Perturbation Theory for Weakly Bound States

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The presence of level energy branch points as a function of perturbation parameter is characteristic for two cases when the applicability of perturbation theory is violated for a discrete level (several close levels and a level close to the continuous-spectrum boundary). A modified perturbation theory developed in the present paper for the second case yields the level width, providing the level becomes quasistationary under action of the perturbation.

1. The condition for applicability of ordinary perturbation theory (PT) for a discrete eigenvalue of the Hamiltonian $H = H^{(0)} + \lambda V^{(1)}$ ($H^{(0)}$ is the unperturbed Hamiltonian, $\lambda V^{(1)}$ is the perturbation, and λ is a parameter) is violated if two eigenvalues of the unperturbed problem, $E_1^{(0)}$ and $E_2^{(0)}$,

$$H^{(0)}\Psi_m^{(0)} = E_m^{(0)}\Psi_m^{(0)}, \tag{1}$$

are close to each other. In this case the problem calls for a special analysis, which is similar to the PT for a degenerate state and leads to the following expression for the energy levels[1]:

$$E_{1,2} = {}^1/_2(E_1^{(0)} + E_2^{(0)} + \lambda V_{11}^{(1)} + \lambda V_{22}^{(1)}) \pm [{}^1/_4(E_1^{(0)} - E_2^{(0)} + \lambda V_{11}^{(1)} - \lambda V_{22}^{(1)})^2 + \lambda^2 |V_{12}^{(1)}|^2]^{1/2}, \tag{2}$$

where $V_{mn}^{(1)} = \langle \Psi_m^{(0)} | V^{(1)} | \Psi_n^{(0)} \rangle$.

The eigenvalues $E_n(\lambda)$ are different branches of one multiple-valued analytic function $E(\lambda)$. From this point of view, formula (2) is an approximation of the function $E(\lambda)$ in the region of interest to us, such that account is taken of the presence of two branch points:

$$\lambda_{br}^{(+)} = \frac{E_2^{(0)} - E_1^{(0)}}{V_{11}^{(1)} - V_{22}^{(1)} \pm 2i|V_{12}^{(1)}|}, \tag{3}$$

symmetrically arranged about the real axis λ.

States with low binding energy are important both in atomic physics (negative ion) and in nuclear physics (deuteron). In this case the condition for applicability of PT is violated because of the proximity of the boundary of the continuous spectrum (which we shall choose as the null point of the energy), so that it is necessary to take into account effectively an infinite number of states of the continuum. This can be done in simplest fashion by considering the Jost function $f_l(k, \lambda)$ of the complete problem (with perturbation (where k is the momentum ($E = k^2/2$) and l is the orbital angular momentum; we assume now that both $H^0 = -{}^1/_2\nabla^2 + V(r)$ and $V^{(1)}(r)$ are spherically symmetrical. The zeroes of the function $f_l(k, \lambda)$, as is well known, correspond to bound and quasi-stationary states.

The trajectories of the zeroes as functions of the potential were investigated in detail by Demkov and Drukarev[2]. With decreasing depth of the potential well, the zero that describes the bound state moves downward along the imaginary axis in the plane of the complex momentum k. Moving upwards in opposition is the zero corresponding to the virtual state. After coalescing at a certain point k_{br} on the imaginary axis in the lower k half-plane, the zeroes become complex (if $l \neq 0$, then $k_{br} = 0$). Obviously, k_{br} is a branch point of the function $k(\lambda)$ (or of the function $E(\lambda) = {}^1/_2 k(\lambda)^2$).

The presence of this point must be taken into account in PT for weakly-bound states, if this point lies close to the origin. We emphasize that for the ground s state the corresponding zero of the Jost function may be "unpaired" (see[2]), so that there is no coalescence point at all.

2. Let us analyze first the case of the s states. According to[2], the point k_{br} lies close to the point $k = 0$ if the effective radius ρ for scattering by the potential is negative and has a large absolute magnitude in comparison with the radius R of the potential well; in this case

$$k_{br} \approx i/\rho. \tag{4}$$

If we know the energy $E_1^{(0)} = {}^1/_2 k_1^{(0)2}$ and the wave function $\varphi_0^{(1)}(r)$ of the weakly-bound state

$$-\frac{1}{2}\frac{d^2}{dr^2}\varphi_1^{(0)} + V\varphi_1^{(0)} = E_1^{(0)}\varphi_1^{(0)}, \tag{5}$$

then we can approximately determine ρ:

$$\rho \approx 2\int_0^\infty \left[\exp(2ik_1^{(0)}r) - \frac{\varphi_1^{(0)}(r)^2}{\varphi_1^{(0)}(R)^2}\right] dr. \tag{6}$$

The simplest approximate expression for the function $k(\lambda)$, which takes into account the presence of the indicated branch point, is

$$k(\lambda) = k_1^{(0)} - a + \lambda b \pm \sqrt{a^2 + 2\lambda ac}, \tag{7}$$

where a, b, and c are certain constants, which we shall define later; the plus sign corresponds to the bound state at $\lambda = 0$ ($k(0) = k^{(0)}$). Expression (7) is analogous to (2) and differs from it only in that here there is only one branch point $\lambda_{br} = -a/2c$, corresponding to the unphysical sheet of the complex energy. Assume that we know in addition to $k_1^{(0)}$ and $\varphi_1^{(0)}$ also the position of the virtual level $k_2^{(0)}$ closest to the origin and the corresponding wave function $\varphi_2^{(0)}$. It is then necessary to put $a = (k_1^{(0)} - k_2^{(0)})/2$ in order to satisfy $k(0) = k_2^{(0)}$ when choosing the minus sign in (7). The constants b and c can be determined from the condition that when (7) is expanded in powers of λ in the vicinity of the point $k_1^{(0)}$ it is necessary to satisfy the equality

$$k_1 = k_1^{(0)} + \lambda U_{11} + O(\lambda^2), \tag{8}$$

where

$$U_{11} = \int_0^\infty V^{(1)}\varphi_1^{(0)}(r)^2\, dr \left[k_1^{(0)}\int_0^\infty (\varphi_1^{(0)}(r)^2 - \varphi_1^{(0)}(R)^2 \cdot$$

$$\times \exp\{2ik_1^{(0)}r\})\,dr + \frac{1}{2i}\varphi_1^{(0)}(R)^2\Big]^{-1},$$

and also from the analogous condition for the point $k_2^{(0)}$. Equation (8) agrees with ordinary perturbation theory and is valid for bound as well as for virtual and quasistationary states (see[3]); it can be obtained from (12), as will be shown in detail below for the case $k_1^{(0)} = 0$.

The final formula for $k(\lambda)$ is

$$k(\lambda) = {}^1/_2(k_1^{(0)} + k_2^{(0)} + \lambda U_{11} + \lambda U_{22}) \pm [{}^1/_4(k_1^{(0)} - k_2^{(0)})^2 + {}^1/_2\lambda(U_{11} - U_{22})(k_1^{(0)} - k_2^{(0)})]^{1/2}. \quad (10)$$

3. The case of arbitrary l can be considered by first constructing the PT for the limiting case of a level with zero energy $E^{(0)} = 0$. To this end we expand the left side of the equation defining the $k(\lambda)$ dependence,

$$f_l(k, \lambda) = 0, \quad (11)$$

in powers of λ and equate the expansion coefficients to zero. At $\lambda = 0$ the function $f_l(k, \lambda)$ goes over into the Jost function of the unperturbed problem, which in the case of interest to us has, by definition, a zero at the point $k = 0$:

$$f_l(0, 0) = 0. \quad (12)$$

Introducing the notation

$$f_{mn} = \frac{\partial^{m+n} f_l(k, \lambda)}{\partial k^m \partial \lambda^n}\Big|_{k=\lambda=0},$$

we obtain at $l = 0$, in first order in λ,

$$f_{10}k(\lambda) + f_{01}\lambda = 0, \quad (13)$$

which leads, when account is taken of the formulas given in the Appendix for f_{mn}, to the following expression for the energy:

$$E = -2\lambda^2\left[\int_0^\infty \varphi_0^{(0)}(r)^2 V^{(1)}\,dr \Big/ \varphi_0^{(0)}(R)^2\right]^2, \quad (14)$$

i.e., the s term always touches the boundary of the continuous spectrum[4]. Thus, for weakly bound s states the PT should be modified already in first order.

If $l \neq 0$, then the zeroes of the Jost function always coalesce at the point $k = 0$, which is thus a branch point ($\lambda_{br} = 0$) of the function $K(\lambda)$, unlike the s states, where the position of the branch point depends on the potential.

As shown in the Appendix, $f_{mn} = 0$ if m is odd and $m < 2l$. It is easy to verify that this leads to the following expansion for $k(\lambda)$:

$$k(\lambda) = \sum_{j=1}^{l} a_j\lambda^{j-1/2} + \sum_{j=2l}^{\infty} b_j\lambda^{j/2}, \quad (15)$$

where, for example, a_1 is determined from the condition ${}^1/_2 a_1^2 f_{20} + f_{01} = 0$:

$$a_1 = \pm\left[2\int_0^\infty V^{(1)}\varphi_l^{(0)}(r)^2\,dr \Big/ \int_0^\infty \varphi_l^{(0)}(r)^2\,dr\right]^{1/2} \quad (16)$$

etc. The series for $E(\lambda) = {}^1/_2 k(\lambda)^2$, up to the l-th order inclusive, then coincides with the series obtained in the ordinary PT. Following this, however, is a term of order $\lambda^{l+1/2}$, which at the corresponding sign of λ becomes imaginary. Such a zero of the Jost function describes a quasistationary state with width

$$\Gamma(\lambda) = 2\mathrm{Im}\,E(\lambda) = 2|a_1 b_{2l}(\lambda - \lambda_{br})^{l+1/2}| + O(|\lambda - \lambda_{br}|^{l+3/2}). \quad (17)$$

The coefficient b_{2l} is determined from the equation

$$a_1 b_{2l} f_{20} + \frac{1}{(2l+1)!}a_1^{2l+1} f_{2l+10} = 0,$$
$$b_{2l} = \frac{ia_1^{2l}}{4\int_0^\infty \varphi_l^{(0)}(r)^2\,dr}\left[\frac{\varphi_l^{(0)}(R)R^l}{(2l-1)!!}\right]^2. \quad (18)$$

The character of the relation[1] $\Gamma(\lambda) \sim (\lambda - \lambda_{br})^{l+1/2}$ is indicated in a somewhat implicit form in[1,2,5], but no formula is given there for the corresponding coefficient. It is interesting that the quantity

$$\lim_{\lambda\to 0}\left|\frac{\Gamma(\lambda)}{E(\lambda)^{l+1/2}}\lambda^{-l}\right|$$

does not depend on $V^{(1)}$ and thus characterizes, at a given l, the trajectories of the zeroes of the Jost function for any perturbation.

Formally, the reason why it is impossible to calculate the $(l+1)$-st term in ordinary PT when applied to a level with zero energy is that the correction of order n to the wave function $\varphi^{(n)}(r)$ behaves like r^{2n-l} as $r \to \infty$. Therefore the normalization integral for $\varphi = \sum_n \lambda^n\varphi^{(n)}$, calculated with allowance for terms of order λ^l, diverges at the upper limit.

4. Returning to the problem of PT for a weakly bound state, we see that up to l-th order we can use the ordinary PT for the energy:

$$E \approx \sum_{n=0}^{l} \lambda^n E^{(n)}. \quad (19)$$

A more accurate expression for the next-order correction can be obtained by the method described below. Using the approximation (19), we obtain the branch point λ_{br} of the function $E(\lambda)$ as a solution of the equation $E(\lambda_{br}) = 0$. We write a more exact expression for $E(\lambda)$, which takes into account the presence of a branch point of the required character

$$E(\lambda) = \sum_{n=0}^{l+1} c_n\lambda^n + a_1 b_{2l}(\lambda - \lambda_{br})^{l+1/2}. \quad (20)$$

The coefficient $a_1 b_{2l}$ can be calculated in accordance with formulas (16) and (18) using the unperturbed wave function for the energy $E^{(0)}$. The remaining coefficients c_n are chosen such that the first l terms in the expansion of expression (20) in powers of λ coincide with (19), and the $(l+1)$-st term is of the form $\lambda^{l+1}E^{(l+1)}$.

Thus, at $l = 1$ we obtain

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + a_1 b_{21}[(\lambda - \lambda_{br})^{3/2} - (-\lambda_{br})^{3/2} - {}^3/_2(-\lambda_{br})^{1/2} - {}^3/_8(\lambda_{br})^{-1/2}]. \quad (21)$$

Depending on the choice of the sign in formula (16) for a_1, expression (21) at small $|\lambda|$ will correspond to a zero of the Jost function on a physical or unphysical sheet of complex energy, i.e., in the upper or lower half-plane of the momentum k.

It must be emphasized that if the state under consideration becomes quasistationary, then its width can be determined from formula (10) for $l = 0$ and from formula (21) and its analog for $l > 0$. In the latter case $\Gamma(\lambda)$ is expressed with the aid of (17) also if $E^{(0)}$ differs from zero but is small. It is known that calculation of the widths of the quasistationary states is a complicated

[1] We emphasize that this relation also holds in such a form when $l = 0$.

problem. The expressions obtained by us are simple and do not assume that the interaction with the continuous spectrum is small. There are problems in which it is necessary to know precisely the $\Gamma(\lambda)$ dependence near the point where the level goes into the continuous spectrum. Thus, for example, it determines the low-energy part of the spectrum of electrons emitted by detachment from a negative ion[4]. In this case the real potential is not spherically symmetrical. However, recognizing that the low-energy scattering by any scatterer is similar to scattering by a spherical center[6], we can generalize our result to include also this case. Indeed, the wave function of a discrete level at the boundary of the continuous spectrum, at large values of r, is given by

$$\Psi^{(0)}\mathbf{r} \sim c_l r^{-l-1} Y_l(\Omega) + O(r^{-l-2}) \qquad (22)$$

($Y_l(\Omega)$ is a certain normalized spherical function and c_l is a coefficient), making it possible to characterize the state by a certain integer l. For example, if the potential has only an inversion center, we have $l = 0$ for even levels and $l = 1$ for odd ones (we do not consider the possibility of "accidental" vanishing of the coefficient c_l). In formulas (16)–(18) for the width it is necessary to change over from one-dimensional integrals to three-dimensional ones and to replace $\varphi_l^{(0)}(R)R^l$ by c_l.

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APPENDIX

The Jost function (which we defined in accord with[5]) can be represented in the form

$$f_l(k) = A_l(k) + ik^{2l+1}B_l(k),$$

where A_l and B_l are even functions of k[7]. From this we get directly $f_{mn} = 0$ if m is odd and $m < 2l$;

$$f_{2l+10} = i(2l+1)!\,B_l(0) = -\frac{i}{2}\frac{(2l)!!}{(2l-1)!!}\varphi_l^{(0)}(R)R^l,$$

and from now on the solution $\varphi_l^{(0)}(\mathbf{r})$ of the Schrödinger equation is assumed to be normalized by the condition

$$\lim_{r\to 0} r^{-l-1}\varphi_l^{(0)}(r) = 1.$$

Newton[8] has shown that if (12) is satisfied, then

$$f_{10} = -i\varphi_0^{(0)}(R), \quad l = 0;$$

$$f_{20} = -\frac{2}{(2l+1)}\frac{1}{\varphi^{(0)}(R)R^l}\int_0^\infty \varphi_l^{(0)}(r)^2\,dr, \quad l \neq 0.$$

For f_{01} we readily obtain the expression

$$f_{01} = \frac{2}{(2l+1)\varphi_l^{(0)}(R)R^l}\int_0^\infty V^{(1)}\varphi_l^{(0)}(r)^2\,dr.$$

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