Diverging perturbation-theory series and classical mechanics

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A summation of the diverging perturbation-theory series yields expressions for the energies of levels (real, virtual, and quasistationary) in terms of the coefficients of the perturbation theory, E_k. Taking the limit of classical mechanics reveals the asymptotic behavior of the highly excited levels with $l = n - 1 \gg 1$, confirming the results of the summation of the perturbation-theory series.

1. Considerable progress has recently been achieved in calculating higher orders of perturbation theory particularly in quantum mechanics.[1–4] For the anharmonic oscillator, the Stark and Zeeman effects in the hydrogen atom, and the screened Coulomb potential

$$V(r) = - r^{-1} f(\mu r), \quad \hbar = m = e = 1, \tag{1}$$

the new perturbation-theory methods make it a simple matter to calculate very high orders of perturbation theory for the energy of a level, E_k (up to $k = 100$–200 in the case of the ground state[1–3]). However, the perturbation-theory series in quantum mechanics and field theory generally diverge because of the factorial growth of $|E_k|$ as $k \to \infty$ (Ref. 5). Consequently, methods for summing diverging series are indispensable for reconstructing the energy from the perturbation-theory coefficients. Methods used for this purpose are the Pade approximants, Borel transformations, etc. All of these methods make use of the circumstance that the higher orders of perturbation theory contain more information than could be found through a simple calculation of the perturbation-theory polynomials.

Let us examine the results of the summation of a divergent perturbation-theory series for the particular case of potentials[2)] of the type in (1).

2. The level energies in the limit $\mu \to 0$ can be represented by formal Rayleigh-Schrödinger series

$$E^{(nl)}(\mu) = \sum_{k=0}^{\infty} E_k^{(nl)} \mu^k, \quad \mu \to 0 \tag{2}$$

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(n is the principal quantum number, l is the orbital angular momentum, and $0 \leqslant l \leqslant n-1$). The calculation of the coefficients E_k for an arbitrary screening $f(\mu_r)$ can be reduced to recurrence relations which are convenient for numerical calculations. For $l = n - 1$ (the lowest level with the given l), these relations were derived in Ref. 3, where tables of E_k were also given. As the screening parameter increases, we reach a value $\mu = \mu_{cr}(n, l)$ at which the binding energy vanishes, and the bound nl level becomes a virtual level ($l = 0$) or a quasistationary level ($l \geqslant 1$). It has been shown[6,7] that in the discrete spectrum ($0 < \mu < \mu_{cr}$) the perturbation-theory series for many potentials can be summed successfully by means of Pade approximants. For example, for a Yukawa potential we find $\mu_{cr}(l+1, l) = 1.190\,612$; 0.2201; 0.09134; 0.04983; and 6.250×10^{-3} and 7.730×10^{-4} for $l = 0$, 1, 2, 3, 10, and 30, respectively.[3)]

We have continued these calculations into the region $\mu > \mu_{cr}$. For $l = 0$, a summation of the perturbation-theory series by means of Pade approximants determines the energies of the virtual ns levels at least up to $\mu \sim 10\mu_{cr}$ (Ref. 7). These results are confirmed by a numerical solution of the integral Lippmann-Schwinger equations continued analytically to the second sheet of the energy.[9] To calculate the position and width of the Breit-Wigner resonances $E^{(nl)} = E_0 - i\Gamma/2$ at $\mu > \mu_{cr}$; $l \neq 0$, we need to combine the method of Pade approximants with a conformal mapping $\mu \rightarrow z(\mu)$ (see Refs. 7 and 8 for the details). Some of the results are shown in Figs. 1 and 2. The widths calculated here agree with the threshold behavior $\Gamma_{nl}(\mu) \approx C_{nl}(\mu - \mu_{cr})^{l+1/2}$ as $\mu \rightarrow \mu_{cr}(n, l)$. The constants C_{nl} can be found numerically without any difficulty.

These results demonstrate the effectiveness of summing perturbation-theory series. Although the convergence of the series of Pade approximants $[L/L+j]$ with $j = 0, \pm 1$ and $L \rightarrow \infty$ is good, we believe it is necessary to verify the results through a summation by an independent method.

3. At $n \sim l \gg 1$, the effective potential in the Schrödinger equation, $U(r) = -r^{-1}f(\mu r) + l(l+1)/2r^2$, contains a deep, narrow minimum into which a classical particle slides. If $l = n - 1 (n_r = 0)$, we can ignore quantum fluctuations around the classical minimum in the limit $n \rightarrow \infty$ (their amplitude is proportional to $1/n$). Setting $E^{(nl)} = \epsilon/2n^2$, $\nu = n^2\mu$ and $x = \mu r$, we find the equations

$$\epsilon = x^2 f'^2 - f^2, \quad \nu = xf - x^2 f', \tag{3}$$

which specify the parametric functional dependence of ϵ on ν and which determine the point of the minimum, $x_0(\nu)$. Taking into account quantum fluctuations near x_0, we can evaluate several terms of the $1/n$ expansion:

$$\epsilon(\nu, l = n-1) = \epsilon^{(0)} + \frac{\epsilon^{(1)}}{n} + \frac{\epsilon^{(2)}}{n^2} + \ldots, \tag{4}$$

where $\epsilon^{(0)}(\nu)$ is determined by Eq. (3), and the first quantum correction is

$$\epsilon^{(1)} = -[g^2 - g^{3/2}h^{1/2}]_{x=x_0}, \quad g = f - xf', \; h = f - xf' - x^2 f'' \tag{5}$$

(there is a regular method for evaluating the subsequent corrections $\epsilon^{(k)}$). As a rule, $\epsilon^{(0)}$ is a monotonically increasing function of ν up to $\nu = \nu_*$, where we have $h(\nu_*) = 0$, and where the two classical solutions join (see the "beak" in Fig. 1). As $\nu \rightarrow \nu_*$, $\epsilon^{(0)}$ and $\epsilon^{(1)}$ have singularities of the types $(\nu_* - \nu)^{3/2}$ and $(\nu_* - \nu)^{1/2}$. If $\nu > \nu_*$, then $x_0(\nu)$, $\epsilon^{(0)}$ and

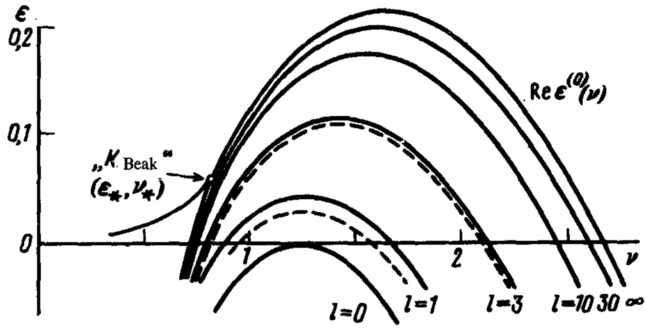

FIG. 1. The Yukawa potential. The energies of the states with $l = n - 1$ found through a summation of the perturbation-theory series in terms of the variables $\epsilon = 2n^2 E^{(nl)}$ and $\nu = n^2 \mu$. The dashed lines show two terms of the $1/n$ expansion in (4). For $l = 10$ and 30, these curves coincide with the solid curves (at the scale of this figure).

$\epsilon^{(1)}$ become complex. Such a solution has no meaning in classical mechanics, but in quantum mechanics it is the solution that determines the asymptotic behavior of E_0 and Γ as $n \to \infty$.

Figures 1 and 2 show the results calculated for $f(x) = e^{-x}$ (a Yukawa potential). The classical asymptotic behavior $\epsilon^{(0)}(\nu)$ at $\nu < \nu_{cr}$ is extremely close to the exact solutions of the Schrödinger equation beginning at $n \sim 10$. The first quantum correction improves the accuracy at $\nu > \nu_{cr}$ also (see the dashed lines in Figs. 1 and 2). Here are some typical numbers: for $\nu = \nu_{cr} = 0.735\,759$ we have $\epsilon^{(0)} = 0$, and for $l = 10$ we have $\epsilon_1 = -0.014\,414$ and $\epsilon_2 = -0.014\,038$ (here $\epsilon_i = \epsilon^{(0)} + \epsilon^{(1)} n^{-1} + \ldots + \epsilon^{(i)} n^{-i}$); according to Ref. 7, we have $\epsilon_{pert} = -0.014\,040$. The $1/n$ expansion thus completely verifies the results found through the summation of the divergent perturbation-theory series.

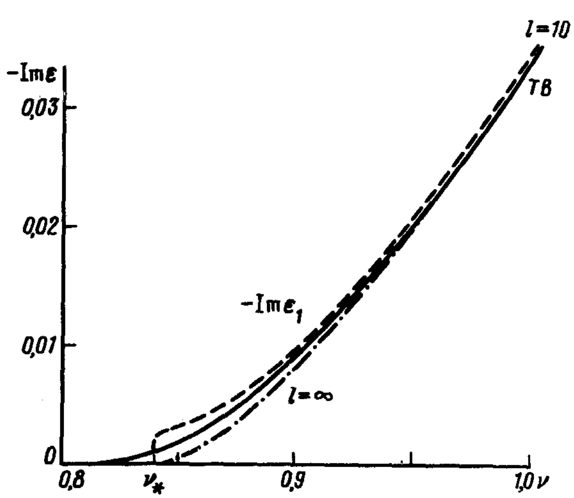

FIG. 2. Values of $-\text{Im}\epsilon = n^2 \Gamma_{nl}$ for states with $l = n - 1$ in a Yukawa potential. Solid line—Summation of series (2) (perturbation theory); dashed line—the first two terms of a $1/n$ expansion ($l = 10$).

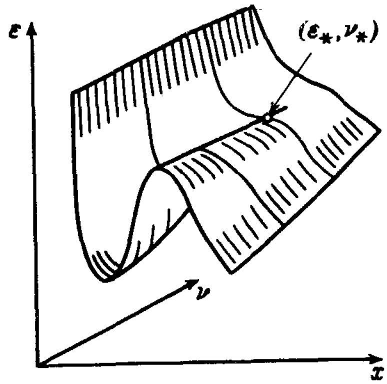

FIG. 3.

In a study of a screening of a general type, as in (1), it is useful to appeal to catastrophe theory.[10] Figure 3 shows the relief of the surface of the effective potential energy $\epsilon = -2\nu(f(x)/x) + (\nu^2/x^2)$. The projection of the surface onto the (ϵ, ν) plane results in a "beak" singularity (Fig. 1). Near the point (ϵ_*, ν_*), the equation of the surface can be put in the standard form[4)]

$$z^3 + az + b = 0, \tag{6}$$

where $a = 6kx_*^{-3}(\nu - \nu_*)$ and $b = \epsilon - \epsilon_* + 2f'(\nu - \nu_*)$,

$$k = xf''' + 3f'', \quad z = \frac{x}{x_*} - 1 + 3\left(\frac{\nu}{\nu} - 1\right)\left(1 + \frac{x^3 f'''}{3g}\right)^{-1},$$

and all the derivatives are evaluated at the point $x = x_* = x_0(\nu_*)$. For the two classical solutions which join at the vertex of the beak we have

$$\epsilon_\pm = \epsilon_* + c_1(\nu - \nu_*) \pm c_2(\nu_* - \nu)^{3/2} + \dots,$$
$$c_1 = -2f'(x_*), \quad c_2 = 2^{5/2}\left[(3f'' + xf''')/x^3\right]^{3/2}_{x = x_*}, \tag{7}$$

in agreement with Fig. 1.

We note that $\epsilon^{(0)}, \epsilon^{(1)}, \dots$, have an imaginary part only after the solutions join $(\nu > \nu_*)$. For finite values of n and l, on the other hand, a width Γ_{nl} arises even at $\nu = \nu_{cr}(n, l)$, but at $\nu_{cr} < \nu < \nu_*$ it is extremely small and decreases rapidly with increasing l (Fig. 2). On the other hand, Γ_{nl} is a weak function of l at $\nu > \nu_*$.

In summary, the classical solutions continued analytically into the region of complex coordinates determine the width of the Breit-Wigner resonances (except near the threshold, $\mu \approx \mu_{cr}$).

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2)In particular, the function $f(x) = \exp(-x)$ corresponds to a Yukawa potential; $f(x) = x/(e^x - 1)$ corresponds to a Hulthén potential; etc.

3)For more details, see Refs. 7 and 8, where tables of μ_{cr} are given for Yukawa and Hulthén potentials, and tables of the bound-state energies are given as functions of μ/μ_{cr}, according to calculations based on a summation of the perturbation-theory series.

4)In catastrophe theory, the situation in Fig. 3 is called a "Whitney cusp."

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