Comment on: 'A simple analytical expression for bound state energies for an attractive Gaussian confining potential'

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Abstract. We discuss a recently proposed analytical formula for the eigenvalues of the Gaussian well and compare it with the analytical expression provided by the variational method with the simplest trial function. The latter yields considerably more accurate results than the former for the energies and critical parameters.

In a recent paper Köksal [1] proposed a simple analytical expression for the eigenvalues of the attractive Gaussian potential

$$V(r) = -\gamma e^{-\lambda r^2} \tag{1}$$

where $\gamma > 0$ is the well depth and $\lambda > 0$ determines its width. From the expansion of the potential-energy function about its minimum $V(r) = -\gamma(1 - \lambda r^2 + \frac{\lambda^2}{2} r^4 - \ldots)$ and perturbation theory the author derived an expansion for the energy of the form

$$E_{nl} = E_{nl}^{HO} + \Delta E_{nl}^{(1)} + \Delta E_{nl}^{(2)} + \ldots \tag{2}$$

where $n = 0, 1, \ldots$ and $l = 0, 1, \ldots$ are the radial and angular-momentum quantum numbers, respectively. The first term E_{nl}^{HO} is the sum of the minimum potential energy $-\gamma$ plus the harmonic oscillation about this minimum.

It is well known that the perturbation series (2) is suitable for sufficiently deep wells (sufficiently great γ) [2]. In order to obtain a better expression Köksal rewrote that perturbation expansion in terms of an exponential function. Since the author did not describe the general strategy clearly we conjecture that the main idea is embodied in the following expression

$$E_{nl}^{K} = \frac{1}{2}\left(E_{nl}^{HO} + \gamma\right) - \gamma e^{-\left(E_{nl}^{HO}+\gamma\right)/(2\gamma)} \tag{3}$$

For large γ we expand the exponential function and obtain the first term of the perturbation series (2) exactly and the approximation $-\frac{1}{8\gamma}\left(E_{nl}^{HO} + \gamma\right)^2$ to the second one. Köksal did not discuss the agreement between the analytical formula (3) and the perturbation series (2). Consequently, without further justification this expression can be considered to be an empirical formula and its validity determined solely by the accuracy of the results. It is worth noting that we can write equation (3) without recourse to perturbation theory because we only need the term of order zero.

Köksal carried out some calculations for the particular model parameters $\lambda = 1/a_B^2$ and $\gamma = 400\,Ryd$, where a_B is the Bohr radius and Ryd the Rydberg energy. The approximate formula (3) appears to approach the numerical eigenvalues reasonably well for some values of the quantum numbers. However, we do not know the actual accuracy of the empirical formula (3) because the author did not report results for other well depths. What we already know is that the accuracy of the empirical formula decreases with l and most remarkably with n [1].

The purpose of this comment is to test the accuracy of the empirical formula (3) more extensively and compare it with a simple analytical expression obtained by means of the variational method.

The Schrödinger equation is

$$\begin{aligned} H\psi &= E(\gamma,\lambda)\psi \\ H &= -\frac{\hbar^2}{2m}\nabla^2 + V(r) \end{aligned} \tag{4}$$

where m is the mass of the particle which Köksal chose to be the electron. It is always convenient to work with a dimensionless eigenvalue equation that we easily derive in terms of the dimensionless coordinates $\mathbf{r}' = \mathbf{r}/L$, where L is an appropriate length unit. The Schrödinger equation thus becomes $H'\psi' = E'\psi'$, where $H' = mL^2H/\hbar^2$ and $E' = mL^2E/\hbar^2$. If, for example, we choose $L = \lambda^{-1/2}$ then we obtain

$$\begin{aligned} H' &= -\frac{1}{2}\nabla'^2 - \xi e^{-r'^2} \\ \xi &= \frac{m\gamma}{\lambda\hbar^2} \end{aligned} \tag{5}$$

where $\nabla'^2 = L^2\nabla^2$. Note that E' depends only on the parameter ξ since $E'(\xi) = E(\xi,1) = \xi E(\gamma,\lambda)/\gamma$.

The dimensionless version of the empirical formula (3) is

$$E'^{K}_{nl}(\xi) = \frac{1}{2}\left(2n + l + \frac{3}{2}\right)\sqrt{2\xi} - \xi e^{-\frac{1}{2}\left(2n+l+\frac{3}{2}\right)\sqrt{\frac{2}{\xi}}} \tag{6}$$

so that the discussion of its accuracy is greatly facilitated by the fact that we need to vary just one model parameter. Note that when $\lambda = 1/a_B^2$ then $\xi = \frac{\gamma}{2}\frac{2ma_B^2}{\hbar^2}$ is half the

well depth in Rydberg units $Ryd = \frac{\hbar^2}{2ma_B^2}$. Therefore, the particular values of the model parameters γ and λ chosen by Köksal correspond to $\xi = 200$.

In a recent pedagogical article Fernández [3] discussed the application of the variational method to the one-dimensional Gaussian well (see also [4]). We can apply the same approach to the Gaussian well in three dimensions. Following those papers we choose the simple trial function

$$\varphi(r) = Nr^{l+1}e^{-ar^2} \tag{7}$$

where N is a normalization factor and $a > 0$ is a variational parameter (we drop the primes on the dimensionless variables from now on). The optimal value of a is given by a root of $d\left\langle H_r\right\rangle/da = 0$, where H_r is the radial Hamiltonian

$$H_r = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \xi e^{-r^2} \tag{8}$$

We thus obtain

$$\begin{aligned} \xi &= \frac{(2a+1)^{\frac{2l+5}{2}}}{2^{l-\frac{1}{2}}4a^{\frac{2l+1}{2}}} \\ E_{0l}^{\prime\, var} &= \frac{a\,(2l+1-4a)}{2} \end{aligned} \tag{9}$$

We can proceed in two alternative ways: either, given ξ we solve the first equation numerically for a and then obtain the energy or we obtain both ξ and the energy analytically for a set of values of a (a parametric equation for the energy).

Fig. 1 shows the eigenvalues E'_{0l} for $\xi = 200$ and several values of l calculated by means of equations (6) and (9). The highly accurate eigenvalues provided by the Riccati-Padé method (RPM) [5] can be considered to be exact for present purposes. As discussed above $\xi = 200$ corresponds to the potential parameters chosen by Köksal. We appreciate that $E_{0l}^{\prime\, K}$ deviates from the exact result as l increases. On the other hand, the variational energy $E_{0l}^{\prime\, var}$ deviates so less noticeably that it appears to agree exactly with the exact energy in the scale of the figure.

Fig. 2 compares the approximate ground-state energies $E_{00}^{\prime\, K}$, $E_{00}^{\prime\, var}$ and the exact RPM ones for a range of values of ξ. We appreciate that the variational energy is closer

to the exact one for all values of ξ. However, the empirical expression (6) appears to yield reasonable results for the ground-state energy for all those values of the well depth. Note that the largest potential parameter $\xi = 30$ in Fig 2 is considerably smaller than the one chosen by Köksal. It is well known that the deepest the well the more accurate the results of perturbation theory [2]. For this reason the values of the potential parameters in Fig. 2 pose a good test for any formula based on perturbation theory.

It is also well known that the Gaussian well supports a finite number of bound states and that there are critical values of the potential parameter ξ for which bound states are exactly at the threshold of the continuum spectrum $E = 0$. In other words, there exists a bound-state eigenvalue E'_{nl} provided that $\xi > \xi_{nl}$, where $E'_{nl}(\xi_{nl}) = 0$. Köksal did not discuss this important problem by means of the empirical formula (3) altough it is obvious that we can obtain estimates ξ^K_{nl} from the roots of $E'^K_{nl}(\xi) = 0$. We cannot solve this equation exactly but the numerical calculation is simple enough. On the other hand, from the variational energy (9) we obtain $a_{0l} = (2l + 1)/4$ and the extremely simple analytical formula

$$\xi^{var}_{0l} = \frac{(2l+3)^{\frac{2l+5}{2}}}{8\,(2l+1)^{\frac{2l+1}{2}}} \tag{10}$$

Fig. 3 shows ξ^K_{0l}, ξ^{var}_{0l} and the accurate numerical results obtained by Liverts and Barnea [6]. It is clear that while ξ^K_{0l} merely follows the trend ξ^{var}_{0l} is almost indistinguishable from the exact results in the scale of the figure. More precisely, the accuracy of ξ^K_{0l} decreases noticeably with l while ξ^{var}_{0l} remains remarkably accurate for all l values.

Since the author did not give a clear justification for the empirical formula (3) nor a sound procedure that may be applied to other problems we assume that the sole purpose of the paper was to obtain an empirical formula for the eigenvalues of the Gaussian well. This assumption is supported by the fact that Köksal did not attempt to derive a similar expression for the eigenvalues of the Yukawa potential already treated by the same perturbation method in an earlier paper [7]. On the other hand, the variational method discussed above is not restricted to the Gaussian well and can be easily applied

to the dimensionless Schrödinger equation for the Yukawa potential

$$V(r) = -\frac{\xi}{r}e^{-r} \tag{11}$$

By means of the trial function

$$\varphi(r) = Nr^{l+1}e^{-ar} \tag{12}$$

we obtain the variational parametric formula for the energy

$$\begin{aligned} \xi &= \frac{(l+1)(2a+1)^{2l+3}}{2^{2(l+1)}a^{2l+1}(2a+2l+3)} \\ E'^{var}_{0l} &= \frac{a^2(2l+1-2a)}{2(2a+2l+3)} \end{aligned} \tag{13}$$

and the critical parameters are given by the simple analytical expression

$$\xi^{var}_{0l} = \frac{2^{2l}(l+1)^{2l+3}}{(2l+1)^{2l+1}} \tag{14}$$

Fig. 4 shows the remarkable agreement between this formula and the accurate numerical results of Liverts and Barnea [6].

Finally, we summarize the main conclusions of this comment:

First, Köksal's empirical formula is far less accurate than the analytical expression provided by the simplest variational function. It is true that Köksal's formula applies to states with $n > 0$ while the variational method does not yield simple analytical expressions for such states (the Rayleigh-Ritz method suitable for them should be treated numerically). However, it is also true that Köksal's empirical formula becomes considerably less accurate as n increases [1] and here we have just compared the results for the most favourable case $n = 0$.

Second, the variational method applies to other problems as we have just illustrated by means of the Yukawa potential. For unknown reasons Köksal did not attempt to apply the same approach to other models for which perturbation corrections are already available [2] as it is the case of the Yukawa potential [7].

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[6] Liverts E Z and Barnea N 2011 *J. Phys. A* **44** 375303.

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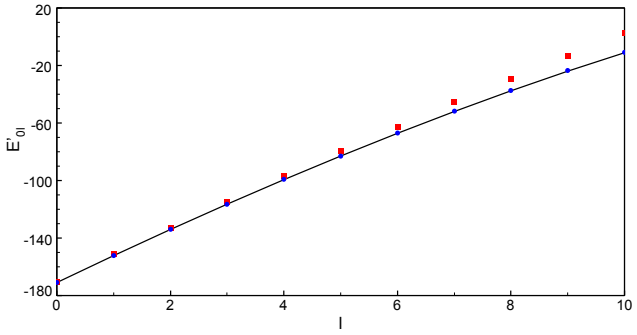

Figure 1. Energy eigenvalues $E_{0l}'^{K}$ (red squares), $E_{0l}'^{var}$ (blue circles) and $E_{0l}'^{exact}$ (solid line) for $\xi = 200$

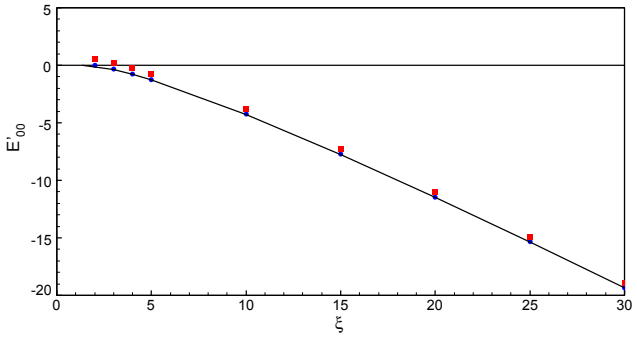

Figure 2. Ground-state energy $E_{00}'^{K}$ (red squares), $E_{00}'^{var}$ (blue circles) and $E_{00}'^{exact}$ (solid line) for a range of ξ values

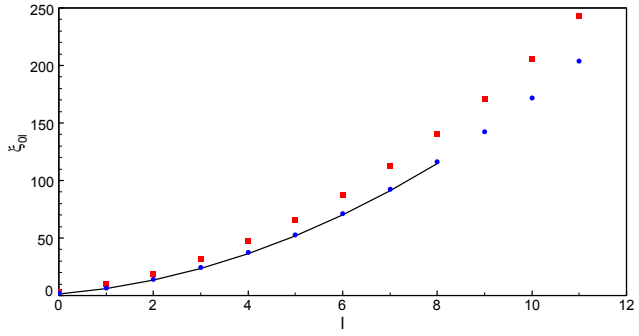

Figure 3. Critical parameters ξ_{0l}^{K} (red squares), ξ_{0l}^{var} (blue circles) and ξ_{0l}^{exact} (solid line)

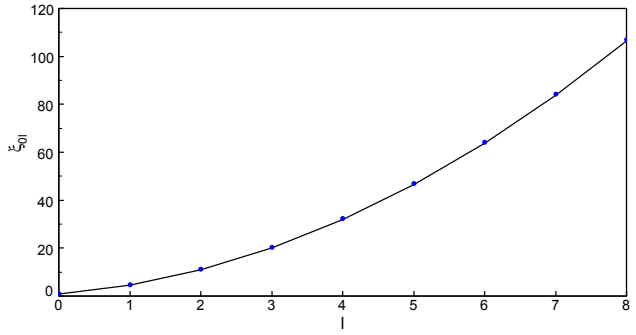

Figure 4. Critical parameters ξ_{0l}^{var} (blue circles) and ξ_{0l}^{exact} (solid line)