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2005 J. Phys. A: Math. Gen. 38 3857

(http://iopscience.iop.org/0305-4470/38/17/010)

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

J. Phys. A: Math. Gen. **38** (2005) 3857–3867 doi:10.1088/0305-4470/38/17/010

Multiple scales analysis of Hamiltonians with short-range potentials

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Received 29 September 2004, in final form 28 January 2005
Published 13 April 2005
Online at stacks.iop.org/JPhysA/38/3857

Abstract

The formal asymptotic expansion in ϵ of the eigenvalues and eigenfunctions of a family of one-dimensional Hamiltonians $-\mathrm{d}^2/\mathrm{d}x^2 + V(x) + 1/\epsilon W(x/\epsilon)$ is considered in the limit $\epsilon \to 0$, using the technique of multiple scales. For sufficiently localized short-range potentials W the $O(\epsilon^0)$ approximation can be found by the usual replacement of the function W by a δ-type distribution. A simple analytical formula is found which expresses the first-order correction in terms of the zeroth-order wavefunction and some moments of the function W.

PACS numbers: 03.65.Ca, 03.65.Ge, 02.30.Mv, 31.15.Md

1. Introduction

In 1931 Kronig and Penney [1] first modelled the potential seen by the electrons in a metal by a train of δ-functions. They were able to determine the exact energy eigenvalues of this model and thus exemplified the appearance of the band structure in metals. Later it was recognized that quite generally the Schrödinger equation for systems with only a discrete number of point potentials can be solved analytically [2] as they merely correspond to some alternative self-adjoint extensions of the free-particle Hamiltonian. In most textbooks on quantum mechanics, it is shown that δ-functions may be used to approximate short-range potentials provided that the other length scales in the system are large compared to the width of the potentials. The approximation of a point interaction by a limit of a family of some regular short-range potentials is called regularization. For other point interactions or in more than one dimension, it is not straightforward to express these as a limit of smooth potentials; for example, for the so-called δ'-potential [3–5] it is still a topic of actual research. In [5] approximations of δ' by local potentials are constructed and proved to converge (in the norm resolvent sense).

In the following, we will discuss in some sense the inverse question, as to whether it is possible to describe a short-range potential perturbation theoretically, starting from a δ-function in 0th order and treating the width of the potential as the small parameter. We are especially interested in deriving some simple expressions for the lowest order corrections to isolated energy eigenvalues and wavefunctions which are due to the finite width of the potential.

We will restrict ourselves to the study of the one-dimensional Hamiltonians

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) + \frac{1}{\epsilon}W(x/\epsilon) \tag{1}$$

where ϵ is a small parameter characterizing the width of the short-range potential $1/\epsilon W(x/\epsilon)$, which in the limit $\epsilon \to 0$ shall converge to a δ-function. Hence $W(x) \in L^1(\mathbb{R})$. This condition has to be sharpened when higher order corrections are considered. In the following, we shall assume that $\exp(a|x|)\, W(x) \in L^1(\mathbb{R})$ for some $a > 0$, as any long-range part may be included into the function $V(x)$, which we assume to be sufficiently well behaved, i.e., C^∞. An example of an admissible function W is a Gaussian $W(x/\epsilon) = \exp(-x^2/\epsilon^2)$. The functions in the range of definition of the operator H shall fulfil homogeneous boundary conditions on the boundary points $x_A < 0$ and $x_B > 0$. For the special case that $V(x) = 0$ and range of definition $\mathcal{D} \subset L^2(\mathbb{R})$, the ground state asymptotics has been carefully studied by Albeverio *et al* [2, 6], which made use of the fact that in the absence of V the Hamiltonian (1) is unitarily equivalent to $1/\epsilon^2(-\mathrm{d}^2/\mathrm{d}x^2 + \epsilon W(x))$, whose ground state asymptotics is known.

It is not possible to simply expand $W(x/\epsilon)$ in a power series in ϵ, as this function is essentially divergent at $\epsilon = 0$. Another possibility would be a moment expansion for the function W. If we define a functional Q which acts on functions $F(x)$, which are sufficiently smooth and localized (for a precise characterization of the domain cf [7, 8]), as

$$Q : F(x) \to 1/\epsilon \int W(x/\epsilon)F(x)\,\mathrm{d}x \tag{2}$$

we may replace the integral kernel $W(x/\epsilon)$ by its moment expansion

$$\frac{1}{\epsilon}W(x/\epsilon) \sim \frac{1}{\epsilon}\sum_{j=0}^{\infty}\frac{(-1)^j}{j!}\langle W(y)y^j\rangle_0\delta^{(j)}(y) = \sum_{j=0}^{\infty}\frac{(-\epsilon)^j}{j!}\langle W(y)\rangle_j\delta^{(j)}(x), \tag{3}$$

with $y = x/\epsilon$ and the definition of the nth moment $\langle f\rangle_n = \int_{-\infty}^{\infty}\mathrm{d}y f(y)y^n$. In the last step, we used the relations

$$\epsilon^{j+1}\delta^{(j)}(x) = \delta^{(j)}(y), \tag{4}$$

which can easily be derived from the fact that

$$\theta(x) = \theta(y), \tag{5}$$

and from $\mathrm{d}/\mathrm{d}y = \epsilon\mathrm{d}/\mathrm{d}x$. Here $\theta(x)$ is Heaviside's step function. We cannot use this moment expansion to construct a perturbation expansion for the Schrödinger equation linked with Hamiltonian (1), as the solutions of the zeroth-order equation have discontinuous first derivative and thus are not even in the space of test functions for tempered distributions[3].

Nevertheless some kind of moment expansion appears still desirable. As we have (at least) two well-separated length scales in the problem—one ~ 1 ($\hat{=}\epsilon^0$), the scale of the 0th order problem, and the other $\sim\epsilon$, the width of the narrow potential—it appears promising

[3] Colombeau [9, 10] has developed a mathematical formalism, the 'generalized function algebra', which allows one to treat products of distributions and which has been applied successfully to physical problems [11, 12]. It might be that the perturbation expansion in terms of moments can be consistently formulated in this method. However, in practice, regularizations similar to those performed in this paper have to be performed in that method, too.

to try a multiple scales expansion [13, 14]. While quite popular in engineering sciences, this method is only rarely used in quantum mechanics [15] and then mostly in the time domain (cf [16] for an application to chemical kinetics). A notable exception is the article by Hagedorn [17], which perhaps is conceptually closest to our analysis. Hagedorn studies the Born–Oppenheimer expansion with multiple scales techniques. He introduces two variables x and y to separate adiabatic from semiclassical behaviour. He uses operators that change dependence on the variable x into dependence on y to be able to treat x and y as if they were independent variables and so to provide a uniqueness criterion in the expansion.

The main new idea in the following will be to make extensive use of equations (4) and (5) to shift divergencies between the two length scales and thus avoid secular contributions. We shall call this shifting procedure 'balancing'.

The objective of the paper is twofold. On the one hand, we want to demonstrate that the method of multiple scales can be used to calculate advantageously perturbational corrections due to the finite range of the interactions. The method may be useful in a much broader range of quantum mechanical problems than the one studied. On the other hand, we will derive in section 2 explicit formulae for the first-order correction in ϵ to the energy and wavefunction which are new in this generality. The main results are equations (13), (26) and (29), which express the first-order corrections in terms of moments (24) of the function W and the zeroth-order wavefunction. The application of these final formulae does not require that the reader go through the derivation; only the zeroth-order wavefunction and some moments of the function W have to be calculated.

For the special case that the first-order correction vanishes we will also derive the second-order correction. In section 3 we show that these corrections coincide with exact results for some model systems that allow analytic solution.

2. Multiple scales analysis

Let $x = \epsilon y$. With $\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\partial}{\partial x} + \frac{1}{\epsilon}\frac{\partial}{\partial y}$, we rewrite the Hamiltonian (1) as

$$H = -\frac{1}{\epsilon^2}\frac{\partial^2}{\partial y^2} - \frac{2}{\epsilon}\frac{\partial^2}{\partial y \partial x} - \frac{\partial^2}{\partial x^2} + V(x) + \frac{1}{\epsilon}W(y). \tag{6}$$

We expand the eigenfunction and energy in series in ϵ,

$$\psi = \sum_i \epsilon^i \psi_i \qquad \text{and} \qquad E = \sum_i \epsilon^i E_i. \tag{7}$$

As in the limit $\epsilon \to 0$ the potential $1/\epsilon W(x/\epsilon)$ converges to a δ-function, we know that the expansion for both E and ψ generically starts with the term $O(\epsilon^0)$. Only if $\langle W\rangle_0 = 0$, will the zeroth-order term be absent. If $\langle W\rangle_0 \neq 0$, we assume that $\langle W\rangle_1 = 0$. This can always be achieved by an appropriate choice of the origin.

From now on, we treat the variables x and y as independent ones, but we will still make use of the identities (4) and (5) to avoid the appearance of either secular terms or terms that would violate the boundary conditions. Secular terms are contributions to ψ which change order on a replacement of x/ϵ by y or y by x/ϵ. Typical secular terms are powers of x or y. We will see that we can combine the boundary condition and the requirement that no secular terms shall appear in the single statement that

$$\psi_i(x, y) \sim f_i(x) + O(\epsilon^\infty) \tag{8}$$

in the limit $y \to \pm\infty$ with $f_i(x)$ independent of the sign of y. This is consistent with the view that functions of the variable y should make only a local contribution on the length scale

$O(\epsilon)$ and decay exponentially with increasing y; we may speak of an inner expansion. On a length scale $O(\epsilon^0)$, the terms that contribute to that outer expansion will depend only on x.

If we insert expressions (6) and (7) for H, ψ and E into the Schrödinger equation $H\psi = E\psi$ and collect like orders of ϵ, we get the perturbation expansion which begins with terms of order ϵ^{-2}.

Second order:

$$-\frac{1}{\epsilon^2}\frac{\partial^2\psi_0}{\partial y^2} = 0. \tag{9}$$

The general solution of this equation is a function linear in y with arbitrary dependence on x. To be non-secular, ψ_0 has to be a function of x only, $\psi_0(x, y) = \psi_0(x)$. The dependence on x will be determined from the higher order equations. The function $\psi_0(x)$ will have to fulfil the same boundary conditions as $\psi(x)$.

First order:

$$\frac{1}{\epsilon}\left\{-\frac{\partial^2\psi_1}{\partial y^2} + W(y)\psi_0\right\} = 0. \tag{10}$$

When the zeroth moment $\langle W(y)\rangle_0$ does not vanish, integration over y leads to secular terms, which increase $\propto |y|$ for large y. To avoid these terms, we add $-1/\epsilon\ \langle W\rangle_0\delta(y)\psi_0(x)$ to the first-order equation (10) and, as a counterbalance, $\langle W\rangle_0\delta(x)\psi_0(x)$ which is of zeroth order in ϵ and will show up in equation (14). This is the 'balancing' procedure which we shall use excessively when treating higher orders.

Integration with respect to y would lead to

$$\psi_1 = \int^{(2)y}[W - \langle W\rangle_0\delta(y)]\psi_0(x) + f_1(x). \tag{11}$$

Here we use the notation $\int^{(n)y}[f(y)] = \int^y \mathrm{d}y' \int_{-\infty}^{y'} \mathrm{d}y'' \cdots \int_{-\infty}^{y^{(n-1)}} \mathrm{d}y^{(n)} f(y^{(n)})$ with the constant of integration chosen in such a way that the result does not contain a constant term. While it is clear that we had to subtract the zeroth moment $\langle W\rangle_0\delta(x)$ from $W(x)$ to avoid secular terms we will now argue that it is also necessary to subtract the first moment[4] $-\langle W\rangle_1\delta'(x)$ although a W with nonzero first moment does not lead to secular terms as such. Instead integration over y gives a y-dependent term which has a sigmoid form when the first moment $\langle W(y)\rangle_1$ is non-vanishing. Specifically (and after replacing y by x/ϵ) we would get

$$\psi_1(x_{A/B}) \sim -\tfrac{1}{2}\langle W\rangle_1 \operatorname{sgn}(x_{A/B})\psi_0(x_{A/B}) + f_1(x_{A/B}) + O(\epsilon^\infty). \tag{12}$$

But later we will see that not only ψ_0 and ψ_1, but also f_1, will have to fulfil asymptotically the same homogeneous boundary conditions, which is not possible[5]. Therefore we will subtract the 1st moment $-1/\epsilon\ \langle W\rangle_1\delta'(y)\psi_0(x)$ from equation (10) and, as a counterbalance, add $-\epsilon\langle W\rangle_1\delta'(x)\psi_0(x)$, which will show up in the first-order equation (22).

We find

$$\psi_1 = \int^{(2)y}[W - \langle W\rangle_0\delta(y) + \langle W\rangle_1\delta'(y)]\psi_0(x) + f_1(x) = \int^{(2)y}[\tilde{W}]\psi_0(x) + f_1(x). \tag{13}$$

Here we use the abbreviation $\tilde{f}(y) = f(y) - \langle f\rangle_0\delta(y) + \langle f\rangle_1\delta'(y)$.

Zeroth order:

$$-\frac{\partial^2\psi_2}{\partial y^2} - 2\frac{\partial^2\psi_1}{\partial y\partial x} + W(y)\psi_1 - \frac{\partial^2\psi_0}{\partial x^2} + V(x)\psi_0 + \langle W\rangle_0\delta(x)\psi_0(x) = E_0\psi_0. \tag{14}$$

[4] Due to our definition of the potential W this can only happen if $\langle W\rangle_0 = 0$. The reasoning also applies to the equations for the higher order corrections where the corresponding moments generically will not vanish.

[5] This can easily be seen, e.g., for the special boundary conditions $\psi_{0/1}(x_A) = \psi_{0/1}(x_B)$ and $f_1(x_A) = f_1(x_B)$.

Here, a new class of inhomogeneous terms appears, which may inject secular terms into the perturbation series: those terms, which depend only on x and not on y, are solutions of the homogeneous equation and would therefore give rise to solutions that increase linearly with y. They cannot be cancelled by subtraction of some δ-functions and hence have to vanish identically. This condition determines ψ_0 completely,

$$-\frac{\partial^2\psi_0}{\partial x^2} + V(x)\psi_0 + \langle W\rangle_0\delta(x)\psi_0(x) = E_0\psi_0. \tag{15}$$

This kind of singular Schrödinger equation is discussed in any text book on quantum mechanics. A rigorous discussion can be found in [18, 19]. Thus we have recovered the result that the function $1/\epsilon W(x/\epsilon)$ converges to $\langle W\rangle_0$ times a δ-function. The function $\psi_0(x)$ generically will have a discontinuous derivative at $x = 0$, so that we cannot allow for a δ-function when balancing. This is the reason why we chose $\langle W\rangle_1 = 0$ if $\langle W\rangle_0 \neq 0$. In the special case $\langle W\rangle_0 = 0$, the first moment $\langle W\rangle_1$ will in general be non-vanishing. However, $\psi_0'(x)$ is continuous in that case, so that the balancing term containing a δ-function is well defined[6].

The equation that determines ψ_2 now reads

$$\frac{\partial^2\psi_2}{\partial y^2} = -2\frac{\partial^2\psi_1}{\partial y\partial x} + W(y)\,\psi_1. \tag{16}$$

This equation is still not in its final form but we will have to modify it, subtracting δ-functions in y to remove secular contributions.

Let us first discuss the last term on the right-hand side: we add $(-\langle W\rangle_0\delta(y) + \langle W\rangle_1\delta'(y))$ $f_1(x)$ and $\epsilon\langle W\rangle_0\delta(x)f_1(x)$ and $-\epsilon^2\langle W\rangle_1\delta'(x)f_1(x)$ which will show up in equations (22) and (30), respectively. Furthermore we add

$$\left(-\left\langle W\int^{(2)y}[\tilde{W}]\right\rangle_0\delta(y) + \left\langle W\int^{(2)y}[\tilde{W}]\right\rangle_1\delta'(y)\right)\psi_0 \tag{17}$$

to the zeroth order and balance it again with terms which are of first and second order in ϵ.

Balancing the term $-2\frac{\partial^2\psi_1}{\partial y\partial x}$ is more tricky. This term does induce secular terms in ψ_2 and is discontinuous in x. We shall first remove the discontinuity in x, as it impedes introduction of the δ-functions necessary to remove secular terms.

We split $\psi_0(x)$ into a part with continuous first derivative and a part with discontinuous derivative,

$$\psi_0(x) = \tfrac{1}{2}\langle W\rangle_0\psi_0(0)G_0(x)|x| + F_0(x). \tag{18}$$

Here $F_0(x)$ and $G_0(x)$ are C^1 with $F_0(0) = \psi_0(0)$, $G_0(0) = 1$ and $G_0'(0) = 0$. Furthermore we choose $G(x_{A/B}) = G'(x_{A/B}) = 0$. While we still have great freedom in the choice of $G_0(x)$, the function $F_0(x)$ results as a solution of

$$\left\{-\frac{\partial^2}{\partial x^2} + V(x) - E_0\right\}F_0 = \frac{1}{2}\langle W\rangle_0\psi_0(0)(E_0 - V(x))G_0(x)|x| \tag{19}$$

with the same boundary conditions as $\psi_0(x)$. As $G_0(x)$ is continuous, so $F_0''(x)$ will be, which will prove important for balancing. Using relation (5), we get rid of the terms discontinuous in x: we subtract the discontinuous part $-\langle W\rangle_0 G_0(x)\,\mathrm{sgn}(x)\int^y[\tilde{W}]\psi_0(0)$

[6] In [3, 4] it is shown that the *δ'-point interaction* cannot be approximated by a potential with vanishing average. This point interaction is characterized by the fact that its eigenfunctions are discontinuous $\lim_{\gamma\to 0}(\psi(|\gamma|) - \psi(-|\gamma|)) \propto \psi'(0)$. There is no contradiction with the appearance of a *δ'-distribution* in equations (13), (29) determining the first-order corrections in the case $\langle W\rangle_0 = 0$. Especially $\psi_0(x)$ will remain continuous. After replacement of y by x/ϵ it can be seen that $\psi_1(x)$ is continuous, too.

and balance it in the same order by $-\langle W\rangle_0 G_0(x)\,\mathrm{sgn}(y)\int^y[\tilde{W}]\psi_0(0)$. All the remaining terms are C^1 in x so that we have no problems in balancing them. To that end we subtract $(-\langle W\rangle_0\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\rangle_1\delta(y)+\langle W\rangle_0\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\rangle_1\delta'(y))\psi_0(0)$ and balance it with terms $-\epsilon\,\langle W\rangle\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\rangle_0\delta(x)\psi_0(0)$ and $\epsilon^2\,\langle W\rangle\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\rangle_1\delta'(x)\psi_0(0)$.

From the term $-2\int^y[\tilde{W}]F_0'(x)\int^{(3)y}[\tilde{W}]$ we subtract $-2\langle\int^{(2)y}[\tilde{W}]\rangle\delta'(y)F_0'(x)$ and balance it by adding $-2\epsilon^2\langle\int^{(2)y}[\tilde{W}]\rangle\delta'(x)F_0'(x)$.

Hence the final equation for ψ_2, is

$$\frac{\partial^2\psi_2}{\partial y^2}=-2\int^y[\tilde{W}]F_0'(x)-\langle W\rangle_0\Big(\widetilde{\mathrm{sgn}(y)\int^y}[\tilde{W}]\Big)\psi_0(0)G_0(x)+2\left\langle\int^{(2)y}[\tilde{W}]\right\rangle\delta'(y)F_0'(x)+W\widetilde{\int^{(2)y}}[\tilde{W}]\psi_0(x)+\tilde{W}f_1(x). \tag{20}$$

We find

$$\psi_2=\int^{(2)y}\left[W\widetilde{\int^{(2)y}}[\tilde{W}]\right]\psi_0(x)-2\int^y\left[\widetilde{\int^{(2)y}}[\tilde{W}]\right]F_0'(x)+\left\langle\int^{(2)y}[\tilde{W}]\right\rangle F_0'(x)-\langle W\rangle_0\int^{(2)y}\left[\widetilde{\mathrm{sgn}(y)\int^y}[\tilde{W}]\right]\psi_0(0)G_0(x)+\int^{(2)y}[\tilde{W}]f_1(x)+f_2(x). \tag{21}$$

First order:

$$\epsilon\Bigg[-\frac{\partial^2\psi_3}{\partial y^2}-2\frac{\partial^2\psi_2}{\partial y\partial x}+W(y)\psi_2+\Bigg(\left\langle W\int^{(2)y}[\tilde{W}]\right\rangle_0-\langle W\rangle_0\left\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\right\rangle_0-\langle W\rangle_0\int^{2y}[\tilde{W}]\Big|_{y=0}\Bigg)\delta(x)\psi_0-\langle W\rangle_1\delta'(x)\psi_0-\frac{\partial^2\psi_1}{\partial x^2}+V(x)\psi_1+\langle W\rangle_0\delta(x)\psi_1(x)\Bigg]=\epsilon(E_0\psi_1+E_1\psi_0). \tag{22}$$

We have added $\epsilon\langle W\rangle_0\int^{2y}[\tilde{W}]\delta(x)\psi_0$ in the third line and subtracted $\epsilon\langle W\rangle_0\int^{2y}[\tilde{W}]\big|_{y=0}\delta(x)\psi_0$ in the second. Both terms are easily seen to balance each other by replacing $\delta(x)$ by $1/\epsilon\delta(y)$. This balancing is made unique by demanding that no terms dependent on y and containing $\delta(x)$ remain at the same time, as they would lead to a singular ψ_3. The part of ψ_1 which is proportional to ψ_0 solves the homogeneous equation in the third line. Hence the terms on the second and third line will be independent of y and we are left with an inhomogeneous equation for $f_1(x)$

$$-\frac{\partial^2 f_1}{\partial x^2}+V(x)f_1+\langle W\rangle_0\delta(x)f_1(x)-E_0f_1=(E_1-B\delta(x)+\langle W\rangle_1\delta'(x))\psi_0(x), \tag{23}$$

with

$$B=\left\langle W\int^{(2)y}[\tilde{W}]\right\rangle_0-\langle W\rangle_0\left\langle\mathrm{sgn}(y)\int^y[\tilde{W}]\right\rangle_0-\langle W\rangle_0\int^{2y}[\tilde{W}]\Big|_{y=0}=\left\langle W\int^{(2)y}[\tilde{W}]\right\rangle_0+\langle W\rangle_0\int^{2y}[\tilde{W}]\Big|_{y=0}. \tag{24}$$

Table 1. For a step pulse, a Gaussian and a Pöschl–Teller potential, the corresponding values of $\bar{B}$ are given.

$W(y)$	$\bar{B}$
$\theta(y+1/2)-\theta(y-1/2)$	1/6
$1/\sqrt{\pi}\exp(-y^2)$	0.398 942
$1/2\cosh^{-2}(y)$	1/2

The inhomogeneous equation for f_1 has a solution only if the inhomogeneity on the rhs is orthogonal to the homogeneous solution $\psi_0(x)$. This condition determines E_1. In the generic case $\langle W\rangle_0 \neq 0$ and $\langle W\rangle_1 = 0$ we find by partial integration

$$B = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y\, W(x)|x-y|W(y) \tag{25}$$

and

$$E_1\langle\psi_0|\psi_0\rangle = B\psi_0^2(0). \tag{26}$$

If we scale $W \to \alpha W$, the quantity B will be proportional to α^2 whence we introduce $\bar{B} := B/\langle W\rangle_0^2$, which will depend only on the shape of the function W but not on its strength.

In the exceptional case $\langle W\rangle_0 = 0$ and $\langle W\rangle_1 \neq 0$, the first-order energy correction will be

$$E_1\langle\psi_0|\psi_0\rangle = \langle W\rangle_1\psi_0(0)\psi_0'(0). \tag{27}$$

If we had not balanced the first moment already in -1^{st} order, equation (23) would be identical to the homogeneous equation (15) with E_0 fixed, but with boundary conditions $f_1(x_{A/B}) = 0$. In general, these boundary conditions are different from those for ψ_0, $\psi_0(x_{A/B}) = \psi(x_{A/B})$. In that case equation (15) could not be solved. Thus we have *a posteriori* justified the balancing of the first moment. This argumentation can be seen to hold also for higher order corrections.

The first-order correction to the wavefunction can easily be determined: the ansatz $f_1(x) = g_1(x)\psi_0(x)$ gives

$$-\frac{\partial^2 g_1}{\partial x^2}\psi_0 - 2\frac{\partial g_1}{\partial x}\frac{\partial\psi_0}{\partial x} = (E_1 - B\delta(x) + \langle W\rangle_1\delta'(x))\psi_0. \tag{28}$$

A special solution is

$$f_1(x) = -\psi_0(x)\int_0^x \mathrm{d}x' \frac{1}{\psi_0^2(x')}\int_0^{x'} \mathrm{d}x''\psi_0^2(x'')(E_1 - B\delta(x'') + \langle W\rangle_1\delta'(x'')). \tag{29}$$

In table 1 the first-order corrections $\bar{B}$ for a step pulse, a Gaussian and a Pöschl–Teller potential are compared. It can be seen that on descending the table, the functions displayed produce increasingly less accurate representations of the δ-function.

2.1. Higher orders and general structure of the perturbation expansion

We have shown how relations (5) and (4) can be used to systematically eliminate divergent or secular terms from the equations. However, the complexity of the equations that determine the higher order corrections increases rapidly.

While the moment expansion of the function W contains derivatives $\delta^{(n)}$ of all orders, in the perturbation series constructed only δ and δ' will show up. The ultimate reason behind this is the fact that we are studying a differential equation which is second order in y: if $f(x, y)$ is a function which falls off faster than any power of $|y|$, the same will hold true for

$\int^y [f(\tilde{x}, y)] = \int^y [f(x, y) - \langle f \rangle_0 \delta(y) + \langle f \rangle_1 \delta'(y)]$ and $\int^{(2)y} [f(\tilde{x}, y)]$. These are the only kinds of integrals that have to be evaluated when the differential equation in any order are solved.

There remains, however, one problem: when balancing, we generate terms of the form $\delta(x) f(x, y)$ and $\delta'(x) f(x, y)$. For these terms to be well defined, the function $f(x, y)$ has to be C^0 or even C^1 respectively. While we can balance any discontinuities using relation (5), we do not see a general mechanism to guarantee that the functions $f(x, y)$ become C^1 although we were able to satisfy this condition individually in all equations up to $O(\epsilon)$.

The evaluation of the second-order correction to the energy is most interesting when the first-order correction vanishes, which is seen to be the case when $\psi(0) = 0$. As an example, we consider the bound states with vanishing angular momentum in a three-dimensional central symmetric potential $V(r)$. After the substitution $\psi(r) = 1/r\phi(r)$, the equation for $\phi(x)$ is identical to equation (1) when we define $V(-x) = V(x)$ and $\psi(-x) = -\psi(x)$. Here, $\phi(r)$ is the wavefunction of the system. The calculation of the perturbation series is much simplified by $\delta(x)\psi(x) = 0$, which also implies that $F_0'(x) = \psi_0'(x)$.

Collecting terms second order in ϵ and concentrating on the contributions independent of y, we find that the energy E_2 can be determined from the equation

$$-\frac{\partial^2 f_2}{\partial x^2} + V(x) f_2 - E_0 f_2 = E_2 \psi_0 + 2 \left\langle \int^{(2)y} [\tilde{W}] \right\rangle_0 \delta'(x) \psi_0'. \tag{30}$$

The inhomogeneous term appeared when we balanced the zeroth-order equation. Equation (30) only has a solution when $E_2 = 2\langle \int^{(2)y} [\tilde{W}] \rangle_0 (\psi_0'(0))^2$ (we assume ψ_0 to be normalized). As can be shown by partial integration, we can alternatively write $E_2 = \langle W \rangle_2 (\psi_0'(0))^2$. Apparently, the non-vanishing correction of lowest order E_n is proportional to the lowest non-vanishing moment $W_n(y)$.

2.2. Multiple narrow potentials

It is easy to enlarge considerably the range of applicability of the results just derived to the case that several spiked potentials are present, i.e., instead of $1/\epsilon W(x/\epsilon)$, we will assume a potential of the form $1/\epsilon \sum_i W_i((x - x_i)/\epsilon)$. The zeroth-order approximation consists of a train of δ-functions $\sum_i \langle W_i \rangle_0 \delta(x - x_i)$ with x_i being the centre of gravity of the functions $W_i((x - x_i)/\epsilon)$. The first-order correction can then be evaluated as a sum of the first-order energies or wavefunctions determined from equations (26) and (13), respectively, with $\psi_0(0)$ replaced by $\psi_0(x_i)$ and y replaced by $y_i = (x - x_i)/\epsilon$.

3. Comparison with exactly solvable models

In the case $V(x) = 0$ and range of definition $x \in]-\infty, \infty[$, our expression for E_1 coincides with the results of Albeverio *et al*. However, these did not calculate the asymptotics of the wavefunction. For an attractive Pöschl–Teller potential $1/\epsilon W(x/\epsilon) = -1/(2\epsilon)[\cosh(x/\epsilon)]^{-2}$, we know the ground state wavefunction in dependence of ϵ, so that we can compare the approximation for the wavefunction. Also eigenenergies of the Pöschl–Teller potential are known analytically and we can expand them into a series in ϵ. With $A = 1/(2\epsilon)(\sqrt{1 + 2\epsilon} - 1) = 1/2 - \epsilon/4 + \epsilon^2/4 + O(\epsilon^3)$, we find

$$E = -A^2 \sim -\frac{1}{4} + \frac{\epsilon}{4} + O(\epsilon^2). \tag{31}$$

The ground state wavefunction is

$$\psi(x) = C \left[\cosh\left(\frac{x}{\epsilon}\right) \right]^{-\epsilon A}, \tag{32}$$

for which we can find asymptotic expressions. For $|x| \gg \epsilon$ (outer expansion) we find

$$\psi(x) \sim C\left(\frac{1}{2}\right)^{-\epsilon A} \exp(-A|x|) = C\left[1 - |x|/2 + \epsilon\left(|x|/4 + \frac{\ln 2}{2}\right) + O(\epsilon^2)\right], \tag{33}$$

while for $|x| \sim O(\epsilon)$ (inner expansion) we find

$$\psi(x) \sim C\{1 - \epsilon/2 \ln[\cosh(x/\epsilon)] + O(\epsilon^2)\}. \tag{34}$$

We may compare with the results of the preceding section. The normalized lowest order wavefunction is $\psi_0(x) = 1/\sqrt{2}\exp(-|x|/2)$, so that $\psi_0^2(0) = 1/2$, thence the first-order correction to the energy is $\epsilon \bar{B}\langle W\rangle_0^2\psi_0^2(0)/\langle\psi_0|\psi_0\rangle = \epsilon/4$, which coincides with equation (31). Furthermore,

$$\psi_0 \int^{(2)y} [\tilde{W}] = C\exp(-|x|/2)\left[-\frac{1}{2}\ln\cosh\left(\frac{x}{\epsilon}\right) + \frac{1}{2}\left|\frac{x}{\epsilon}\right|\right] \tag{35}$$

and

$$f_1(x) = \frac{\bar{B}}{2}\langle W\rangle_0^2|x|\psi_0(x) = \frac{1}{4}|x|\psi_0(x). \tag{36}$$

so that

$$\begin{aligned}\psi(x) \sim \psi_0(x)\left\{1 - \left[\epsilon\frac{1}{2}\ln\cosh\left(\frac{x}{\epsilon}\right) - \frac{1}{2}|x|\right] + \epsilon\frac{1}{4}|x|\right\} + O(\epsilon^2)\} \sim C\{1 - |x|/2 \\ - \left[\epsilon\frac{1}{2}\ln\cosh\left(\frac{x}{\epsilon}\right) - \frac{1}{2}|x|\right] + \epsilon\frac{1}{4}|x|\right\} + O(\epsilon^2)\} \text{ for } x \sim O(\epsilon).\end{aligned} \tag{37}$$

For $x = O(\epsilon^0)$ the term in square brackets is $\epsilon/2\ln 2 + O(\epsilon^\infty)$ so that the expansion (37) reduces to the outer expansion (33). For $x = O(\epsilon)$ expression (37) reproduces also the inner expansion (34). Therefore, the first-order correction is uniform.

As a check for other boundary conditions, which are not invariant under scaling, we consider a step function $W(y) = \theta(y + 1/2) - \theta(y - 1/2)$, and a box potential $V(x) = 0$ for $|x| < 1$, as the corresponding problem can be solved analytically. The eigenenergies corresponding to symmetric eigenfunctions are determined as solutions of the equation

$$\sqrt{E}\cot[\sqrt{E}(\epsilon/2 - 1)] = \sqrt{1/\epsilon - E}\tanh[\sqrt{1/\epsilon - E}\epsilon/2]. \tag{38}$$

From the zeroth-order equation $\sqrt{E_0}\cot(\sqrt{E_0}) = -1/2$ we infer the zeroth-order wavefunctions $\psi_0(x) = N\sin\{\sqrt{E_0}(|x|-1)]\}$ and $\psi_0^2(0) = 4E_0/(4E_0 + 3)$. On the other hand, equation (38) can be expanded into a series in ϵ from which we find $E_1 = 2E_0/3(4E_0 + 3) = \psi_0^2(0)/6$ and $E_2 = -E_0\big(-189+196E_0+1104E_0^2+960E_0^3\big)\big/180(4E_0+3)^3$. With $B = 1/6$ for the square potential, the expression for E_1 coincides with formula (26). For large E_0, $E_1 \sim 1/6$ and $E_2 \sim 16/3E_0$. Hence the first- and second-order energy corrections become comparable for $\epsilon = 1/(32E_0)$. The expansion for the odd functions is even simpler and can be used to check the correctness of the second-order result.

4. Conclusion

The aim of the paper was twofold. On the one hand, we have demonstrated that the technique of multiple scales can be used with advantage to derive perturbational expansions for families of Hamiltonians which contain short-range potentials. The perturbation parameter here is the width ϵ of these potentials.

As was expected, the eigenenergies and eigenfunctions in lowest order are solutions of a Schrödinger equation with a Hamiltonian in which the spiked potential is replaced by a Dirac

δ-function. The solution of this Schrödinger equation is well known. We derived the lowest order corrections to this result which are due to the nonzero extent of the spiked potentials. The corrections to the wavefunction are uniform in x. One advantage of the method of multiple scales is that it is not necessary to presuppose some special behaviour under scaling transformations as is the case in related methods, especially the treatment of Albeverio *et al* [2, 6]. Therefore, we could allow for families of Hamiltonians which contain additional slowly varying potentials besides the spiked potentials. In the special case that these slowly varying potentials were absent, our results reduce to the formulae found by Albeverio *et al*. The method of multiple scales allowed us to separate the corrections to the wavefunction into short-range contributions relevant on a scale ϵ and long-range contributions, which influence the wavefunction on a scale ϵ^0. Indeed, the long-range corrections, e.g., $f_1(x)$ are given as solutions of inhomogeneous differential equations, like of equation (23), in which only moments of the potential W occur in combination with some δ- or δ'-distribution. Hence the method implements directly the idea of a moment expansion. However, this expansion turns out to be much more complicated than the expansion (3), which stood at the beginning of our considerations.

On the other hand, we applied the multiple scales technique to a concrete one-dimensional family of Hamiltonians (1) with various spiked potentials from which we chose as examples, potentials of rectangular shape or of Gaussian and Pöschl–Teller type. Simple formulae for the first-order corrections to the eigenenergies and eigenfunctions were derived, namely formulae (26), (25) and (11), (29), respectively. The results have been compared with some special cases, for which the whole perturbation series can be derived by other methods.

Acknowledgments

One of us (FD) would like to thank Professor S H Lin for his hospitality and the IAMS of the Academia Sinica for financial support.

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