A self consistent technique for singular potentials

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Abstract. A technique used by Edwards and Singh [8] in the study of polymers is used to provide a simple analytic procedure for calculating the upper bound of the energies of a class of singular potentials. The accuracy of our procedure turns out to be better than 1%.

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Attractive potentials with a strong repulsive core are common in nuclear physics and molecular physics. A class of such potentials that have been studied extensively [1–6,9] in the last two decades is the class represented by $V(r) = r^2 + \frac{\lambda}{r^\alpha}$. Of particular interest is the ground state energy of a particle in this potential. In three dimensional space, the solution of $H\psi = E\psi$ for the $l = 0$ state reduces to

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left(r^2 + \frac{\lambda}{r^\alpha}\right) u = Eu \tag{1}$$

where $\psi = u/r$ and the boundary conditions on u is that it vanishes at $r = 0$. For $\alpha \geq 3$, these potentials exibit the so called Klauder phenomenon [4] where perturbation theory has to be ordered in fractional powers of λ, rather than integer powers for $\lambda \ll 1$. For $\alpha = 2$, the model is exactly solvable and as one raises α beyond 2, the difficulty that is going to set in at $\alpha = 3$ makes its presence felt by making convergence of numerical procedures slow. Very recently Hall and Saad [7] have adopted a clever variational scheme that yields accurate answers with much less labour. In this note we adopt an old argument of Edwards and Singh [8], set up to deal with a situation in polymers, to obtain a simple analytic formula for getting the upper bound of the ground state energy which is within 1% of the accurate variational and numerical results of Hall and Saad [7] for all λ. Specifically, we compare with Hall and Saad over a range of 6 decades in λ for $\alpha = 2.5$. The method of Edwards and Singh [8] exploits a neighboring exact result and uses selfconsistency. To implement it, we write,

$$\begin{aligned} H = &-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + r^2 + \lambda\beta\langle\frac{1}{r^{\alpha-2}}\rangle\frac{1}{r^2} \\ &+ \frac{\lambda}{r^\alpha} - \lambda\beta\langle\frac{1}{r^{\alpha-2}}\rangle\frac{1}{r^2} \end{aligned} \tag{2}$$

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$$\begin{aligned} = &-\frac{\mathrm{d}2}{\mathrm{d}r^2} + r^2 + \frac{A}{r^2} \\ &+ \lambda\left[\frac{1}{r^\alpha} - \beta\langle\frac{1}{r^{\alpha-2}}\rangle\frac{1}{r^2}\right] \\ = &\, H_0 + \lambda H' \end{aligned} \tag{3}$$

where

$$A = \lambda\beta\langle\frac{1}{r^{\alpha-2}}\rangle \tag{4}$$

$$H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + r^2 + \frac{A}{r^2} \tag{5}$$

$$H' = \lambda \times \left[\frac{1}{r^\alpha} - \beta\langle\frac{1}{r^{\alpha-2}}\rangle\frac{1}{r^2}\right]. \tag{6}$$

The eigenvalues and eigenfunctions of H_0 are exactly known. We first choose β by requiring that the first order perturbation correction to eigenvalues of H_0 vanish. This implies (we will always focus on the ground state) that $\langle H' \rangle = 0$ and hence

$$\beta = \left[\langle\frac{1}{r^{\alpha-2}}\rangle\langle\frac{1}{r^2}\rangle\right]^{-1} \langle\frac{1}{r^\alpha}\rangle \tag{7}$$

where all averages are taken with respect to the ground state of H_0. With this choice of β,

$$A = \lambda\langle\frac{1}{r^\alpha}\rangle/\langle\frac{1}{r^2}\rangle. \tag{8}$$

The ground state energy is given by (using the known spectrum) of H_0,

$$E = 2 + \sqrt{1 + 4A} \tag{9}$$

Table 1. Results for the ground state energy of a particle with the potential $V(r) = r^2 + \frac{\lambda}{r^\alpha}$ for $\alpha = 2.5$, obtained by self consistent method.

λ	E (Eq. (12))	E_{HS}
0.001	3.00406	3.00404
0.01	3.0385	3.0375
0.1	3.28	3.27
1.0	4.35	4.32
5.0	6.34	6.30
10.0	7.79	7.74

The ground state wave function is

$$\psi = N\mathrm{e}^{-r^2/2} r^{\frac{E-1}{2}} \tag{10}$$

$$\left\langle \frac{1}{r^\alpha} \right\rangle = \Gamma\left(\frac{E-\alpha}{2}\right) / \Gamma(E/2) \tag{11}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \Gamma\left(\frac{E-2}{2}\right) / \Gamma(E/2). \tag{12}$$

Using equations (11) and (12), equation (9) becomes

$$(E-2)^2 - 1 = 4\lambda \frac{\Gamma(\frac{E-\alpha}{2})}{\Gamma(\frac{E-2}{2})}. \tag{13}$$

The answer is exact at $\lambda = 0$ and at $\alpha = 2$ for all λ. It can be used at $\alpha = 3$ which is where the Klauder phenomenon sets in but is inaccurate at that point. In Table 1, we show the energy coming from equation (13), and the accurate variational and numerical values of Hall and Saad which we denote by E_{HS}.

As we can see from Table 1, over a range of λ spanning 4 decades, we can achieve 1% accuracy with a formula as simple as that of equation (13).

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