[3(1-\alpha_1^2)^2/8\alpha_1](31-11\alpha_1^2)^{-1}, \\ E_1^{(4)} &= -\frac{(1-\alpha_1^2)^4}{\alpha_1}\frac{3}{(31-11\alpha_1^2)^2} \\ &\quad \times\left(\frac{1}{5-\alpha_1^2}+\frac{14}{37-17\alpha_1^2}+\frac{189}{64(43-23\alpha_1^2)}-\frac{1}{512(31-11\alpha_1^2)}\right), \end{aligned}\right\} \tag{5.17}$$

and α_i is the positive real root of

$$10\lambda\alpha_1^3+\alpha_1^2-1=0.$$

This formula covers all ranges of λ, and like $\bar{E}_0^4$, even for $\lambda\to\infty$ the error is 0.013%, while $E_0^{(0)}+E_0^{(2)}$ has at most an error of 0.17%, and the simplest expression $E_1^{(0)}$ gives an error of 1.25% only (see figure 4 and table 2).

For $\lambda\gg 1$ we obtain instead of (5.13):

$$\bar{E}_1^{(4)} = E_1^{(0)}+E_1^{(2)}+E_1^{(4)} = 2.393\,3259\lambda^{1/3}+0.357\,8943\lambda^{-1/3}+\ldots. \tag{5.18}$$

This should be compared with the exact values (cf HMM, table 1)

$$E_1^{(e)} = 2.393\,64402\lambda^{1/3}+0.357\,80\lambda^{-1/3}+\ldots.$$

For small λ our α_1 is given by

$$\alpha_1 = 1-5\lambda+\tfrac{5}{2}(5\lambda)^2-8(5\lambda)^3+\tfrac{231}{8}(5\lambda)^4+\ldots \tag{5.19}$$

and we get

$$\begin{aligned} E_1^{(0)} &= \tfrac{3}{2}+\tfrac{3}{4}(5\lambda)-\tfrac{3}{4}(5\lambda)^2+\tfrac{3}{2}(5\lambda)^3-\tfrac{63}{16}(5\lambda)^4+\ldots, \\ E_1^{(2)} &= -\tfrac{3}{40}(5\lambda)^2+\tfrac{183}{400}(5\lambda)^3-\tfrac{2193}{4000}(5\lambda)^4+\ldots, \\ E_1^{(4)} &= -\tfrac{33717}{256000}(5\lambda)^4+\ldots, \end{aligned} \tag{5.20}$$

and therefore

$$\bar{E}_1^{(4)} = \tfrac{3}{2}+\tfrac{15}{4}\lambda-\tfrac{165}{8}\lambda^2+\tfrac{3915}{16}\lambda^3-\tfrac{5910345}{2048}\lambda^4+\ldots. \tag{5.21}$$

We believe these to be also the correct coefficients and the discussion given for $i=0$ is also valid here, since $E_1^{(3)}=0$ and $E_1^{(5)}\neq 0$.

6. The small-λ regime for higher excited states ($i\geqslant 2$)

As the calculation of perturbations due to $H_i^{(I)}$ higher than the third order becomes quite complicated for $i\geqslant 2$, we will be content with our second-order perturbation formulae (3.1), (3.2) and (4.4).

For small λ the solution of (3.2) is given by

$$\alpha_i = 1-\tfrac{1}{2}y_i+\tfrac{5}{2}(\tfrac{1}{2}y_i)^2+\ldots. \tag{6.1}$$

We see that $(1-\alpha_i^2)$ is proportional to y_i, or λ, so the factor $(1-\alpha_i^2)^2$ in front of $E_i^{(2)}$ is proportional to λ^2. Hence for small λ we retain only terms proportional to λ in

the rest of $E_i^{(2)}$. We can thus rewrite $E_i^{(2)}$ in the following form:

$$E_i^{(2)} \approx -\lambda^2\left(\frac{1}{\alpha_i^2}\right)\left[\frac{(i+4)(i+3)(i+2)(i+1)}{16[4+(2i+5)6\lambda]}-\frac{i(i-1)(i-2)(i-3)}{16[4+(2i-3)6\lambda]}\right.$$
$$\left.+\frac{(i+2)(i+1)i(i-1)}{(2i+1)^2}\left(\frac{i(i-1)}{2+(2i+3)3\lambda}-\frac{(i+2)(i+1)}{2+(2i-1)3\lambda}\right)\right] \qquad (\lambda \ll 1). \tag{6.2}$$

Together with $E_i^{(0)}$ for small λ

$$E_i^{(0)} \approx (i+\tfrac{1}{2})+\tfrac{3}{4}[1+2i(i+1)]\lambda-\frac{9}{4}\frac{(2i^2+2i+1)^2}{2i+1}\lambda^2+\ldots \tag{6.3}$$

we obtain a formula for $(E_i^{(0)}+E_i^{(2)})$, which resembles the formula (HMM (1.17)) if we put $1/\alpha_i^2$ equal to 1. But $1/\alpha_i^2$ is equal to 1 plus terms proportional to λ, so that it is a little arbitrary to keep λ otherwise and not in α_i. Still, (6.2) is not a consistent expansion in powers of λ. If we neglect consistently all terms proportional to λ^3, then we get

$$E_i^{(2)} \approx [(4i^4+8i^3-25i^2-29i-3)/8(2i+1)]\,\lambda^2+\ldots$$

and finally we obtain

$$E_i^{(0)}+E_i^{(2)} \approx (i+\tfrac{1}{2})+\tfrac{3}{4}(2i^2+2i+1)\lambda-\tfrac{1}{8}(34i^3+51i^2+59i+21)\lambda^2+\ldots. \tag{6.4}$$

This agrees with the results for $i=0,1$ in § 5 up to order λ^2, as it should.

Now if we let $i\to\infty$, but keep $\lambda i=\beta$ finite and small, we get

$$(E_i^{(0)}+E_i^{(2)})/(i+\tfrac{1}{2}) \approx 1+\tfrac{3}{2}\beta-\tfrac{17}{4}\beta^2+\ldots. \tag{6.5}$$

This agrees with the formula (HMM (1.18b)) for small β. We retained terms up to λ^2, so that in the coefficient of β^2, β should be put to zero. We will give the formulae valid for any β in § 8. The formula (HMM (1.18b)) is not valid for $\beta \geqslant 1$, as will be seen in § 8, while our formula (8.3) is valid also for large β.

7. The large-λ regime for higher excited states ($i \geqslant 2$)

For $i=0,1$, we already gave a fourth-order calculation in § 5. We use here also our second-order formulae (3.1), (3.2) and (4.4), and expand them for large λ. In this case α_i is given by

$$\alpha_i \approx (y_i)^{-1/3}(1-\tfrac{1}{3}y_i^{-2/3}+\tfrac{1}{9}y_i^{-4/3}+\ldots), \qquad y_i=6\lambda[(2i^2+2i+1)/(2i+1)]. \tag{7.1}$$

So, if we expand in powers of $y_i^{-1/3}$ (or $\lambda^{-1/3}$), and express our result in the form

$$E_i^{(0)}+E_i^{(2)} \approx \lambda^{1/3}(\varepsilon_i^{y(2)}+\alpha_i^{y(2)}\lambda^{-2/3}+\beta_i^{y(2)}\lambda^{-4/3}+\ldots) \tag{7.2}$$

as in HMM, our formula for $\beta_i^{y(2)}$ becomes too elaborate, so we will only give our expression for ε_i^{y} and α_i^{y};

$$\varepsilon_i^{y(2)}=\left(\frac{6(2i^2+2i+1)}{2i+1}\right)^{1/3}\left\{\tfrac{3}{4}(i+\tfrac{1}{2})+\frac{1}{36(2i^2+2i+1)}\right.$$
$$\left.\times\left[\left(\frac{2i+1}{4}\right)^2\left(-\frac{(i+4)(i+3)(i+2)(i+1)}{8i^2+16i+7}+\frac{i(i-1)(i-2)(i-3)}{8i^2-1}\right)\right.\right.$$

$$+2(i+2)(i+1)i(i-1)\left(-\frac{i(i-1)}{8i^2+12i+5}+\frac{(i+2)(i+1)}{8i^2+4i+1}\right)\Bigg]\Bigg\}, \tag{7.3}$$

$$\alpha_i^{y(2)}=\left(\frac{6(2i^2+2i+1)}{2i+1}\right)^{-1/3}\Bigg[\Big[\tfrac{1}{2}(i+\tfrac{1}{2})-\frac{1}{36(2i^2+2i+1)}$$
$$\times\Bigg\{\left(\frac{2i+1}{4}\right)^2\Bigg[\frac{(i+4)(i+3)(i+2)(i+1)}{8i^2+16i+7}\left(\frac{8i+3}{8i^2+16i+7}-\frac{5}{3}\right)$$
$$+\frac{i(i-1)(i-2)(i-3)}{8i^2-1}\left(\frac{8i+5}{8i^2-1}+\frac{5}{3}\right)\Bigg]$$
$$+2(i+2)(i+1)i(i-1)\Bigg[\frac{i(i-1)}{8i^2+12i+5}\left(\frac{4i+1}{8i^2+12i+5}-\frac{5}{3}\right)$$
$$+\frac{(i+2)(i+1)}{8i^2+4i+1}\left(\frac{4i+3}{8i^2+4i+1}+\frac{5}{3}\right)\Bigg]\Bigg\}\Big]\Big]. \tag{7.4}$$

The first terms of (7.3) and (7.4) come from $E_i^{(0)}$, and will be called $\varepsilon_i^{y(0)}$ and $\alpha_i^{y(0)}$ respectively.

This formula can be compared with the corresponding numerical values given in HMM, tables 1 and 2, which will be done in § 9 and is summarised in our table 4. Contrary to the case of small λ in § 6, where 'our' perturbation theory contains the 'usual' perturbation theory, here our higher-order contributions $E_i^{(3)}$, $E_i^{(4)}\ldots$ always bring a small numerical correction also for the coefficients of the leading terms (proportional to $\lambda^{1/3}$, $\lambda^{-1/3}\ldots$).

8. The large-i regime for arbitrary finite $i\lambda$

For large i, it is more convenient to use

$$j=i+\tfrac{1}{2} \tag{8.1}$$

as variable. Then our second-order perturbation results (3.1) and (4.4) have a more symmetrical form:

$$\varepsilon_i^{(0)}\equiv E_i^{(0)}/j=\tfrac{1}{4}(3/\alpha_i+\alpha_i),$$
$$\frac{E_i^{(2)}}{j}=\left(\frac{1-\alpha_i^2}{6}\right)^2\frac{1}{2\alpha_i(j^2+\frac{1}{4})}$$
$$\times\Bigg[\left(\frac{j}{2}\right)^2\left(-\frac{(j^2+4j+\frac{7}{4})(j^2+4j+\frac{15}{4})}{8j^2+8j+1-\alpha_i^2(8j-1)}+\frac{(j^2-4j+\frac{7}{4})(j^2-4j+\frac{15}{4})}{8j^2-8j+1+\alpha_i^2(8j+1)}\right)$$
$$+2(j^2-\tfrac{1}{4})(j^2-\tfrac{9}{4})\left(-\frac{(j^2-2j+\frac{3}{4})}{8j^2+4j+1-\alpha_i^2(4j-1)}\right.$$
$$\left.+\frac{(j^2+2j+\frac{3}{4})}{8j^2-4j+1+\alpha_i^2(4j+1)}\right)\Bigg] \tag{8.2}$$

where

$$y_i\alpha_i^3+\alpha_i^2-1=0, \qquad y_i=6\lambda\left(\frac{2i^2+2i+1}{2i+1}\right)=6\lambda j\left(1+\frac{1}{4j^2}\right).$$

After some algebra we arrive at

$$\frac{E_i^{(2)}}{j}=\left(\frac{1-\alpha_i^2}{12}\right)^2\frac{1}{\alpha_i}\left(\frac{4j^2}{4j^2+1}\right)\left(\frac{32(j^2-1/16j^2)(j^2-\frac{9}{4})(5-\alpha_i^2)}{(8j^2+1+\alpha_i^2)^2-16j^2(1-\alpha_i^2)^2}\right.$$
$$\left.-\frac{8j^4(7+\alpha_i^2)+4j^2(1+45\alpha_i^2)-\frac{1}{2}(61-149\alpha_i^2)}{(8j^2+1+\alpha_i^2)^2-64j^2(1-\alpha_i^2)^2}\right).$$

This is still valid for any $j(=i+\frac{1}{2})$. Now let $j\to\infty$, keeping $j\lambda\equiv\Lambda$ finite, large or small. For any i and λ, α_i is always between 0 and 1, as can be clearly seen from figure 3. Then we get

$$\frac{E_i^{(2)}}{j}\approx\frac{1}{8\alpha_i}\left(\frac{1-\alpha_i^2}{12}\right)^2\left[(13-5\alpha_i^2)-\frac{1}{4j^2}(216+85\alpha_i^2-17\alpha_i^4+8\alpha_i^6)+\ldots\right].\dagger$$

So our formula for large j is given by

$$\varepsilon_i^{(2)}=\frac{E_i^{(0)}+E_i^{(2)}}{(i+\frac{1}{2})}=\frac{1}{4}\left(\frac{3}{\alpha_i}+\alpha_i\right)+\frac{1}{8\alpha_i}\left(\frac{1-\alpha_i^2}{12}\right)^2(13-5\alpha_i^2). \tag{8.3}$$

This is our formula for large i and any finite $\Lambda=(i+\frac{1}{2})\lambda$. α_i is given as usual, which covers quite well large and small Λ. For small $\Lambda(\sim y_i)$ we use (6.1), and inserting this into (8.3) we get (6.3), as we should. For large $\Lambda(\sim y_i)$ we use (7.1); inserting this into (8.3) and expanding up to the power $\Lambda^{-2/3}$ we get

$$E_i^{(0)}+E_i^{(2)}\approx\lambda^{1/3}\left[\frac{(6)^{1/3}}{8}\left(\frac{877}{144}\right)(i+\tfrac{1}{2})\left(i+\frac{1}{2}+\frac{1}{4(i+\frac{1}{2})}\right)^{1/3}\right.$$
$$\left.+\frac{1}{8(6)^{1/3}}\left(\frac{103}{27}\right)(i+\tfrac{1}{2})\left(i+\frac{1}{2}+\frac{1}{4(i+\frac{1}{2})}\right)^{-1/3}\lambda^{-2/3}+\ldots\right]$$
$$\approx\lambda^{1/3}\left[1.383\,346\left(i+\frac{1}{2}+\frac{1}{16(i+\frac{1}{2})}\right)^{4/3}+0.262\,422(i+\tfrac{1}{2})^{2/3}\lambda^{-2/3}+\ldots\right]. \tag{8.4}$$

This should be compared with the more accurate value (Hioe and Montroll 1975 (IV. 16*a*))

$$E_i^{(e)}=\lambda^{1/3}\left[1.376\,507\left(i+\frac{1}{2}+\frac{0.0265}{i+\frac{1}{2}}\right)^{4/3}+0.268\,055(i+\tfrac{1}{2})^{2/3}\lambda^{-2/3}+\ldots\right].$$

Except that we get $\frac{1}{16}=0.0625$ in place of 0.0265 in the first term, the agreement here is also satisfactory, especially in view of the fact that we used only 'our' second-order perturbation formula.

Thus our formula (8.3) for large i covers really well all ranges of finite $\Lambda=(i+\frac{1}{2})\lambda$. The formula (HMM (1.18*b*)) covers only small Λ, whereas our formula (8.3) (which gives (6.3) in this case) is equally well suited and, as we have shown in figure 5, our

† Now we neglect the $(1/4j^2)$ term. In view of the large numerical coefficient one may be afraid that this could be dangerous for some range of finite $\Lambda=j\lambda$. As we have assumed j large and Λ finite, small Λ ($\alpha_i\to 1$) means j exceedingly large, so that the $1/4j^2$ term can be safely neglected in spite of its large numerical coefficient. And for large Λ ($\alpha_i\to 0$) we neglected $216/4j^2$ in comparison with 13, which is also all right for, say, $j>10$ because $E_i^{(2)}$ itself is only a small correction to $E_i^{(0)}$.

Table 1. The ground state energies $E_0^{(j)}$, equation (5.12).

λ	α_0	$E_0^{(0)}$	$-E_0^{(2)}$	$-E_0^{(4)}$	$\bar{E}_0^{(2)}$	$\bar{E}_0^{(4)}$	$E_0^{(e)}$
0.002	0.994 088	0.501 491	0.000 001	0.000 000	0.501 490	0.501 490	0.501 490
0.010	0.972 055	0.507 288	0.000 031	0.000 000	0.507 257	0.507 257	0.507 256
0.10	0.818 869	0.560 308	0.001 107	0.000 058	0.559 201	0.559 143	0.559 146
0.5	0.598 194	0.701 661	0.004 847	0.000 365	0.638 337	0.637 972	0.637 992
1.0	0.500 000	0.812 500	0.007 500	0.001 255	0.805 000	0.803 745	0.803 771
2.0	0.410 704	0.964 405	0.010 797	0.002 050	0.953 609	0.951 560	0.951 568
50	0.148 277	2.547 585	0.038 763	0.008 898	2.508 822	2.499 924	2.499 709
200	0.093 827	4.008 446	0.062 564	0.014 580	3.945 882	2.931 302	3.930 331
1000	0.054 977	6.827 91	0.107 757	0.025 277	6.720 154	6.694 877	6.694 221
8000	0.027 509	13.635 34	0.216 122	0.050 826	13.419 22	13.368 39	13.366 91
20000	0.020 271	18.501 87	0.293 451	0.069 039	18.208 42	18.139 38	18.137 23

Table 2. The first excited state energies $E_1^{(j)}$, equation (5.17).

λ	α_1	$E_1^{(0)}$	$-E_1^{(2)}$	$-E_1^{(4)}$	$\bar{E}_1^{(2)}$	$\bar{E}_1^{(4)}$	$E_1^{(e)}$
0.002	0.990 242	1.507 427	0.000 007	0.000 000	1.507 420	1.507 420	1.507 419
0.01	0.955 401	1.535 792	0.000 142	0.000 000	1.535 649	1.535 649	1.535 648
0.10	0.754 878	1.773 387	0.003 717	0.000 186	1.769 670	1.769 484	1.769 503
0.5	0.525 166	2.339 117	0.013 391	0.001 457	2.325 726	2.324 269	2.324 406
1.0	0.433 105	2.759 937	0.019 749	0.002 516	2.740 188	2.737 672	2.737 892
2.0	0.352 469	3.323 946	0.027 536	0.003 876	3.296 411	3.292 535	3.292 868
50	0.125 329	9.023 373	0.094 359	0.015 390	8.929 014	8.913 624	8.915 096
200	0.079 204	14.233 53	0.151 155	0.025 039	14.082 38	14.057 34	14.059 23
1000	0.046 383	24.271 97	0.259 880	0.043 274	24.012 09	24.968 81	23.972 21
8000	0.023 204	48.491 72	0.520 862	0.086 907	47.970 85	47.883 95	47.890 77
20000	0.017 098	65.803 58	0.707 157	0.118 028	65.096 42	64.978 39	64.986 68

Comparison of our calculated values with the exact values $E_i^{(e)}$, taken from table IIA of Hioe and Montroll (1975). $E_i^{(j)}$ is our jth-order calculation, and $\bar{E}_i^{(2)} = E_i^{(0)} + E_i^{(2)}$, $\bar{E}_i^{(4)} = E_i^{(0)} + E_i^{(2)} + E_i^{(4)}$ $(i = 0, 1)$.

Table 3. E_2, E_3, E_8, equation (4.4). $E_i^{(0)} = (i+\frac{1}{2})\varepsilon_i^{(0)}$, $\bar{E}_i^{(2)} = (i+\frac{1}{2})(\varepsilon_i^{(0)} + \varepsilon_i^{(2)}) = (i+\frac{1}{2})\bar{\varepsilon}_i^{(2)}$, $E_i^{(e)} = (i+\frac{1}{2})\varepsilon_i^{(e)}$. $E_i^{(0)}(\bar{E}_i^{(2)})$ are our calculated lowest (with second-order correction) energy levels, from (3.1), (3.2) ((4.4)). $E_i^{(e)}$ are exact values taken from tables IIA, IIB, IIC of Hioe and Montroll (1975).

λ	$\varepsilon_2^{(0)}$	$\bar{\varepsilon}_2^{(2)}$	$\varepsilon_2^{(e)}$	$\varepsilon_3^{(0)}$	$\bar{\varepsilon}_3^{(2)}$	$\varepsilon_3^{(e)}$	$\varepsilon_8^{(0)}$	$\bar{\varepsilon}_8^{(2)}$	$\varepsilon_8^{(e)}$
0.002	1.007 682	1.007 681	1.007 681	1.010 497	1.010 501	1.010 498	1.024 397	1.024 451	1.024 449
0.006	1.022 396	1.022 390	1.022 389	1.030 305	1.030 343	1.030 339	1.067 594	1.067 961	1.067 924
0.01	1.036 354	1.036 343	1.036 338	1.048 799	1.049 775	1.048 884	1.105 504	1.106 310	1.106 199
0.05	1.149 601	1.149 729	1.149 592	1.192 308	1.193 240	1.193 450	1.362 349	1.367 747	1.366 444
0.1	1.255 298	1.255 850	1.255 450	1.320 552	1.323 360	1.322 538	1.567 474	1.577 016	1.573 996
0.3	1.536 962	1.539 270	1.537 913	1.651 281	1.658 635	1.656 164	2.059 991	2.079 055	2.073 229
0.5	1.729 408	1.733 072	1.731 010	1.872 784	1.883 163	1.879 543	2.376 580	2.401 351	2.393 552
0.7	1.882 003	1.886 750	1.885 312	2.047 043	2.059 733	2.055 219	2.621 785	2.650 804	2.641 529
1	2.068 951	2.075 005	2.071 717	2.259 407	2.274 828	2.269 258	2.917 599	2.951 587	2.940 582
2	2.517 306	2.526 375	2.521 552	2.765 877	2.787 501	2.779 235	3.614 370	3.659 794	3.644 692
50	6.958 084	6.992 653	6.974 796	7.723 295	7.797 861	7.769 327	10.294 75	10.438 47	10.389 92
200	10.999 65	11.055 71	11.020 57	12.214 66	12.334 64	12.287 22	16.307 00	16.536 69	16.458 87
1000	18.760 00	18.856 76	18.806 94	20.849 86	21.056 20	20.976 89	27.858 78	28.252 69	28.119 01
8000	37.490 01	37.684 22	37.584 24	41.673 48	42.087 10	41.927 29	55.699 19	56.487 92	56.218 32
20000	50.875 29	51.139 02	51.003 60	56.560 14	57.121 77	56.898 61	75.592 08	76.662 75	76.295 92

Table 4. $E_i^{(0)}$, $\bar{E}_i^{(2)}$ for $\lambda \to \infty$, (7.3), (7.4). Equations (7.3) and (7.4) are valid for large λ. $E_i^{(0)}/\omega = \lambda^{1/3}(\varepsilon_i^{y(0)} + \alpha_i^{y(0)}\lambda^{-2/3} + \ldots)$ ... is our lowest-order result. $\bar{E}_i^{(2)}/\omega = \lambda^{1/3}(\varepsilon_i^{y(2)} + \alpha_i^{y(2)}\lambda^{-2/3} + \ldots)$ ... with our second-order corrections. $\varepsilon_i^{(e)}$ and $\alpha_i^{(e)}$ are the corresponding exact values, taken from tables 1 and 2 of HMM. The author is indebted to C B Lang and L Mathelitsch for computational aid in obtaining this table.

i	$\varepsilon_i^{y(0)}$	$\varepsilon_i^{y(2)}$	$\varepsilon_i^{(e)}$	$\alpha_i^{y(0)}/(i+\frac{1}{2})^{+2/3}$	$\alpha_i^{y(2)}/(i+\frac{1}{2})^{2/3}$	$\alpha_i^{(e)}/(i+\frac{1}{2})^{2/3}$
0	0.681 4202	0.670 6040	0.667 9863	0.218 40	0.224 83	0.228 06
1	2.423 739	2.397 677	2.393 644	0.265 66	0.271 29	0.273 05
2	4.684 999	4.709 304	4.696 795	0.271 59	0.265 22	0.268 16
3	7.291 111	7.363 548	7.335 730	0.273 31	0.263 79	0.268 20
4	10.166 496	10.287 822	10.244 309	0.274 04	0.263 24	0.268 13
5	13.267 428	13.439 319	13.379 337	0.274 41	0.262 96	0.268 10
6	16.564 699	16.789 097	16.711 890	0.274 62	0.262 81	0.268 08
7	20.037 121	20.316 011	20.220 850	0.274 75	0.262 71	0.268 08
8	23.668 476	24.003 803	23.889 994	0.274 84	0.262 65	0.268 07
9	27.445 866	27.839 509	27.706 394	0.274 91	0.262 60	0.268 07
10	31.358 742	31.812 501	31.659 457	0.274 95	0.262 57	0.268 06
100, 101	1.362 85 $\times(i+\frac{1}{2})^{-4/3}$	1.383 35 $\times(i+\frac{1}{2})^{-4/3}$	1.376 507 $\times(i+\frac{1}{2})^{-4/3}$	0.275 16	0.262 42	0.268 055

formula (8.3) and (HMM (1.18*b*)) deviate near $\Lambda \sim 1$, as expected. Our formula also covers the intermediate Λ region well and connects smoothly with the correct result for large Λ.

9. Intermediate regime of i and λ. Numerical results

For intermediate magnitudes of i and λ we must return to formula (3.1) for our lowest order, and (4.4) for our second-order corrected results. First, for $i=0$, we obtain from our fourth-order formula (5.12) the numerical results summarised in table 1. For this calculation we still need only a desk computer. For $i=1$, from the corresponding formula (5.17), we obtain the results of table 2. As will be seen the maximal errors (in the case of large λ) are less than 0.012% and 0.013%, respectively.

For the states with $i \neq 0, 1$ we must be content with the much more inaccurate formula (4.4). We have listed as examples the lowest- ((3.1)) and second-order ((4.4)) results for $i=2$, 3 and 8 in table 3. The accuracy of our approximation procedure can be most clearly seen from figure 4, where we plot the ratio of our results to the exact values as a function of λ. We see that in general $E_i^{(0)} < E_i^{(e)} < \bar{E}_i^{(2)} = E_i^{(0)} + E_i^{(2)}$, and $|R_i^{(2)} - 1| = |(\bar{E}_i^{(2)} - E_i^{(e)})/E_i^{(e)}|$ are much smaller than $|R_i^{(0)} - 1| = |(E_i^{(0)} - E_i^{(e)})/E_i^{(e)}|$ for any i.

This means 'our' second-order perturbation calculations improve 'our' lowest-order results essentially, for all ranges of λ. In table 4 we have summarised our calculated $E_i^{(0)}$ and $\bar{E}_i^{(2)}$ for the limiting case of large λ (equations (7.2), (7.3), (7.4)), and even for this case we see that the agreement is satisfactory.

10. Concluding remarks and discussion

As we have seen, our method and the required numerical calculations are extremely simple; they contain only one adjustable parameter α_i for given i and λ in the special combination $y_i = 6\lambda(2i^2+2i+1)/(2i+1)$. We see that the largest error occurs at $\lambda \to \infty$ and $i=0$. The other extreme case, $i \to \infty$, is less inaccurate. And even for the ($\lambda \to \infty$, $i=0$) case 'our' fourth-order perturbation reduces the error to 0.01%. From these numerical results we are quite certain that if we calculate $E_i^{(3)}$ and $E_i^{(4)}$ also for $i \geq 2$, then everything is expected to agree within, say, about 0.01%.

As our method is simple enough, we may apply our method also to a pair of coupled oscillators with quartic coupling, as discussed in HMM. We have to introduce two parameters α_1 and α_2 for each oscillator. Our preliminary calculations show that our approach is also successful in this case. We will discuss these problems in a forthcoming paper.

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