Perturbation theory for quasistationary levels

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A perturbation-theory formula is derived for the energies of quasistationary states (resonances) in the semiclassical approximation. This formula is valid for resonances either below or above the barrier. It is illustrated for several potentials, for which a comparison can be made with exact solutions.

1. A perturbation theory for quasistationary states has been studied by several authors.[1–3] Because of the exponential growth of the Gamow wave function at infinity, integrals which arise in the process diverge and must be regularized. The perturbation-theory formulas derived in Refs. 2 and 3 are therefore not completely transparent, since they contain an operation of taking a limit [an example is Zeldovich's lim $\exp(-\alpha r^2)$ as $\alpha \to +0$; Ref. 2].

2. Let us examine this question in the semiclassical approximation, in which this difficulty can be overcome completely. Assuming that the (real) potential $U(x)$ has a barrier, and that it satisfies the condition for a semiclassical treatment, we use a modified quantization rule incorporating a finite transmission of the barrier.[4–6] Varying this equation with respect to the potential, we find the (first-order) perturbation-theory formula

$$\delta E = \frac{\int_{x_0}^{x_1} \delta U(x) p^{-1} dx + \xi(a) \int_{x_1}^{x_2} \delta U(x)(-p^2)^{-1/2} dx}{\int_{x_0}^{x_1} p^{-1} dx + \xi(a) \int_{x_1}^{x_2} (-p^2)^{-1/2} dx}, \tag{1}$$

where $\delta E = \delta E_r - \frac{i}{2}\, \delta\Gamma$,

$$\xi(a) = \frac{1}{2\pi}\left[\ln(ia) - \psi\left(\frac{1}{2} + ia\right)\right], \tag{2}$$

$$a = \frac{1}{\pi}\int_{x_1}^{x_2} (-p^2)^{1/2} dx, \tag{3}$$

and $\psi(z)$ is the logarithmic derivative of the gamma function. Here x_i are turning points, where $x_0 < x < x_1$ is a classically allowed region, and $x_1 < x < x_2$ is a classically forbidden (below-barrier) region (see Fig. 1 in Ref. 5); $p = p(x,E)$ is the semiclassical momentum. For quasistationary states the energy $E = E_r - i\Gamma/2$, the turning points $x_i(E)$, etc., are complex.

Let us examine two limiting cases of expression (1).

A. **Below-barrier resonances**

In this case we have a parameter $a \gg 1$ and

$$\xi(a)=\frac{1}{48\pi a^2}\left(1+\frac{7}{40a^2}+\ldots\right)+\frac{i}{2}e^{-2\pi a}. \tag{4}$$

Substituting this expansion into (1), and separating the real part and the imaginary part, we find corrections to the position and width of the resonance. In particular, we find

$$\delta E_r=\langle\delta U\rangle+0(1/n^2), \tag{5}$$

where the terms on the order of $1/n^2$ receive contributions from only the corrections $\hbar^2$, $\hbar^4$, etc., in the WKB method, calculated for the classically allowed region [the contributions from the below-barrier region associated with the function $\xi(a)$ cancel out[1)]]. We will not reproduce the corresponding formula nor discuss it here. For the level width we find

$$\frac{\delta\Gamma}{\Gamma}=(\langle\delta U\rangle-\langle\delta U\rangle')T', \tag{6}$$

where $\hbar=m=1$, and where

$$\langle f\rangle=\frac{2}{T}\int_{x_0}^{x_1}f(x)p^{-1}dx, \quad \langle f\rangle'=\frac{2}{T'}f(x)|p|^{-1}dx, \tag{7}$$

$$T=2\int_{x_0}^{x_1}p^{-1}dx, \quad T'=2\int_{x_1}^{x_2}|p|^{-1}dx. \tag{7a}$$

We can thus assume that the energy E and the turning points are real in (5)–(7), since $\mathrm{Im}E=-\Gamma/2$ is exponentially small. Here T is the period of the classical oscillations of a particle between turning points x_0 and x_1, $\langle f\rangle$is the expectation value of the function $f(x)$ calculated from the semiclassical wave function, and T' and $\langle f\rangle'$ are the corresponding quantities for below-barrier motion, analyzed by the imaginary-time method.[7,8]

It can be seen from (6) that the correction $\delta\Gamma$ depends on the potential perturbation δU not only in the above-barrier region but also in the region of classical motion. These two corrections enter (5) with opposite signs. This situation can be clarified with the help of the following example. We imagine that a perturbation $\delta U(x)>0$ lies exclusively in the small interval Δx. If Δx is in the below-barrier region, the barrier rises, and we have $\delta\Gamma<0$. If Δx is instead in the interval (x_0,x_1), where the particle is localized for the most part, then there is an increase in the energy of the level (at a fixed barrier), so we have $\delta\Gamma>0$. This accounts for the signs in Eq. (6).

B. **Above-barrier resonances** $(E_r>U_m)$

As was shown in Refs. 9 and 10, we have $\pi/2<\arg a<\pi$ in this case, and in place of (4) we find $\xi(a)=i+0(a^{-2})$. Expression (1) then becomes

$$\delta E=\oint_C\delta U(x)(p^2)^{-1/2}dx/\oint_C(p^2)^{-1/2}dx, \tag{8}$$

where the integration contour C encloses the turning points x_0 and x_2 , which lie in the complex plane,[2)] and where the cut for the function $[p^2(x)]^{-1/2}$ is drawn from x_0 to x_2. The same result, (8), follows directly from the generalized quantization condition derived in Ref. 10 for an above-barrier resonance. This agreement is independent confirmation of Eq. (1).

3. We will illustrate the equations derived here with the help of several model potentials, for which a comparison can be made with exact solutions.

a) We first consider the parabolic barrier

$$U(r)=-\frac{1}{2}\,\omega^2(r-R)^2,\quad 0<r<\infty. \tag{9}$$

The Schrödinger equation with $l=0$ has an exact solution which satisfies the Sommerfeld radiation condition as $r\rightarrow\infty$:

$$\chi_0(r)=\mathrm{const}D_{-1/2-ia}([1-i]\omega^{1/2}[r-R]).$$

In the semiclassical approximation, using the asymptotic expression for the parabolic cylinder function, we find

$$\omega R^2[(1-\epsilon)^{1/2}-\epsilon\ \mathrm{arctanh}(1-\epsilon)^{1/2}]=2\pi(n-1/4),$$

$$\Gamma_n=\frac{\omega}{2}(\mathrm{arctanh}\ (1-\epsilon)^{1/2})^{-1}\exp(-2\pi a),\quad a=-E_n/\omega, \tag{10}$$

where $\epsilon=-E/V_0$, $V_0=-U(0)=\frac{1}{2}\,\omega^2R^2$ (the first of these equations determines the position of the level), and $n=1,2,\ldots$. Here we can vary both the oscillator frequency ω and the radius R. From (10) we find

$$\frac{\delta\Gamma}{\Gamma}=-\pi\omega R^2\frac{(1-\epsilon)^{1/2}}{\mathrm{arctanh}\ (1-\epsilon)^{1/2}}\left(\frac{\delta\omega}{\omega}+2\frac{\delta R}{R}\right) \tag{11}$$

(for below-barrier resonances we would have $0<\epsilon<1$). The same result is found from (6) by assuming $\delta U(r)=-\omega(r-R)^2\delta\omega+\omega^2(r-R)\delta R$ and by taking the turning points to be $r_0=0$ and $r_{1,2}=R(1\mp\epsilon^{1/2})$.

b) For the potential

$$V(r)=-\frac{\alpha^2}{2r^2}-\frac{1}{8}\,\omega^2r^2 \tag{12}$$

the Schrödinger equation can be solved in terms of Whittaker functions for an arbitrary angular momentum l. The effective potential differs from (12) only in that we make the replacement $\alpha\rightarrow g=[\alpha^2-(l+1/2)^2]^{1/2}$ and in that the potential has a barrier under the condition $\alpha>l+1/2$. We will examine this case. Varying the frequency ω in (12), we find [from both Eq. (6) and the exact solution]

$$\frac{\delta\Gamma}{\Gamma}=\frac{\pi g}{\ln(1+\epsilon^{-1})}\frac{\delta\omega}{\omega}. \tag{13}$$

Here now $\epsilon=(E-U_m)/2U_m$, where $U_m=-\frac{1}{2}g\omega$ is the maximum value of the potential.

c) Similar results are found for the potential

$$U(r)=-\frac{g^2}{2r^2}+\frac{\zeta}{r}, \tag{14}$$

which has the form of the effective potential in the Dirac equation for electron states close to the boundary of the lower continuum.[11]

In the examples discussed here, the dependence of $\delta\Gamma$ on ϵ (i.e., the dependence on the level energy) is not trivial. We thus regard the agreement with the exact solutions as convincing confirmation of Eq. (6). Another limiting case, specifically, Eq. (8), has been tested in the example of an anharmonic oscillator: $U(x)=\frac{1}{2}x^2-gx^3$, with $\delta U=-x^3\delta g$. In the limit $g\to\infty$ we have $x_0\approx-(E/g)^{1/3}$ and $x_2\approx(E/g)^{1/3}\exp(i\pi/3)$. Accordingly, the integrals in (8) reduce to gamma functions. As a result, we find $\delta E_n/E_n=\frac{2}{5}\delta g/g$ and

$$\delta\Gamma_n\approx k(n+1/2)^{6/5}g^{-3/5}\delta g, \quad n\gg1, \tag{15}$$

where

$$k=\left(\frac{10}{27}\pi^3\right)^{1/5}[2\Gamma(5/6)/\Gamma(1/3)]^{6/5}\sin\frac{\pi}{5}\approx0.780.$$

The same expression follows from the asymptotic expression for the energy $\tilde{E}_n(g)\sim g^{2/5}$ in the strong-coupling limit.[10,12] Treating the oscillatory term in $U(x)$ as a perturbation, and using (8), we can easily calculate the correction $\sim g^{-4/5}$ to the leading term of the asymptotic expression $\tilde{E}_n(g)$ at $g\gg1$.

4. In general, including the case of resonances close to the crest of the barrier, in which case we have $E_r\approx U_m$ and $|a|\sim1$, we need to use perturbation-theory formula (1), which determines both δE_r and $\delta\Gamma$. This formula requires some straightforward numerical calculations; it can apparently be used in a variety of physical problems.

The approach outlined above can be generalized to the multidimensional case. For a system with $f>1$ degrees of freedom, and for which variables can be separated in the Schrödinger equation, it is possible to construct a perturbation-theory formula analogous to (1). However, we do not have room here to go through this derivation. We defer this question, as well as the incorporation of terms on the order of $1/n^2$ in (5), to a more detailed paper.

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[1)]It can be shown that we have $a\sim n$, where n is the quantum number of the level. At the same time, we know that the formal parameter $\hbar$ of the semiclassical expansion becomes $1/n$ in the final expressions. The terms on the order of a^{-2} and $\hbar^2$ should thus be treated simultaneously.

[2)]Not the points x_0 and x_1, which bound the region of classical motion (as in the case of a discrete spectrum).

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