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Perturbation theory for the triple-well anharmonic oscillator: II

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Abstract. Asymptotic formulae of the energy eigenvalues for the states which 'originate' from the middle well of the one-dimensional Schrödinger equation with the potential $U(x) = x^2(R^2 - x^2)^2/8R^4$ are analysed. In particular, the relation between eigenvalues for modal and non-modal solutions is determined analytically to the next higher approximation, and compared with available numerical data.

1. Introduction

In our previous paper (Damburg and Propin 1982, to be referred to as I) we studied perturbation theory at large order for the one-dimensional Schrödinger equation

$$d^2\psi/dx^2 + [2E - x^2(R^2 - x^2)^2/4R^4]\psi = 0 \tag{1}$$

where R is a large parameter. Here we continue to study this problem for the states which 'originate' from the middle well. Their energy eigenvalues can be approximated by the perturbation expansion

$$E_0 = \tfrac{1}{2}n + \tfrac{1}{4} - (6n^2 + 6n + 3)/4R^2 + \dots. \tag{2}$$

In I, it was shown that an exponentially small shift should be added to E_0 in order to make the asymptotic expansion for E more consistent. For modal solutions of equation (1), we obtained

$$E_{\mathrm{m}} = E_0 + \delta E, \tag{3}$$

where

$$\delta E = (-1)^{n+1} \frac{R^{3n+3/2} \exp(-\frac{1}{4}R^2)}{2^{n/2+5/4}\Gamma(\frac{1}{2}n + \frac{3}{4})\Gamma(n+1)} \left(1 - \frac{72n^2 + 120n + 63}{8R^2} + \dots\right). \tag{4}$$

In I we considered also non-modal solutions of equation (1),

$$E_{\mathrm{nm}} = E_0 + \tfrac{1}{2}\mathrm{i}\gamma, \tag{5}$$

where

$$\tfrac{1}{2}\gamma = \delta E. \tag{6}$$

In I we were not quite consistent in taking into account the sign of γ and had instead of (6) $\gamma = 2|\delta E|$. But that was insignificant for the results presented in I. Comparison of the results obtained by use of asymptotic formulae with the results of exact numerical solution of equation (1) was presented in I. Numerical data for non-modal solutions were taken from Benassi *et al* (1979). Overall agreement appeared to be excellent. Nevertheless, we must point out that formula (6) was only approximate, and now turn to its improvement.

2. Terms $\exp(-\frac{1}{2}R^2)$ in solutions of (1)

Recollecting that in order to find δE in I we were using the substitution $n \to n+\lambda(n)$, let us now extend it by one step, namely

$$n \to n+\lambda(n+\lambda(n)) = n+\lambda(n)+\lambda(n)\,\mathrm{d}\lambda(n)/\mathrm{d}n+\ldots. \tag{7}$$

Substituting (7) into (2), we obtain with accuracy of up to terms of $O(\lambda^3)$

$$E_{\mathrm{m}} = E_0+\delta E+\delta E', \tag{8}$$

where

$$\delta E' = \frac{R^{6n+3}\exp(-\frac{1}{2}R^2)}{2^{n+3/2}[\Gamma(\frac{1}{2}n+\frac{3}{4})\Gamma(n+1)]^2}\{3\ln R-\tfrac{1}{2}\ln 2-\tfrac{1}{2}\psi(\tfrac{1}{2}n+\tfrac{3}{4})-\psi(n+1)$$
$$-[(72n^2+96n+51)[3\ln R-\tfrac{1}{2}\ln 2-\tfrac{1}{2}\psi(\tfrac{1}{2}n+\tfrac{3}{4})-\psi(n+1)]$$
$$+72n+48]/4R^2+\ldots\}. \tag{9}$$

In order to obtain non-modal solutions, we substitute

$$n \to n+\mathrm{i}\lambda(n+\mathrm{i}\lambda(n)) = n+\mathrm{i}\lambda(n)-\lambda(n)\,\mathrm{d}\lambda(n)/\mathrm{d}n+\ldots \tag{10}$$

into equation (2) and obtain

$$E_{\mathrm{nm}} = E_0+\tfrac{1}{2}\mathrm{i}\gamma'-\delta E'. \tag{11}$$

The level width γ' is now defined as

$$\tfrac{1}{2}\gamma' = \tfrac{1}{2}\gamma-\delta E'', \tag{12}$$

where

$$\delta E'' = \frac{\pi R^{6n+3}\exp(-\frac{1}{2}R^2)}{2^{n+3/2}[\Gamma(\frac{1}{2}n+\frac{3}{4})\Gamma(n+1)]^2}\left(1-\frac{72n^2+96n+51}{4R^2}+\ldots\right). \tag{13}$$

By using numerical methods for solving (1), we can calculate values $\frac{1}{2}\gamma'$ and $E_{\mathrm{m}}-\mathrm{Re}\,E_{\mathrm{nm}}$. These two quantities coincide for large R with accuracy of up to terms of $O(\exp(-\frac{1}{2}R^2))$, as was shown in I. Namely, in such an approximation the formula (6) was obtained. By taking into account terms $\sim\exp(-\frac{1}{2}R^2)$, we have the improved relation

$$\Delta = (E_{\mathrm{m}}-\mathrm{Re}\,E_{\mathrm{nm}})-\tfrac{1}{2}\gamma' = 2\delta E'+\delta E''. \tag{14}$$

3. Comparison with the numerical data

In table 1 we compare results for values of Δ obtained for the ground state by use of the asymptotic formula (14) with numerical results. We take numerical values of Δ from data presented in I.

Table 1.

$n=0$

$g=\sqrt{2}/R$	Δ_{num}	$\Delta_{as}=2\delta E'+\delta E''$
0.20	-0.101×10^{-6}	0.1359×10^{-7}
0.22	0.682×10^{-6}	0.6909×10^{-6}
0.24	0.1166×10^{-4}	0.1252×10^{-4}
0.26	0.9440×10^{-4}	1.0891×10^{-4}
0.28	0.4395×10^{-3}	0.5489×10^{-3}
0.30	0.1366×10^{-2}	0.1801×10^{-2}

As seen from table 1, the agreement between asymptotic and numerical results for Δ is satisfactory, except for $g=0.20$. We note that in formula (14) we obtained only two terms; the next terms in expansion in powers of R^{-2} would improve agreement still more. Discrepancy between the data for $g=0.20$ we tentatively attribute to the sensitivity of such a minute value of Δ to a small inaccuracy in the numerical result for the non-modal solution.

In conclusion, we should make one essential comment. It is useless to take into account the term $\delta E'$ when calculating E_m or Re E_{nm} by using the asymptotic formulae (8) or (11), because the intrinsic error of the asymptotic expansion for E_0 is larger than $\delta E'$, as follows from the analysis presented in I.

References

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