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Relationship Between the Level Splitting and the Large Order Behaviour of Perturbation Theory

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ABSTRACT. The relationship between the splitting of asymptotically degenerate energy levels and the large order behaviour of the Rayleigh-Schrödinger perturbation expansion is investigated in the case of a periodic potential.

Recently a group of authors (Damburg *et al.* 1984) has given a mathematical justification of an approximate formula relating the rate of divergence of the Rayleigh-Schrödinger perturbation series to the level splitting. The approximate formula was tested previously (Brézin and Zinn-Justin 1979) by application to the expansion of the H_2^+ ground state energy in inverse power of the distance between the protons, and, in fact, was used to determine numerically the large order behaviour of the expansion. As pointed out by these authors, the divergence rates of expansions for other cases, such as the anharmonic oscillator, have been understood previously, the case of H_2^+ being different, since in this case the expansion is not directly Borel summable (Brézin *et al.* 1977).

Using a dispersion relation representation of the energy eigenvalue E as a function of some coupling parameter h^2, the coefficient of the r th term of the perturbation expansion of E can be related to the discontinuity across its cut. Thus (ignoring possible subtractions)

$$E(h) = \frac{1}{\pi} \int_0^\infty \frac{\mathcal{I}m\, E(h^1)}{h^1 - h}\, dh^1 = - \sum_{r=1}^{\infty} \frac{Ar}{h^r}$$

where

$$A_r = \frac{1}{\pi} \int_0^\infty h^{1^{r-1}}\, \mathcal{I}m\, E(h^1)\, dh^1 \qquad (1)$$

The formula relating $\Im m E$ to the tunneling contribution $\frac{1}{2}\,\triangle E$ to the real part of the ground state energy has been given by Bogomolny and Fateyev (1977) for the double-well potential, *i.e.*

$$\Im m E = \pi \left(\frac{1}{2}\,\triangle E\right)^2 \tag{2}$$

In the following we seek the corresponding formula for the case of a periodic potential.

Properties of the Perturbation Expansion for the Eigenvalues of the Periodic Potential

We consider the perturbation expansion for the eigenvalues E of the equation

$$Y'' + [E - 2h^2 \cos 2x]\, Y = 0 \tag{3}$$

subject to periodic boundary conditions.

The dominant contribution to the splitting of asymptotically degenerate eigenvalues of (3) was first calculated by Goldstein (1929). A more recent calculation with higher order correction terms has been given by Dingle and Müller (1962). In the latter, the splitting was obtained in terms of the deviation $q-q_0$ of an approximately odd quantum number q from an exact integer $q_0 = 2n+1$, $n = 0, 1, 2, \ldots$.

Thus

$$E(q, h) = E(q_0, h) + (q-q_0)\left(\frac{\partial E}{\partial q}\right)_{q_0} + \ldots \tag{4}$$

and

$$q-q_0 = \mp 2 \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{(16h)^{\frac{1}{2}q_0} e^{-4h}}{[\frac{1}{2}(q_0-1)\,!} \left[1+O\left(\frac{1}{h}\right)\right] \tag{5}$$

the upper sign referring to even and the lower to odd eigenfunctions. We use this result in order to establish empirically the relationship corresponding to (2). To this end, we require the discontinuity of E (h) across its cut from h=0 along the positive real axis. The discontinuity of E, or rather the corresponding imaginary part, has been calculated by Stone and Reeve (1978). We extract the following expression

$$\Im m\, E(h) \simeq \frac{(16h)^{q_0+1} e^{-8h}}{4\,\{[\frac{1}{2}(q_0-1)]\,!\}^2} \tag{6}$$

From (5) and (6) we deduce

$$\mathcal{I}m\ E \simeq \left(\frac{\partial E}{\partial q}\right)_{q_0} \pi \left(\frac{q-q_0}{2}\right)^2 \tag{7}$$

where we have used the dominant terms of the expansion (see *e.g.* Dingle and Müller 1962)

$$E\ (q,h) = -\ 2h^2 + 2hq + \ldots$$

Using (4) we can rewrite (7) in the more appealing form

$$\mathcal{I}m\ (q-q_0) \simeq \pi \left(\frac{q-q_0}{2}\right)^2 \tag{8}$$

This formula seems to underline the fundamental significance of the parameter q.

The behaviour of the late terms A_r of the eigenvalue expansion has been calculated by Dingle and Müller (1964) and Dingle (1964) by solving appropriate recurrence relations, and by Stone and Reeve (1978) by using the dispersion relation. We can demonstrate the agreement of the results of both methods as follows.

Inserting (6) into (1) we obtain the expression

$$E = -\ \sum_r \frac{2^{2n}(r+2n+1)!}{\pi\ (8h)^{+}\ (n!)^2} \tag{9}$$

where $n = \frac{1}{2}\ (q_0-1)$. In the work of Dingle and Müller (1964; eq. 32) the r th term was shown to be given by

$$r^{th}\ \text{term} \simeq -\ \frac{r\,!\ r^{q-1}}{\{\ [\frac{1}{4}(q-1]!\ [\frac{1}{4}(q-3)]!\}^2\ (8h)^{r-1}} \tag{10}$$

for r large and $q = q_0$. Using

$$\frac{r\,!}{(r+m)!} \simeq \frac{1}{rm}\ \{1-0(\frac{1}{r})\}$$

and the duplication formula for Γ (z) eq. (10) becomes

$$-\ \frac{(r+2n)\ !\ 2^{2n}}{\pi\ (8h)^{r-1}\ (n\ !)^2}$$

in agreement with (9) if we raise r by 1.

We have thus demonstrated the relationship between the level splitting and the large order behaviour of the perturbation expansion in the case of the periodic potential.

Analogous calculations can be performed for the case of the double-well potential using the level splitting calculated by Mansour and Müller-Kirsten (1982) and a calculation of the large order behaviour as by Müller-Kirsten (1980).

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العلاقة بين إنشطار المستويات والسلوكية الكبيرة المرتبة لنظرية الإضطراب

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تم تحري العلاقة بين إنشطار مستويات الطاقة المفككة تقريباً والسلوكية الكبيرة المرتبة لمفكوك الإضطراب لرايلي ـ شرودنجر بالنسبة للجهد ذي الطبيعة الدورية.