Divergent series in quantum mechanics

Large-order behavior of the perturbation series:

its derivation and applications

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Luminy

Motivation

Is there a way how to learn more about perturbation series other than by calculating more and more perturbation coefficients?

This is important especially in cases when we cannot calculate much.

Simple quantum-mechanical systems are simple enough to permit numerical checks of general considerations.

Derivation

Let us consider the problem of the hydrogen atom in a constant magnetic field $\vec{B} = (0, 0, B)$. Neglecting the motion of the nucleus and the effect of the spin, Schrödinger equation for this system reads

$$\left[-\frac{\nabla^2}{2} - \frac{1}{r} + \frac{B\,L_z}{2} + \frac{B^2}{8}(x^2 + y^2)\right]\psi = E\psi. \tag{1}$$

where the atomic units are used.

Since Eq. (1) has axial symmetry we introduce the cylindric coordinates $x = \rho\cos\varphi$, $y = \rho\sin\varphi$, $z = z$.

The ground state is independent of the coordinate φ; Eq. (1) reads

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right]\psi = \left[V(\rho, z) - 2E\right]\psi, \tag{2}$$

where

$$V(\rho, z) = -\frac{2}{(\rho^2 + z^2)^{1/2}} + \frac{B^2}{4}\rho^2. \tag{3}$$

Searching for the perturbative solution of the problem

$$E = \sum_{n=0}^{\infty} E_n \left(\frac{B^2}{8}\right)^n \tag{4}$$

we find that this series diverges. The reason is that the energy E is not analytic function in the vicinity of the point $B = 0$.

Dispersion relation

Analytic continuation: for complex B^2 Schrödinger equation is solved with the boundary condition $\psi(\rho \to \infty) \to e^{-(B^2/8)^{1/2}\rho^2}$, where in the upper half of the complex plane we take $B^2 = |B^2|e^{i\arg(B^2)}$ and in the lower half $B^2 = |B^2|e^{-i\arg(B^2)}$.

Now, approaching the value $-|B^2|$ from the upper half of the complex plane leads to the boundary condition $\psi(\rho \to \infty) \to e^{-i|B^2/8|^{1/2}\rho^2}$, while approaching this value from the lower half leads to $\psi(\rho \to \infty) \to e^{+i|B^2/8|^{1/2}\rho^2}$. These different boundary conditions yield different signs of the imaginary part of the energy $\Im[E(B^2)]$. Therefore, the energy E has for real negative values of B^2 the discontinuity $2i\Im[E(-|B^2| + i\varepsilon)]$, $\varepsilon > 0$. Cauchy theorem then yields dispersion relation (Simon, Bender and Wu)

$$E(B^2) = -\frac{1}{\pi}\int_0^\infty d\lambda \frac{\Im[(\lambda)]}{\lambda + B^2/4}, \tag{5}$$

where

$$\lambda = -\frac{B^2}{4} \tag{6}$$

Imaginary part of the energy is given by the time-independent version of the continuity equation for the probability density

$$\Im[E] = \frac{J}{2 < \psi|\psi >}, \tag{7}$$

where the probability flux J in the ρ direction equals

$$J = -\frac{1}{2i}\int_{-\infty}^{\infty} dz \lim_{\rho\to\infty} \rho \left[\psi^* \frac{\partial}{\partial\rho}\psi - \psi\frac{\partial}{\partial\rho}\psi^*\right] \tag{8}$$

and the norm of the wave function reads

$$< \psi|\psi >= \int_0^{\infty} d\rho \int_{-\infty}^{\infty} dz\rho|\psi|^2. \tag{9}$$

By expanding both sides of the dispersion relation in powers of B^2 one gets the dispersion relation for the perturbation coefficients

$$E_n = \frac{(-1)^{n+1}2^n}{\pi}\int_0^{\infty} d\lambda \frac{\Im\left[E(\lambda)\right]}{\lambda^{n+1}} \tag{10}$$

The dominant contribution to the integral comes from the region of λ going to zero.

Physically, for negative B^2 the potential in Eq. (1) has no bound states. However, for small λ the effect of the perturbing potential is weak and the quasistationary states have very long lifetime. The probability flux in Eq. (8) can then be calculated from WKB wave function and the norm in Eq. (9) from hydrogenic wave function.

Multidimensional WKB approximation

The main obstacle in carrying out the program described above is the construction of the WKB wave function. The standard formulation of the WKB approximation as applied to Eq. (2) leads to the non-separable non-linear partial differential equation

$$\left(\frac{\partial S_0}{\partial \rho}\right)^2 + \left(\frac{\partial S_0}{\partial z}\right)^2 = V(\rho, z) - 2E, \tag{11}$$

that is difficult to solve.

The simplification of the problem of calculation of the imaginary part of the energy from Eq. (7) comes out from the fact that the tunneling of the particle takes place in the neighborhood of the line $z = 0$:

$$V(\rho, z) = -\frac{2}{(\rho^2 + z^2)^{1/2}} - \lambda\rho^2. \tag{12}$$

Consequently, we do not need to know the wave function in all space, but only in the neighborhood of this line.

Approximation in transversal direction

In the vicinity of the ρ axis the potential $V(\rho,z)$ given by Eq. (3) can be expanded as

$$V(\rho,z)=V_0(\rho)+V_2(\rho)z^2+V_4(\rho)z^4+\ldots. \tag{13}$$

Then, the wave function of the particle in the direction transversal to tunneling can be written as

$$\psi(\rho,z)=e^{f(\rho)+h(\rho)z^2+q(\rho)z^4+\ldots}. \tag{14}$$

This says nothing else than close to the minimum of the potential in the direction perpendicular to tunneling we can approximate the exact wave function by the wave function of the harmonic oscillator. This approximation can be further improved by considering anharmonic terms.

Inserting the expansions (13) and (14) into Eq. (2) and comparing the terms of the zeroth, second and fourth order of z we get successivelly

$$f'(\rho)^2+f''(\rho)+\frac{f'(\rho)}{\rho}+2h(\rho)=-2E-\lambda\rho^2-\frac{2}{\rho}, \tag{15}$$

$$2f'(\rho)h'(\rho)+h''(\rho)+\frac{h'(\rho)}{\rho}+4h(\rho)^2+12q(\rho)=\frac{1}{\rho^3}, \tag{16}$$

$$2f'(\rho)q'(\rho)+h'(\rho)^2+q''(\rho)+\frac{q'(\rho)}{\rho}+16h(\rho)q(\rho)=-\frac{3}{4\rho^5}. \tag{17}$$

Approximation in longitudinal direction

In the direction of the tunneling we approximate the wave function as follows. The dominant contribution to tunneling comes from the classically forbiden region. In this region the terms $-2E$ and $-\lambda\rho^2$ are of the same order of magnitude. To make these terms of the same order in λ we make the scaling in the coordinate ρ

$$\rho = \lambda^{-1/2} u. \tag{18}$$

Expanding Eq. (2) *after* this scaling we get approximation of the wave function in the classically forbiden region.

To get clue how to expand the functions $f(u)$, $h(u)$ and $q(u)$ in the powers of $\lambda^{1/2}$ we use the fact that for $u \to 0$ we have to recover the wave function of the hydrogen atom. For the ground state it reads

$$\psi_{1s} = e^{-r} = e^{-\sqrt{\rho^2+z^2}} = e^{-\rho - z^2/(2\rho) - z^4/(8\rho^3)+\dots} = \tag{19}$$

$$e^{-u/\lambda^{1/2} - \lambda^{1/2} z^2/(2u) - \lambda^{3/2} z^4/(8u^3)+\dots}.$$

Therefore, we expand the functions $f(u)$, $h(u)$ and $q(u)$ as follows

$$f(u) = \frac{f_0(u)}{\lambda^{1/2}} + f_1(u) + f_2(u)\lambda^{1/2} + \dots, \tag{20}$$

$$h(u) = h_0(u)\lambda^{1/2} + h_1(u)\lambda + \dots \tag{21}$$

and

$$q(u) = q_0(u)\lambda^{3/2} + \dots . \tag{22}$$

By inserting these expansions into Eqs. (15)-(17) and comparing the terms of the same order of λ we get equations for the functions $f_0(u)$,

$$f_0'(u) = -\sqrt{1-u^2}, \tag{23}$$

$h_0(u)$

$$2f_0'(u)h_0'(u) + 4[h_0(u)]^2 = 0, \tag{24}$$

$f_1(u)$

$$2f_0'(u)f_1'(u) + f_0''(u) + \frac{1}{u}f_0'(u) + 2h_0(u) = -\frac{2}{u}, \tag{25}$$

and so on. These equations can be integrated. The suggested approximation of the wave function leads to the systematic expansion of the imaginary part of the energy in the powers of $\lambda^{1/2}$. The details can be found in

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Large-order behavior of the perturbation energies for the hydrogen atom in magnetic field

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Proceeding in the described way one gets for the ground state

$$\Im[E] = 2^{7/2}\lambda^{3/4}e^{-\pi/(2\lambda^{1/2})}\left(1 + R_1\lambda^{1/2} + \ldots\right). \tag{26}$$

By inserting this equation into Eq. (10) we obtain for the large-order behavior

$$E_n^{lo} = \frac{2^5}{\pi^{3/2}}(-1)^{n+1}\left(\frac{2^{3/2}}{\pi}\right)^n\left(2n + \frac{1}{2}\right)!\left(1 + \frac{R_1\pi}{2\left(2n + \frac{1}{2}\right)} + \ldots\right), \tag{27}$$

The exact form of the coefficient R_1 for the ground state is

$$R_1 = -\pi + \frac{3}{2\pi} - \frac{7\zeta(3)}{4\pi} = -3.33372436736865 \tag{28}$$

What means large in large order behavior of the perturbation series?

order	exact	leading	corrected
1	2.	4.9276703	-5.3940291
2	-17.666667	-62.908944	10.297521
3	620.11111	1822.9663	354.32799
4	-39958.143	-94199.588	-36165.971
5	0.38621356 10^7	0.76164415 10^7	0.38179394 10^7
6	-0.51361160 10^9	-0.88746280 10^9	-0.51567964 10^9
7	0.89650348 10^{11}	0.14081280 10^{12}	0.89958962 10^{11}

Applications

Summation to the smallest term

$$E = \sum_{n=0}^{N} E_n \left(\frac{B^2}{8}\right)^n + \Delta E_N \tag{29}$$

$$\Delta E_N = \pi^{1/2} 2^5 \left(-\frac{B}{8}\right)^{2N+2} \int_0^\infty dt e^{-t} t^{1/2+N} \frac{1 + R_1(\pi/(2t))^2 + \dots}{B^2 + (\pi/t)^2}$$

For $B = 0.2$ and $N = 5$ inclusion of ΔE_N improves the result by two orders of magnitude.

Borel transformation

The large-order behavior of the perturbation series yields singularity of the Borel transform.

$$\Delta E_N = \int_0^\infty dt e^{-t} t^b C_b(Bt), \tag{30}$$

$$C_b(Bt) = \sum_{n=N+1}^{\infty} \frac{E_n (Bt)^{2n}}{8^n (2n+b)!}. \tag{31}$$

This can be used for efficient Borel summation of the series by means of the conformal transformation that maps the cut Bt plane onto a circle

$$u = \frac{\sqrt{1+(Bt/\pi)^2}-1}{\sqrt{1+(Bt/\pi)^2}+1}, \ (Bt)^2 = 4\pi^2 \frac{u}{1-u^2}. \tag{32}$$

Borel transform and the energy can then be calculated via convergent series

$$C_b(u) = \sum_{n=N+1}^{\infty} A_n u^n \tag{33}$$

and

$$\Delta E_N = \sum_{n=N+1}^{\infty} A_n \int_0^{\infty} dt e^{-t} t^b \left(\frac{\sqrt{1+(Bt/\pi)^2}-1}{\sqrt{1+(Bt/\pi)^2}+1} \right)^n, \tag{34}$$

respectively.

Sequence transformations

Let us consider partial sums

$$s_m = \sum_{n=0}^{m} E_n \left(\frac{B^2}{8}\right)^n = \sum_{n=0}^{m} a_n, \tag{35}$$

where for large n

$$a_n = \left(\frac{4}{\pi}\right)^{5/2} (-1)^{n+1} \left(\frac{B^2}{\pi^2}\right)^n \left(2n + \frac{1}{2}\right)! \tag{36}$$

For large m, the partial sums s_m behave as

$$s_m = \left(\frac{4}{\pi}\right)^{5/2} (-1)^{m+1} (2m+1/2)! \left(\frac{B}{\pi}\right)^{2m} \times \tag{37}$$

$$\left(d_0 + \frac{d_1}{m+1} + \frac{d_2}{(m+1)^2} + \ldots\right) + s.$$

We are thus led to a sequence transformation

$$s_m = a_m \left(d_0 + \frac{d_1}{(m+q_1)} + \frac{d_2}{(m+q_1)(m+q_2)} + \ldots + \right. \tag{38}$$

$$\left. + \frac{d_{l-2}}{(m+q_1)(m+q_2)\ldots(m+q_{l-2})}\right) + s,$$

where q_i, $i = 1, 2, \ldots, l-2$ are arbitrary coefficients that have to be determined from some additional requirement.

Equations (38) represent a system of l equations for l unknowns $d_0, d_1, \ldots, d_{l-2}$ and s.

Heuristic principle

If we extend the meaning of the limit to the sequence $(-1)^{n+1}(2n+1/2)!$, that is if we say that such a sequence exhibits "regular oscillations" and its generalized limit is zero, then the divergent regular oscillations $d_0 a_m$, $d_1 a_m$, ... are singled out and the remaining constant term s approaches with increasing n the generalized sum of the series $\Sigma_{n=0}^{\infty} a_n$.

Curved escape paths

Let us generalize previous considerations to the case when the escape path is not straight line. Let us consider Schrödinger equation

$$\varepsilon^2 \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] \psi = \left[v(x,y) - E \right] \psi, \tag{39}$$

where ε is some small parameter, e.g. the Planck constant and the potential $v(x,y)$ and energy E could, in principle, be parametrically dependend on ε. Expanding the wave function and the potential as

$$\psi(x,y) = \exp \left\{ \frac{1}{\varepsilon} S_0(x,y) + S_1(x,y) + \ldots \right\} \tag{40}$$

and

$$v(x,y) - E = v_0(x,y) + \varepsilon v_1(x,y) + \ldots \tag{41}$$

we get from Eq. (39) at the leading order of ε

$$\left(\frac{\partial S_0}{\partial x} \right)^2 + \left(\frac{\partial S_0}{\partial y} \right)^2 = v_0(x,y). \tag{42}$$

What is difficult is to find solution to this equation. Equations for higher order terms in Eq. (40), e.g. $S_1(x,y)$, are linear.

Expansion in y

In the neighbourhood of the x-axis, the potential can be expanded as

$$v_0(x,y) = V_0(x)+V_2(x)y^2+V_4(x)y^4+\ldots+\gamma\left[V_1(x)y + V_3(x)y^3 + \ldots\right], \tag{43}$$

where the meaning of the parameter γ will be made clear. We have seen that in the case of the straight escape path corresponding to $\gamma = 0$, the particle moves inside the potential that is in the first approximation parabolic. Then, the wave function of the particle is in the first approximation that of the harmonic oscillator, namely

$$S_0(x,y,\gamma=0) = f(x) + h(x)y^2/2! + \ldots. \tag{44}$$

Now, the first key idea toward the solution of Eq. (42) is that for $\gamma \neq 0$, the wave function of the particle is in the first approximation that of the *shifted* harmonic oscillator, namely

$$S_0(x,y) = f(x) + g(x)y + h(x)y^2/2! + p(x)y^3/3! + q(x)y^4/4! + \ldots. \tag{45}$$

By inserting this expansion into Eq. (42) and comparing the powers of the same order of y we get successively

$$f'^2 + g^2 = V_0(x), \tag{46}$$

$$f'g' + gh = \frac{\gamma}{2} V_1(x), \tag{47}$$

$$f'h' + g'^2 + qp + h^2 = V_2(x), \tag{48}$$

and so on. Here, the prime denotes the differentiation with respect to x.

Expansion in γ

The second key idea is that vanishing of the terms proportional to the odd powers of y in case $\gamma = 0$ suggests the following expansion of the functions in Eq. (45):

$$f(x) = f_0(x) + \gamma^2 f_2(x) + \gamma^4 f_4(x) + \ldots, \tag{49}$$

$$g(x) = \gamma g_1(x) + \gamma^3 g_3(x) + \ldots, \tag{50}$$

$$h(x) = h_0(x) + \gamma^2 h_2(x) + \ldots, \tag{51}$$

and so on. Inserting these expansions into Eqs. (46)-(48) and comparing the terms of the same order of γ we obtain equations for the function $f_0(x)$

$$f_0'^2 = V_0(x), \tag{52}$$

$h_0(x)$

$$f_0' h_0 + h_0^2 = V_2(x), \tag{53}$$

$g_1(x)$

$$f_0' g_1' + g_1 h_0 = V_1(x)/2, \tag{54}$$

$f_2(x)$

$$f_0' f_2' + g_1^2 = 0 \tag{55}$$

and so on. These equations can be integrated. It is evident that the simultaneous expansion of the wave function in y and γ is mutually consistent. Since γ determines how much the escape path of the particle deviates from the straight line, going to higher orders of γ one has to take into account the behavior of the wave function at larger distances from the x-axis. To describe this behavior one has to go to higher powers of y.

One can show that the described approximation of the wave function yields systematic expansion of the probability flux in the direction of the x-axis in powers of ε and γ.

Further details can be found in

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Multidimensional WKB approximation for particle tunneling

Phys. Rev. A **72**, 024101 (2005).