How do supersingular perturbations generate non-Taylor series?

2005 J. Phys. A: Math. Gen. 38 L331

(http://iopscience.iop.org/0305-4470/38/20/L01)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) L331–L336 doi:10.1088/0305-4470/38/20/L01

LETTER TO THE EDITOR

How do supersingular perturbations generate non-Taylor series?

S K Bandyopadhyay[1], K Bhattacharyya[1] and J K Bhattacharjee[2]

[1] Department of Chemistry, The University of Burdwan, Burdwan 713 104, India
[2] Department of Theoretical Physics, Indian association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India

E-mail: pchemkb@yahoo.com and tpjkb@iacs.res.in

Received 25 October 2004
Published 3 May 2005
Online at stacks.iop.org/JPhysA/38/L331

Abstract
We show that a suitable choice of the zero-order problem can lead directly to the emergence of non-Taylor expansions in λ for the ground-state energies of the Hamiltonian family $H(\lambda) = -\nabla^2 + r^2 + \lambda/r^\beta$ in regions $\beta \geqslant 3$. The discussion includes the role of dimension and the right order parameter. The effect of choosing a more general potential of the form $r^\alpha + \lambda/r^\beta$ is also considered.

PACS numbers: 03.65.Db, 31.15.Md

Conventional perturbation theory in quantum mechanics intends to solve an eigenvalue problem $H\Psi_n = E_n\Psi_n$ by taking a solvable Hamiltonian H_0 and a perturbing potential λV, where V defines the nature of the perturbation and λ its strength. The system is defined by the total Hamiltonian $H = H_0 + \lambda V$, with known $H_0\Psi_{n0} = E_{n0}\Psi_{n0}$. It is then customary to express an unknown eigenvalue E_n of H in Taylor series as

$$E_n = E_{n0} + \lambda E_{n1} + \lambda^2 E_{n2} + \cdots. \tag{1}$$

A similar expansion for the eigenstate Ψ_n of H, in the form $\Psi_n = \Psi_{n0} + \lambda\Psi_{n1} + \lambda^2\Psi_{n2} + \cdots$, yields subsequently expressions for the unknown correction terms of the series. Specifically, one finds that

$$E_{n1} = \frac{\langle\Psi_{n0}|V|\Psi_{n0}\rangle}{\langle\Psi_{n0}|\Psi_{n0}\rangle}. \tag{2}$$

If, however, the potential V corresponds to a strong repulsive core near the origin, which is common in certain areas of physical interest, it may so happen that the numerator in (2) diverges, yielding $E_{n1} = \infty$. This is then called a supersingular perturbation [3]. In this case, the leading shift in energy $\Delta E_n = (E_n - E_{n0}) = \lambda E_{n1}$ becomes useless, even when $\lambda \to 0$. Hence, the only way to keep ΔE_n finite is to increase the coupling strength. This may be achieved by choosing some μ as the order parameter that satisfies $\mu \gg \lambda$ as $\lambda \to 0$. If the first-order correction to energy is now denoted by $\bar{E}_{n1}$, it could be finite; consequently, the net first-order shift $\mu\bar{E}_{n1}$ would be finite, at least for small μ. The idea, however, leads to non-Taylor expansions, contrary to (1). Theoretical interest in such problems is therefore obvious.

Perturbative and related studies on the radial states of the Hamiltonian (see, e.g., [1–14] and references therein)

$$H = -\nabla^2 + r^2 + \lambda/r^\beta, \tag{3}$$

in N-dimensions (ND) with

$$\nabla^2 = \sum_{j=1}^{N} \partial^2/\partial x_j^2, \qquad r^2 = \sum_{j=1}^{N} x_j^2, \tag{4}$$

reveal the aforesaid feature very clearly. In the total potential $r^2 + \lambda/r^\beta$, the second part dominates the behaviour near the origin. The singularity at $r = 0$ gets stronger as β increases and, for large enough β, it is the $r \to 0$ behaviour that becomes decisive. For example, the conventional expansion (1) for the ground state breaks down for $\beta \geqslant N$. Instead, a new series gets ordered in fractional powers of λ for $\beta > N$. For $N = 3$, this was explicitly shown in [4]. Later, it was also shown via a scaling argument [13] that this new series involves μ as the order parameter, where $\mu = \lambda^Z$, $Z = (N-2)/(\beta-2)$. Thus, for H in (3), one can write

$$E_0 = E_{00} + \mu\bar{E}_{01} + \cdots = N + \lambda^Z \bar{E}_{01} + \cdots \tag{5}$$

instead of (1). However, it is not easy to show the emergence of (5). Harrell [4] pursued a rather involved scheme to obtain (5) along with $\bar{E}_{01}$ for several β-values (or ranges) in the 3D case. Following his route, it is neither straightforward to generalize the results for arbitrary N nor easy to infer in what ways (5) would change if, for example, we wished to concentrate on a more general H of the form

$$H = -\nabla^2 + r^\alpha + \frac{\lambda}{r^\beta}, \tag{6}$$

in which considerable interest for $\alpha = 4$ has already been shown [12].

In view of the above remarks, our purpose is to explore a straightforward route to arrive at series like (5), more specifically the nature of the leading shift ΔE_0, for H in (6) at $\alpha = 2$ and else. To this end, we employ a better H_0 and Ψ_{00}, following the 'back-to-front' method of Killingbeck [15].

Consider H in (6). It is easy to check that Ψ_0 would go as $\exp[-r^P]$, with $P = 1 - (\beta/2)$, for $\beta > 2$ as $r \to 0$. At the other extreme of $r \to \infty$, Ψ_0 would decay as $\exp[-r^Q]$, with $Q = 1 + (\alpha/2)$. Therefore, we choose our starting normalizable function Ψ_{00} as

$$\Psi_{00} = \exp[-R(r)/2], \tag{7}$$

with $R(r) = Ar^a + Br^{-b}$. If we now define our H_0 as

$$H_0 = -\nabla^2 + V_0 \tag{8}$$

and insist that Ψ_{00} be its lowest eigenfunction with zero eigenvalue, then V_0 becomes

$$V_0 = \left(\frac{aA}{2}\right)^2 r^{2a-2} + \left(\frac{bB}{2}\right)^2 r^{-(2b+2)} - \frac{abAB}{2} r^{a-b-2} - \frac{aA(a+N-2)}{2} r^{a-2} - \frac{bB(b-N+2)}{2} r^{-(b+2)}. \tag{9}$$

For convenience, we now distinguish a few cases and study them separately.

Case I. Let us first take $\alpha = 2$, i.e., the case of H in (3), and set

$$A = 1, \qquad a = 2, \qquad B = \frac{4\sqrt{\lambda}}{\beta - 2}, \qquad b = \frac{\beta}{2} - 1. \tag{10}$$

This means that

$$R(r) = r^2 + \frac{4\sqrt{\lambda}}{\beta - 2} r^{1-\frac{\beta}{2}}, \tag{11}$$

and

$$V_0 = r^2 + \lambda r^{-\beta} - N - 2\sqrt{\lambda} r^{1-\frac{\beta}{2}} - \sqrt{\lambda}\left(1 - N + \frac{\beta}{2}\right) r^{-(1+\frac{\beta}{2})}. \tag{12}$$

Therefore, writing H in (3) as

$$H = h_0 + h_1, \tag{13}$$

with $h_0 = H_0 + N$ that has a ground-state energy N and wavefunction given by (7) and (11), one can choose

$$h_1 = 2\sqrt{\lambda} r^{1-\frac{\beta}{2}} + \sqrt{\lambda}\left(1 - N + \frac{\beta}{2}\right) r^{-(1+\frac{\beta}{2})}. \tag{14}$$

The key observation now is that the leading correction to the ground-state energy induced by h_1 can be calculated using first-order perturbation theory without any difficulty. The structure of Ψ_{00} ensures that there will be no divergence of the correction integral at the origin. We thus get

$$E_0 = N + \frac{\int_0^\infty h_1\, \mathrm{e}^{-R(r)}\, \mathrm{d}^N r}{\int_0^\infty \mathrm{e}^{-R(r)}\, \mathrm{d}^N r}. \tag{15}$$

The following results are now worth mentioning:

(i) In the range $2 < \beta < N$, $R(r)$ in the exponent in the numerator of (15) can be expanded to note that there cannot be any correction of order less than λ.

(ii) At $\beta = (2N - 2)$, the second part of h_1 in (14) vanishes and hence (15) yields neatly

$$E_0 = N + \lambda^{\frac{1}{2}}\, (2/\Gamma(N/2)) \tag{16}$$

at the lowest order, thus identifying $\bar{E}_{01} = 2/\Gamma(N/2)$ in (5).

(iii) For $\beta > (2N - 2)$, the integral appearing in the numerator in (15) has a very clear maximum close to the origin at

$$r_0 \approx \lambda^{\frac{1}{\beta-2}} \left(\frac{4}{\beta + 4 - 2N}\right)^{\frac{2}{\beta-2}} \tag{17}$$

when $\lambda \ll 1$. Also, under such a condition, the second part of h_1 virtually controls the value of the total integral. The denominator contributes a constant value of $\Gamma(N/2)/2$. Therefore, one finds that the leading correction from the actual integral part in (15) is of order λ^S, $S = (2N - 2 - \beta)/(2\beta - 4)$. The pre-factor $\lambda^{1/2}$ in (14) finally yields the same Z as considered in (5).

(iv) While all the results obtained above and the conclusions reached so far agree with Harrell's work [4] for $N = 3$, the area $3 \leqslant \beta < 4$ is yet to be covered. So, we now turn specific attention to this region of β at $N = 3$. The integral in (15) then shows a deep minimum very close to the origin at the same point r_0 given by (17). From (15), the dominant contribution emerges as

$$E_0 = 3 + \frac{4\lambda(4 - \beta)}{\Gamma(3/2)(\beta - 2)} \int_L^\infty r^{2-\beta} \exp[-r^2]\, \mathrm{d}r, \tag{18}$$

where L stands for the lower limit of integration. Putting $L = r_0$, one finds from (18) that $\Delta E_0 \sim \lambda^Z$ again, with $Z = 1/(\beta - 2)$, at the leading order for $\beta > 3$. However, (18) also shows that the dependence will be of the form $\Delta E_0 \sim \ln \lambda$ at $\beta = 3$, agreeing with the actual finding [4]. For $N \neq 3$, similar considerations apply, only the expression for r_0 in (17) may differ.

Table 1. Adequacy of (15) in furnishing the ground-state energies for small λ at $N = 3$. The lower entries denote energies obtained by summing up the perturbation series [4] up to first order.

β	$\lambda = 10^{-6}$	$\lambda = 10^{-8}$
3.1	3.000 069	3.000 001 3
	3.000 073	3.000 001 1
3.5	3.000 413	3.000 0196
	3.000 390	3.000 018 1
4.1	3.002 962	3.000 330 7
	3.002 958	3.000 330 1
4.5	3.007 5	3.001 19
	3.007 2	3.001 15
5.0	3.018	3.003 9
	3.016	3.003 5

(v) We may also provide some numerical estimates to check the workability of (15). Table 1 presents our result at $N = 3$ *vis à vis* the energies obtained from the work of [4] up to first order. For $\lambda \ll 1$, they must agree. A glance at the table reveals the correspondence. Indeed, one needs to reduce λ considerably to achieve a very good conformity. One index of 'smallness' of λ is provided by the virtual λ-independence of the denominator in (15). At larger β, however, the pre-factor at the second term in (14) grows linearly and hence the agreement becomes poorer.

Case II. For H in (6) at arbitrary α, we take

$$A = \frac{4}{\alpha+2}, \qquad a = \frac{\alpha}{2} + 1, \qquad B = \frac{4\sqrt{\lambda}}{\beta-2}, \qquad b = \frac{\beta}{2} - 1. \tag{19}$$

Thus, (11) is changed to

$$R(r) = \frac{4}{\alpha+2} r^{1+\frac{\alpha}{2}} + \frac{4\sqrt{\lambda}}{\beta-2} r^{1-\frac{\beta}{2}}, \tag{20}$$

and (12) to

$$V_0 = r^\alpha + \lambda r^{-\beta} - \left(N - 1 + \frac{\alpha}{2}\right) r^{\frac{\alpha}{2}-1} - 2\sqrt{\lambda} r^{\frac{\alpha-\beta}{2}} - \sqrt{\lambda}\left(1 - N + \frac{\beta}{2}\right) r^{-(1+\frac{\beta}{2})}. \tag{21}$$

Choosing now $H = H_0 + H_1$ with

$$H_1 = \left(N - 1 + \frac{\alpha}{2}\right) r^{\frac{\alpha}{2}-1} + 2\sqrt{\lambda} r^{\frac{\alpha-\beta}{2}} + \sqrt{\lambda}\left(1 - N + \frac{\beta}{2}\right) r^{-(1+\frac{\beta}{2})}, \tag{22}$$

we write $E_0(\lambda)$ for the Hamiltonian (6) as

$$E_0 = 0 + \frac{\int_0^\infty H_1 \, \mathrm{e}^{-R(r)} \, \mathrm{d}^N r}{\int_0^\infty \mathrm{e}^{-R(r)} \, \mathrm{d}^N r}. \tag{23}$$

In relation to (14), an extra λ-independent term in (22) exists. But this term does not affect the major λ-dependent contribution from (23) for $\lambda \ll 1$. Therefore, we may proceed in a manner similar to that followed earlier. Thus, a number of features emerge. The more important ones are the following:

(i) The leading λ-dependent term is of order λ for any β within $2 < \beta < N$.

(ii) At $\beta = (2N - 2)$, the primary correction term is of order $\sqrt{\lambda}$. More explicitly, this term is given by

$$\mu \bar{E}_{01} = \frac{2}{\Gamma\left(2N/(\alpha+2)\right)} \sqrt{\lambda} \left(\frac{\alpha+2}{4}\right)^{\frac{\alpha-\beta}{\alpha+2}}. \tag{24}$$

(iii) For $\beta > (2N - 2)$, a maximum in the numerator of the second part of (23) occurs at r_0, where we again find $r_0 \sim \lambda^{1/(\beta-2)}$, and therefore the overall correction goes as $\lambda^{(N-2)/(\beta-2)}$. The intermediate range may also be analysed (see the discussion around (18)) to arrive at the same characteristic dependence.

Note that all the conclusions reached above are common to both situations, i.e. they are independent of α, except for the numerical values of the coefficients. Thus, we have generalized the earlier scaling result that is known to be valid only for $\alpha = 2$.

Case III. Turning attention to the specific case of $\alpha = 4$ in (6) in 3D [12], let us try to find good estimates of E_0. The problem now becomes highly nontrivial. Looking at (22), we note that the λ-independent term here ($4r$) would make a fairly large contribution from all orders. So, (23) is not expected to perform nicely. Therefore, we choose to proceed through an approximate route, bypassing the direct one. To this end, we rewrite H in (6) as

$$H = h_0 + \sqrt{\lambda} h_1 \tag{25}$$

and define

$$h_0 = H_0 + 4r, \qquad h_1 = 2r^{2-\beta/2} + \left(\frac{\beta}{2} - 2\right) r^{-(1+\beta/2)}. \tag{26}$$

We then assume that

$$E_0 \approx \varepsilon + \sqrt{\lambda} \frac{\int_0^\infty h_1 \, \mathrm{e}^{-R(r)} \, \mathrm{d}^3 r}{\int_0^\infty \mathrm{e}^{-R(r)} \, \mathrm{d}^3 r}, \qquad R(r) = \frac{2}{3} r^3 + \frac{4\sqrt{\lambda}}{\beta - 2} r^{1-\frac{\beta}{2}}, \tag{27}$$

where ε signifies the minimum energy of h_0 when $\lambda = 0$. In other words, ε is the ground-state energy of $-\nabla^2 + r^4$. Denoting the lowest energy of the Hamiltonian $H = -\mathrm{d}^2/\mathrm{d}x^2 + x^4$ by ε_0, one can show that

$$\varepsilon = \left(\frac{5}{3}\right)^{1/3} 3\varepsilon_0. \tag{28}$$

Taking $\varepsilon_0 = 1.060\,362\,09$, one gets ε from (28) as 3.771 594 817. Putting this value in (27), estimates of E_0 for given β and λ are obtained. Here are the two sample results for which near-exact values, shown in parentheses, are available [12]. For $\lambda = 10^{-4}$, we get $E_0 = 3.79$ (3.84) at $\beta = 4$ and $E_0 = 3.95$ (4.09) at $\beta = 6$. The success is notable in view of the approximate nature and simplicity of our scheme, remembering further that $\lambda = 10^{-4}$ is not quite a weak perturbation.

Three more remarks are now in order. First, H_0 in case II or I does contain a supersingular potential part that is mixed with less singular ones. But E_0 in either case is zero. This means that it is not mandatory that we would get non-Taylor expansions for energy whenever supersingular potentials are present. However, Ψ_{00} reveals the odd $\sqrt{\lambda}$-type series on expansion. Secondly, our analysis based on the behaviour in the small-r and large-r region hints clearly that the exact wavefunction for any state of the general Hamiltonian in (6) would be of the form

$$\Psi_n \sim \exp\left[-\tfrac{1}{2}(Ar^a + Br^{-b})\right] \Phi_n, \tag{29}$$

where Φ_n stands for a function that takes due care of the intermediate-r behaviour and also of the nodes, if any. In effect, Φ_n corrects the H_1 part. So, it will also be a function of λ. However, it is unlikely to be as complicated a function of λ as E_n is. This is because the peculiar λ-dependence of E_n originates from the lower limit of the integrals involved in the average potential energy. The B factor in (29) provides this, as we have seen. Thus, while it is traditionally believed that one loses finer features after an averaging, here in studies on supersingular perturbations we may observe the opposite. Finally, the $\sqrt{\lambda}$-dependence of B

in (29) clarifies the vestigial effect [3]. In the limit $\lambda \to 0$, $H(\lambda)$ assumes a λ-independent form, but $\Psi_n(\lambda)$ does not. The latter requires a stronger condition, namely $\sqrt{\lambda} \to 0$, to achieve a similar end. This inequivalence is possibly the root behind the observed non-Taylor series in such contexts.

In summary, we have presented here a simple, straightforward way to show how the primary energy correction may sometimes depend nonlinearly on λ, leading to non-Taylor expansions. Our analysis yields the precise nature of λ-dependence as well. We have also generalized the earlier scaling result to include $H(\lambda)$ in (6) and noted some sort of universality. Further work along similar lines may be rewarding.

References

[1] Klauder J R 1973 *Acta. Phys. Aust.* S **11** 341
[2] Detwiler L C and Klauder J R 1975 *Phys. Rev.* D **11** 1436
[3] Ezawa H, Klauder J R and Shepp L A 1975 *J. Math. Phys.* **16** 783
[4] Harrell E M 1977 *Ann. Phys., NY* **105** 379
[5] Killingbeck J 1982 *J. Phys. B: At. Mol. Phys.* **15** 829
[6] Znojil M 1989 *J. Math. Phys.* **30** 23
[7] Znojil M 1990 *J. Math. Phys.* **31** 108
[8] Aguilera-Navarro V C and Guardiola R 1991 *J. Math. Phys.* **32** 2135
[9] Aguilera-Navarro V C, Fernández F M, Guardiola R and Ros J 1992 *J. Phys. A: Math. Gen.* **25** 6379
[10] Hall R L and Saad N 2000 *J. Phys. A: Math. Gen.* **33** 569
[11] Hall R L, Saad N and Kvickzky A 2001 *J. Phys. A: Math. Gen.* **34** 1169
[12] Killingbeck J, Jolicard G and Grosjean A 2001 *J. Phys. A: Math. Gen.* **34** L367
[13] Bhattacharjee J K and Bhattacharyya S 2003 *J. Phys. A: Math. Gen.* **36** L223
[14] Datta S and Bhattacharjee J K 2003 *Eur. Phys. J.* B **31** 247
[15] Killingbeck J 1977 *Rep. Prog. Phys.* **40** 963