LETTER TO THE EDITOR

Ultraviolet divergence and scaling in a class of singular potentials

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Abstract
For the class of singular potentials $r^2 + \frac{\lambda}{r^\alpha}$, the perturbation theory in λ has an ultraviolet divergence for a range of α which causes the perturbation series to be ordered by λ^Z, where Z is a fraction less than unity. We use a scaling argument to find Z in any dimension N.

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It is quite common in nuclear and chemical physics problems to have a potential which is attractive at large distances and repulsive at short distances. A typical example of such a potential which has been studied extensively [1–21] is $V(r) = r^2 + \frac{\lambda}{r^\alpha}$, where $r^2 = x_1^2 + x_2^2 + \cdots + x_N^2$ in N-dimensional space. Clearly, the potential behaves differently at different length scales. For large r, the attractive oscillator potential dominates, whereas close to the origin the repulsive $r^{-\alpha}$ part far outweighs the confining oscillator potential. This is the well-known spiked oscillator. The singularity in the potential becomes stronger with large values of α, even for $\lambda \ll 1$. Consequently, one focuses on the large α and small λ situations. The minimum of the potential is at $r_0 = (\lambda\alpha)^{1/(2+\alpha)}$ which shifts towards the origin with decreasing λ. Hence, the problem becomes quite insensitive to what happens far away from the origin, and the exact shape of the wavefunction in the vicinity of the origin becomes crucial. For small λ, $\lambda r^{-\alpha}$ can be treated as a perturbation over the oscillator Hamiltonian $H_0 = p^2 + r^2$. It will be seen that for sufficiently singular potentials ($\alpha \geqslant N$) the perturbation theory breaks down because of the ultraviolet divergence coming from the lower limit of the energy integral.

Two salient features of this problem are

- the perturbed operator may not converge to the original one as $\lambda \to 0$ (the Klauder phenomenon) and
- the perturbation series is ordered in fractional powers of λ.

Here, one should note that in the literature people usually talk about the one-dimensional problem with the Hamiltonian $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \frac{\lambda}{x^\alpha}$ defined in the half-space $[0, \infty)$ with the Dirichlet boundary condition that $\psi(x) = 0$ at $x = 0$. As a result one deals with the odd

wavefunctions of the original harmonic oscillator problem, for the unperturbed case. This is identical with the three-dimensional problem we have introduced above ($N = 3$) so far as the ground state is concerned. Using the theory of linear operators along with that of differential equations and exploiting a connection between the WKB method and the Bessel function, Harrel *et al* [2] showed that for $N = 3$ and $\alpha \geqslant 3$ the perturbation series is ordered by $\lambda^{\frac{1}{\alpha-2}}$. It hinted at the existence of the Klauder phenomenon in this case only, in the $\lambda \to 0$ limit. Klauder [22] discussed the problem in the context of a random process driven by $H = H_0 + \frac{\lambda}{x^\alpha}$. It had to do with the fact that for $\alpha \geqslant 1$ and $\lambda > 0$, paths of the random process passing through the origin form a set of measure zero. This work also showed that the convergence problem existed in one dimension (half-space) only.

Recent numerical work of Killingbeck *et al* [21] shows clear evidence of $\lambda^{\frac{1}{\alpha-2}}$ behaviour. Use of scaling and renormalization group arguments in scattering from singular potentials by Adhikari and Frederico [23] inspired us to explore the problem further. Scaling arguments have always helped in finding energy levels of a variety of potentials. For potential λr^μ, scaling the coordinate by a factor γ leads to the relation $E(\lambda) = \frac{1}{\gamma^2} E(\lambda r^{2+\mu})$. Choosing $\gamma = \left(\frac{1}{\lambda}\right)^{\frac{1}{2+\mu}}$ we find $E(\lambda) = E(1)\lambda^{\frac{2}{2+\mu}}$. Since $E(1)$ is a constant, $E(\lambda) \sim \lambda^{\frac{2}{2+\mu}}$. If $\lambda = m\omega^2$ and $\mu = 2$ (simple harmonic oscillator), then $E \propto \omega$ as is well known. For $\mu = 4$, we get another familiar result that $E \propto \lambda^{1/3}$. For $\mu = -1$ and $\lambda = e^2$, we get the hydrogen atom charge dependence $E \propto e^4$. In what follows we will use a scaling argument for the potential $V(r) = r^2 + \frac{\lambda}{r^\alpha}$. This potential is obviously very different from the potential λr^μ considered before because it supports a specific length scale r_0 mentioned above. Consequently, the scaling argument cannot be of the kind shown above. The scaling argument is now going to be more subtle and in what follows we will show how the ordering of perturbation theory by fractional powers of λ can be inferred from a scaling argument. The ability to obtain the exponent is reminiscent of the scaling arguments in critical phenomena. It is interesting to note that this kind of scaling argument was originally explored by Symanzik [24].

We begin by writing down the equation in a dimensionless form

$$-\left[\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_N^2}\right]\psi + \left(r^2 + \frac{\lambda}{r^\alpha}\right)\psi = E\psi \tag{1}$$

with the Hamiltonian given by

$$H = -\nabla_r^2 + r^2 + \frac{\lambda}{r^\alpha}. \tag{2}$$

The unperturbed Hamiltonian

$$H_0 = -\nabla_r^2 + r^2 \tag{3}$$

has a ground state energy $E_0 = N$ and the ground state wavefunction $\psi_g \sim e^{-r^2/2}$. First-order perturbation theory calculates the shift in energy as

$$\begin{aligned}
E_1 &= \frac{\langle\psi_g|\,\lambda r^{-\alpha}\,|\psi_g\rangle}{\langle\psi_g\mid\psi_g\rangle} \\
&= \lambda \frac{\int_0^\infty r^{-\alpha}\,e^{-r^2}\,d^N r}{\int_0^\infty e^{-r^2}\,d^N r} \\
&= \lambda \frac{\Gamma\left(\frac{N-\alpha}{2}\right)}{\Gamma(\frac{N}{2})}
\end{aligned} \tag{4}$$

for $\alpha < N$. For $\alpha = N$, the numerator becomes logarithmically divergent and for $\alpha > N$ it diverges more strongly. Hence, the perturbation series breaks down. Making λ smaller does

not save the situation. For $\alpha \geqslant N$, the only way to produce a reasonable answer is to introduce a cut-off in the lower limit of the integral. This cut-off can be provided by the minimum of the potential which, however, goes to zero as $\lambda \to 0$. The divergence comes from the region close to the origin and hence the integral gets a maximum contribution from the vicinity of the point $r = 0$. Therefore, the numerator of the equation (4) should look like $\int_\epsilon^\infty r^{-\alpha}\,\mathrm{d}^N r$, where ϵ is a very small number. Since ϵ is λ-dependent, we can write

$$\int_\epsilon^\infty r^{-\alpha}\,\mathrm{d}^N r = \lambda^{-\mu} \tag{5}$$

where μ is some positive number, as yet unknown, independent of λ. The negative sign ensures the fact that the integral diverges as $\lambda \to 0$. Therefore,

$$E = E_0 + A\lambda^Z$$
$$= N + A\lambda^Z \tag{6}$$

where A is some number and $Z = 1 - \mu$. The task now boils down to finding out Z. This is of crucial importance as Z will order the perturbation series. To obtain this we use a scaling argument. Let us say

$$H = -\nabla_r^2 + r^2 + \frac{\lambda}{r^\alpha}$$
$$E = E(\lambda) \tag{7}$$

under the scaling $r = \beta R$, the Hamiltonian H becomes

$$H = \frac{1}{\beta^2}\left[-\nabla_R^2 + \beta^4 R^2 + \frac{\lambda\beta^{2-\alpha}}{R^\alpha}\right]$$
$$= \frac{1}{\beta^2}H'. \tag{8}$$

The energy levels of H and H' are related by

$$E = \frac{1}{\beta^2}E'(\omega', \lambda') \tag{9}$$

where

$$\omega' = \beta^2$$
$$\lambda' = \lambda\beta^{2-\alpha}. \tag{10}$$

Let us now carry out the identical perturbation theory for H' as was done for H. This yields

$$E' = N\beta^2 + \lambda\beta^{2-\alpha}\left\langle\frac{1}{R^\alpha}\right\rangle. \tag{11}$$

The expectation value $\left\langle\frac{1}{R^\alpha}\right\rangle$ is given by

$$\left\langle\frac{1}{R^\alpha}\right\rangle = \lambda\frac{\int_0^\infty R^{-\alpha}\,\mathrm{e}^{-\beta^2 R^2}\,\mathrm{d}^N R}{\int_0^\infty \mathrm{e}^{-\beta^2 R^2}\,\mathrm{d}^N R}$$
$$= \frac{\beta^N}{\Gamma\left(\frac{N}{2}\right)}\int_0^\infty R^{N-\alpha-1}\,\mathrm{e}^{-\beta^2 R^2}\,\mathrm{d}R. \tag{12}$$

For the integral in equation (12), the discussion following equation (4) holds once again, and the divergence of this integral $\alpha > N$ leads to the $(\lambda')^{-\mu}$ behaviour of the integral for $\lambda' \to 0$. This allows us to write

$$E' = N\beta^2 + C(\lambda')^Z\beta^N \tag{13}$$

where C is some number. Hence, from equations (9) and (10)

$$
\begin{aligned}
E &= N + C(\lambda')^Z \beta^{N-2} \\
&= N + C(\lambda \beta^{2-\alpha})^Z \beta^{N-2} \\
&= N + C\lambda^Z \beta^{(2-\alpha)Z+(N-2)}.
\end{aligned}
\tag{14}
$$

This has to match equation (6) and requires

$$
\beta^{(2-\alpha)Z+(N-2)} = 1 \qquad \text{or} \qquad Z = \frac{N-2}{\alpha-2}.
\tag{15}
$$

For $N = 3$, we obtain the result $Z = \frac{1}{\alpha-2}$ established by Harrel [2].

We conclude by noting that this result does indeed order the perturbation theory by powers of λ^z. To do this, we need to examine the second perturbation theory which would yield the additional energy E_2 given by

$$
E_2 = \sum_{n\neq 0} \lambda^2 \frac{\langle \psi_g \left| \frac{1}{r^\alpha} \right| \psi_n \rangle \langle \psi_n \left| \frac{1}{r^\alpha} \right| \psi_g \rangle}{E_0 - E_n}.
\tag{16}
$$

In the above we assume that ψ_g and ψ_n are normalized wavefunctions. The important point once again is that the integral for the moment $\langle \psi_g | \frac{1}{r^\alpha} | \psi_n \rangle$ will be dominated by the small r region and in that range the behaviour of $|\psi_n\rangle$ is independent of r for all n and in all spatial dimensions. This can be seen by writing equation (3) in the form $\tilde{H}_0 \tilde{\psi}_0 = E_0 \tilde{\psi}$ where

$$
\tilde{H}_0 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{(N-1)(N-3)}{4r^2} + r^2
\tag{17}
$$

with $\tilde{\psi}$ required to vanish at $r = 0$. The above is true for spherically symmetric states ($l = 0$). For $l \neq 0$, N is replaced by $\bar{N} = N - l$. The energy levels of $\tilde{H}_0$ are $4n + N$, and the wavefunctions are $C_n r^{\frac{N-1}{2}} \mathrm{e}^{-r^2} F\left(-n, \frac{N}{2}, r^2\right)$, where F is the hypergeometric function which is finite at the origin and C_n is the normalization. Since ψ and $\tilde{\psi}$ are related by $\psi_n = \tilde{\psi}_n/r^{(\frac{N-1}{2})}$ the wavefunction $\psi_n = C_n \mathrm{e}^{-r^2} F\left(-n, \frac{N}{2}, r^2\right)$. Near the origin, $\mathrm{e}^{-r^2} \sim 1$, $F \sim$ constant and hence it follows that ψ_n is independent of r for $r \simeq 0$. With this result it follows that $\langle \psi_g | \frac{1}{r^\alpha} | \psi_n \rangle$ has the behaviour $\sim \int r^{-\alpha} \, \mathrm{d}^N r$ which is exactly the behaviour tackled in equation (5). Thus each of the integrals in equation (16) behaves as $\lambda^{-\mu}$ and the overall λ dependence is $\lambda^{2(1-\mu)} = \lambda^{2Z}$. The structure of the mth order perturbation theory requires m such integrals and since the wavefunction of H_0 is always r-independent near the origin, it follows that the λ-dependence of mth order perturbation theory will be λ^{mZ}. Thus, we have shown that by using a suitable scaling argument, the singular behaviour of the perturbation theory for the class of potentials $r^2 + \frac{\lambda}{r^\alpha}$ can be easily handled.

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