RAYLEIGH-SCHROEDINGER COEFFICIENTS FOR SINGULAR PERTURBATIONS OF THE DISCRETE SPECTRUM

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It is shown that the level shift of the even states in the discrete spectrum, produced by the singular perturbation $\lambda|x|^{-\nu}$, can be described by the standard Rayleigh-Schroedinger formulas only for $0 < \nu < 3/2$.

Singular perturbations of the form

$$\lambda W(x) = \lambda|x|^{-\nu} \quad (1)$$

are of considerable interest in mathematical physics and have been examined in a number of publications (see the review paper in [1]). However, a correct perturbation theory of the discrete spectrum has not so far been constructed because it leads to difficulties associated with the removal of divergences that arise when the matrix elements are evaluated.

We shall show here that a Rayleigh-Schroedinger perturbation theory exists in the case of a weak singularity ($1 \leq \nu < 3/2$ in the even case and $1 \leq \nu < 2$ in the odd case).

Consider the purely discrete spectrum of the Schroedinger equation ($\hbar = 2m = 1$)

$$\psi''(x) - (V(x) + \lambda|x|^{-\nu})\psi(x) + E\psi(x) = 0 \quad (2)$$

with an even, smooth confining potential $V(x)$ ($\lim_{x\to+\infty} V(x) = +\infty$, $V'(x) > 0$ for $x > x_0 > 0$, $V(-x) = V(x)$, $V(0) = 0$ for $x \to 0$ $V(x) \simeq C|x|^{\gamma}$, $C, \gamma > 0$).

When $\nu < 2$, (2) has two linearly independent solutions, namely, $\psi_{+\nu}(x)$, $\psi_{-\nu}(x) \in L_2(0, a)$, $a > 0$, whose behavior for $x \to +0$ is

$$\psi_{-\nu}(x) = x(1 + \lambda(2-\nu)(3-\nu)x^{2-\nu} + \ldots), \quad (3)$$

$$\psi_{+\nu}(x) = 1 - \lambda(2-\nu)(\nu-1)x^{2-\nu} + \ldots, \quad \nu \neq 2 - n^{-1}, \quad n = 1, 2, \ldots, \quad (4)$$

$$\psi_{+1}(x) = 1 + \lambda x(\ln x - 1) + \ldots. \quad (5)$$

When $\nu = 2 - n^{-1}$, the form of (4) becomes somewhat different, but this has no effect on any of our subsequent conclusions.

As $\lambda \to 0$, solution (3) becomes identical with the odd solution $\psi_-(x)$ of the unperturbed Schroedinger equation (2) with $\lambda = 0$, and solutions (4) and (5) become identical with the odd unperturbed solution $\psi_+(x)$.

The standard condition for even states

$$\psi'(0)\psi^{-1}(0)=0 \tag{6}$$

cannot be satisfied for the perturbation (1) because $\psi'_{+\nu}(0)$ is singular. We shall therefore construct the even solutions of (2) by performing the even continuation of the mixture of $\psi_{+\nu}$ and $\psi_{-\nu}$ to x < 0:

$$\psi_\alpha(x)=\cos\alpha\psi_{+\nu}(|x|)+\sin\alpha\psi_{-\nu}(|x|),\quad -\pi/2<\alpha<\pi/2. \tag{7}$$

As $x \to 0$, the functions (7), like (3)-(5), satisfy a boundary condition that is independent of E.

The choice $\alpha = \pi/2$ made in [2] leads to the absence of continuity in λ as we pass from the even solutions of (2) ($\lambda = 0$) to the functions given by (3).

The choice of the even solution of (2) in the form given by (7) automatically leads to a change of (2) because the function (7) satisfies the Schroedinger equation with the additional point potential

$$\psi''(x)+(E-V(x)-\lambda W(x)-U(x))\psi(x)=0, \tag{8}$$

$$U(x)=2\delta(x)\frac{d\ln\psi(|x|)}{d|x|}, \tag{9}$$

$$U(x)=\begin{cases} 2\delta(x)|x|^{-1}\sum_{k=1}^{q}\lambda^k h_k(\nu)|x|^{(2-\nu)k}+2\delta(x)\operatorname{tg}\alpha,\ \alpha\neq\frac{\pi}{2}, & (10)\\ \nu\neq 2-n^{-1},\ n=1,\ 2,\ldots,\ h_1(\nu)=-(\nu-1)^{-1},\ q=\varepsilon((2-\nu)^{-1}), & \\ 2\lambda\ln|x|\delta(x)+2\delta(x)\operatorname{tg}\alpha,\quad \nu=1, & (11)\\ \pm 2\delta(x)|x|^{-1},\quad \alpha=\pm\pi/2. & (12)\end{cases}$$

where $\varepsilon(z)$ is the integer part of z and the coefficients $h_k(\nu)$ do not depend on V(x). The expressions given by (10) and (11) were obtained in [10] by functional integration but without the last term.

Different possible choices of the mixing parameter α have been discussed in the literature [2,4].

We shall not examine this question here and will assume that the mixing angle α is given. The λ-independent part of the potential (9) is naturally included in the unperturbed potential as the part that vanishes as $\lambda \to 0$ can be regarded as an additional perturbation which cannot be excluded by any choice of $\alpha \neq \pi/2$.

Let us examine the case $\alpha = 0$ in greater detail. The total perturbation $\lambda W(x)$ in this case has the form ($1<\nu<2,\ \nu\neq 2-n^{-1},\ n=2,3\ldots$)

$$W(x)=|x|^{-\nu}-2(\nu-1)^{-1}|x|^{1-\nu}\delta(x)+\lambda h_2(\nu)|x|^{3-2\nu}\delta(x)+\ldots, \tag{13}$$

and there is no unperturbed potential. Even normalization of the function for the unperturbed potential will be denoted by $\psi_{n+}(x)$, $n=0,1,2,$ and the energy levels by $E^{(0)}_{n+}$ (as $x \to 0$, we have $\psi_{n+}(x)\simeq C_n+d_nx^2+\ldots$).

When $\nu \to 3/2$, the total perturbation is linear in λ (10):

$$W(x)=|x|^{-\nu}-2(\nu-1)^{-1}|x|^{1-\nu}\delta(x) \tag{14}$$

and, despite the fact that each of the terms in the perturbation matrix element

$$W_{kn}=\int_{-\infty}^{\infty}\psi_{k+}W(x)\,\psi_{n+}\,dx \tag{15}$$

diverges, the total matrix element is finite and single-valued:

$$\begin{aligned} W_{kn}&=2\int_{0}^{\infty}\psi_{k+}\psi_{n+}\left(x^{-\nu}-2(\nu-1)^{-1}x^{1-\nu}\delta(x)\right)dx=\\ &=2\lim_{a\to+0}\int_{a}^{\infty}\psi_{k+}\psi_{n+}\left(x^{-\nu}-2(\nu-1)\,x^{1-\nu}\delta(x-a)\right)dx=\\ &=2\lim_{a\to+0}\Big[-(\nu-1)^{-1}x^{1-\nu}\psi_{k+}\psi_{n+}\Big|_{a}^{\infty}-(\nu-1)^{-1}a^{1-\nu}\psi_{k+}(a)\,\psi_{n+}(a)+\\ &+(\nu-1)^{-1}\int_{a}^{\infty}x^{1-\nu}(\psi_{k+}\psi_{n+})'\,dx\Big]=2(\nu-1)\int_{0}^{\infty}(\psi_{k+}\psi_{n+})'\,x^{1-\nu}\,dx. \end{aligned} \tag{16}$$

The matrix element cannot be regularized for $\nu \geq 3/2$: divergences $\sim\lambda$, λ^2 due to the following terms in the point perturbation $U(x)$ (10) are found to remain. Attempts to introduce counterterms into the Schroedinger equation for $\nu \geq 3/2$ (by analogy with quantum field theory) have been found to lead to a contradiction.

When $\nu = 1$, the function $\psi_{+1}(x)$ has a logarithmic singularity [5] and, according to (11), the matrix element for $\alpha = 0$ is

$$W_{kn}=-2\int_{0}^{\infty}\ln x\,(\psi_{k+}\psi_{n+})'\,dx. \tag{17}$$

When $0 < \nu < 1$, the point potential in the matrix element does not provide a contribution, and we have the usual "good" perturbation theory.

Thus, matrix elements for even functions are finite only for $\nu < 3/2$. However, the finiteness of (16) and (17) is not sufficient for the existence of the Rayleigh-Schroedinger coefficients of the perturbation theory series (series in powers of λ) for the energy levels and wave-function projections onto the unperturbed state. The Rayleigh-Schroedinger coefficients may diverge when the sums in the higher orders diverge [1], [5, pp. 163-166]:

$$\left.\begin{aligned} &E_n=\sum_{l=0}^{\infty}\lambda^l\,\Delta E_n^{(l)},\\ &(\psi_{n+1},\ \psi_m)=\sum_{l=0}^{\infty}\lambda^l\,\Delta\psi_{nm}^{(l)},\\ &\Delta E_n^{(0)}=E_n^{(0)},\ \ \Delta E_n^{(1)}=W_{nn},\ \ \Delta E_n^{(2)}={\sum_i}'\,W_{ni}\mu_{in},\\ &\Delta\psi_{nm}^{(0)}=\delta_{nm},\ \ \Delta\psi_{nm}^{(1)}=W_{mn}\mu_{nm}(1-\delta_{mn}), \end{aligned}\right\} \tag{18}$$

where $\psi_n(x)$ are the normalized solutions of the Schroedinger equation (2) and $\mu_{nn}=(E_n^{(0)}-E_k^{(0)})^{-1}$. The convergence of the sums in (18) and, especially, for the higher order corrections, is determined by the behavior of the levels $E_n^{(0)}$ and the matrix elements (16) and (17) for $n \to \infty$.

Highly excited states ($n \gg 1$) are satisfactorily described quasiclassically and quasiclassical functions can also be used in perturbation theory to evaluate the matrix element [5, pp. 206-225].

We shall assume from now on that

$$V(x)=|x|^{\gamma},\ \gamma>0 \tag{19}$$

which significantly simplifies the derivations but has no effect on the final conclusions.

The quasiclassical levels and wave functions in the potential defined by (19) are given, to within an order of magnitude, by

$$\psi_{n+}=N_n k_n^{-1/2}(x)\cos\beta_n(x), \tag{20}$$

where n labels the sequence of states and

$$\beta_n=\int_0^x k_n(y)\,dy, \tag{21}$$

$$k_n(x)=(E_n^{(0)}-x^{\gamma})^{1/2}, \tag{22}$$

$$E_n^{(0)}\sim n^{\frac{2\gamma}{\gamma+2}}, \tag{23}$$

$$N_n\sim n^{\frac{\gamma-2}{2(\gamma+2)}}. \tag{24}$$

Formula (20) is valid only for the internal region, well away from the right turning point x_{n0} (behind which $\psi_n\sim\exp[-2x^{(\gamma+2)/2}(\gamma+2)^{-1}]$).

From (20)-(24), we obtain the following expression for the matrix elements (16) in the case of fixed l and $n\to\infty$:

$$W_{ln}=C\int_0^b(\psi_{l+}\psi_{n+})'\,x^{1-\nu}\,dx=CN_n k_n^{1/2}\int_0^b x^{1-\nu}\psi_{l+}\sin k_n x\,dx, \tag{25}$$

where $x_{l0}<b\ll x_{n0}$,

$$k_n=k_n(0)=E_n^{1/2}\infty n^{\gamma/(\gamma+2)}, \tag{26}$$

and we have carried out differentiation in (25) after expanding the phase (21) in powers of x and retaining only the terms that show the maximum rate of increase for large n. Since $\psi_{l+}(x)$ is smooth and the integrand in (25) has a singularity of the form $x^{1-\nu}=x^{(2-\nu)-1}$, we can use the following well-known formula [16] to find the principal term in the asymptotic behavior of the integral in (25):

$$\int_\alpha^\beta e^{inx}(x-\alpha)^{\xi-1}\varphi(x)\,dx=C\varphi(\alpha)n^{-\xi},\quad 0<\xi<1,\ n\to\infty, \tag{27}$$

which yields the following asymptotic expression for the matrix elements (16):

$$W_{ln}=n^{w_l},\ w_l=(\gamma+2)^{-1}[\gamma(\nu-1)-1]. \tag{28}$$

If on the other hand $l, n\gg 1$, $l/n\infty 1$, similar estimates yield

$$W_{ln}\infty N_l N_n k_l^{1/2}k_n^{1/2}(k_l+k_n)^{\nu-2}, \tag{29}$$

$$W_{nn}\infty n^{w},\ w=(\gamma+2)^{-1}[\gamma(\nu-1)-2]. \tag{30}$$

Among the terms that appear in the Rayleigh-Schroedinger coefficients for the energy levels and wave-function projections [1], [5, pp. 163-166], the most rapidly increasing with ν are the coefficients appearing in the sum of the form

$$\sum_s = \sum'_{i_1, i_2, \ldots, i_s} W_{ni_1}\mu_{i_1 n} W_{i_1 i_2}\mu_{i_2 n} \ldots \mu_{i_s n} W_{i_s m}. \tag{31}$$

The convergence of (31) can be estimated by replacing summation for $i_j \gg 1$, $j = 1, 2 \ldots s$ with integration with respect to $dx_{i_1} dx_{i_2} \ldots dx_{i_s}$ and introducing the s-dimensional polar coordinates, as usual in field theory [7]. After integration with respect to the angles, the sum

$$\sum_s \sim \int^{\infty} \rho^{-1-q_s} d\rho \tag{32}$$

converges as $\rho \to \infty$, or the integral (32) converges, i.e., by hypothesis,

$$q_s(\gamma, \nu) > 0. \tag{33}$$

The Rayleigh-Schroedinger perturbation theory is meaningful if all the Rayleigh-Schroedinger coefficients exist (converge), i.e., condition (33) is valid for all s = 1, 2, ... When $n_{ij} \gg 1, n, m$ fixed, we have

$$\mu_{i_j n} = (E_{i_j}^{(0)} - E_n^{(0)})^{-1} \simeq (E_{i_j}^{(0)})^{-1} \sim \rho^{\mu}, \quad \mu = 2\gamma(\gamma+2)^{-1}. \tag{34}$$

Since the volume element of the s-dimensional space is $dV_s \infty \rho^{s-1} d\rho$, we find that

$$q_s = -2w_b - (s-1)w + s\mu - s, \tag{35}$$

which together with (28), (30), and (34) yields

$$q_s = \gamma(\gamma+2)^{-1}[2s+1-(s+1)\nu]. \tag{36}$$

The converges conditions (33) are equivalent to

$$\nu < 2-(s+1)^{-1}, \quad s = 1, 2, \ldots, \tag{37}$$

i.e., the Rayleigh-Schroedinger coefficients exist for all $\gamma > 0$ and the same condition

$$\nu < 3/2, \tag{38}$$

as for the matrix elements.

In view of the foregoing, we consider that, for $0 < \gamma < 3/2$, we can take (4) or (7) as the even state functions in the discrete spectrum. The behavior of the matrix elements and the Rayleigh-Schroedinger coefficients is then analogous to the behavior for the functions (4). The use of (3) as the even functions [2] is undesirable because of the two-fold degeneracy in parity. These functions must undoubtedly be taken as the odd functions for all ν. The functions can be continued evenly only for $\nu \geq 3/2$, in which case there is no Rayleigh-Schroedinger perturbation theory for the states (4) and (7). To justify this choice ($\alpha = \pi/2$, $\nu \geq 3/2$) and to determine the upper limit of ν for which the Rayleigh-Schroedinger perturbation theory is still valid, we must carry out estimates analogous to (28), (29), (30), and (38) in the even case ($0 \leqslant r \leqslant \infty$, $\psi(r) = \psi_{-\nu}(r)$).

The final result is that instead of (38) we now have

$$\nu<2+(1+s)^{-1}, \tag{39}$$

i.e., all the Rayleigh-Schroedinger coefficients exist for $\nu < 2$. The fact that the Rayleigh-Schroedinger perturbation theory is not valid for $\nu \geq 2$ is not unexpected because such a strong singularity produces a fall on the center (bottom of the well) for $\lambda < 0$ [5, p. 145]. However, for $\nu < 3$, the energy levels can be expanded into a series in powers of λ by methods other than the Rayleigh-Schroedinger perturbation theory [8]. The energy levels are analytic in λ in the even case as well, when $3/2<\nu<2$; $\nu=2$, $|\lambda|<1/4$.

We note that, as the perturbation parameter ν passes through the boundary values $\nu = 3/2$, $\nu = 2$, the exact even and odd functions change their behavior (3), (4) for $x = 0$. The derivative of the even function (4) ceases to be square integrable at $\nu = 3/2$. For the odd function, we have instead of (3) the expression $\psi_{-}(x) \infty x^{\nu/4} \exp(-2\sqrt{\lambda}(\nu-2)^{-1}x^{-(\nu-2)/2}$, $x\to+0$, $\nu>2$, $\lambda>0)$ [5, p. 215].

Since our main conclusions, i.e., the existence of the matrix elements and the Rayleigh-Schroedinger coefficients for $\nu < 3/2$ in the even case and the existence of the Rayleigh-Schroedinger coefficients for $\nu < 2$ in the odd case, is independent of the quantity $\gamma > 0$, the conclusions must also be valid for any smooth even confining potential. This amounts to a rehabilitation (contrary to [9]) of perturbation theory for weakly singular perturbations ($1 \leq \nu < 3/2$) of the even states in the discrete spectrum, so that we may look upon this quantum-mechanical problem as a model of quantum field theory in which Feynman diagrams correspond to the Rayleigh-Schroedinger series.

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