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The HVT technique and the treatment of two basic inequalities

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Abstract

The quantum mechanical hypervirial theorems (HVT) technique is used in treating two basic inequalities relating the ground-state mean square radius of the orbit of a particle in a central potential and its kinetic energy, respectively, to the spacing of the two lowest energy levels ΔE. For quite a wide class of those potentials, the parameters of which also lead to a sufficiently small dimensionless quantity s, the difference between the two sides of each inequality is of order s^3 and higher (while ΔE is of order s and higher), and thus it is expected in general to be quite small.

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The quantum mechanical hypervirial theorems (HVT) technique is an efficient technique in treating quite a few problems, avoiding the use of the wavefunction [1–5]. The aim of this paper is to discuss in this context two basic (in)equalities which are known in the literature. They refer to physically interesting quantities for a particle, in its ground state, moving non-relativistically in a three-dimensional central potential $V = V(r)$.

The first (in)equality relates the mean square radius (msr) of its orbit: $\langle r^2\rangle_{1\mathrm{s}} \equiv \langle r^2\rangle_{00}$ to the spacing between the two lowest energy levels $\Delta E \equiv (E_{1\mathrm{p}} - E_{1\mathrm{s}}) \equiv (E_{01} - E_{00})$:

$$\langle r^2\rangle_{1\mathrm{s}} \leqslant \frac{3\hbar^2}{2\mu(E_{1\mathrm{p}} - E_{1\mathrm{s}})} \tag{1a}$$

where μ is the mass of the particle or its reduced mass if the particle moves in the field of another particle or of a 'core system'.

The second relates the expectation value of its kinetic energy operator to the same energy-level spacing:

$$\langle \hat{T}\rangle_{1\mathrm{s}} \geqslant \tfrac{3}{4}(E_{1\mathrm{p}} - E_{1\mathrm{s}}). \tag{2a}$$

In both relations, the equality sign holds for the harmonic oscillator (HO) potential.

Relations (1a) and (2a) were derived on the basis of the Thomas–Reiche–Kuhn sum rule by Bertlmann and Martin [6, 7] in discussing a special application of them. As was mentioned in [7], however, they were derived originally in an alternative way and quoted in [8]. Reference to them [9] and their extensions [10] has also been useful in discussing single-particle aspects of a Λ in hypernuclei. Since both relations are, unfortunately, in a form of inequality (but for the HO potential), a pertinent question is whether the inequalities 'get saturated' [10], that is whether they become equalities approximately (e.g. within a few per cent). This depends on the functional form (the shape) of the central potential considered and also on the values of its parameters. For the singular Coulomb potential, the deviation from equality is quite large while for other potentials it can become fairly small.

In order to discuss this matter, we write relations (1*a*) and (2*a*) as

$$E_{1\mathrm{p}} - E_{1\mathrm{s}} \leqslant \frac{3\hbar^2}{2\mu\langle r^2\rangle_{1\mathrm{s}}} \tag{1b}$$

or

$$E_{1\mathrm{p}} - E_{1\mathrm{s}} = \frac{3\hbar^2}{2\mu\langle r^2\rangle_{1\mathrm{s}}} + C_1 \qquad C_1 = -|C_1| < 0 \tag{1c}$$

and

$$E_{1\mathrm{p}} - E_{1\mathrm{s}} \leqslant \tfrac{4}{3}\langle\hat{T}\rangle_{1\mathrm{s}} \tag{2b}$$

or

$$E_{1\mathrm{p}} - E_{1\mathrm{s}} = \tfrac{4}{3}\langle\hat{T}\rangle_{1\mathrm{s}} + C_2 \qquad C_2 = -|C_2| < 0 \tag{2c}$$

and express the 'correction terms' C_1 and C_2 in terms of the potential parameters.

In this paper we consider, quite generally, the fairly wide class of central potentials of the form

$$V(r) = -Df(r/R) \qquad 0 \leqslant r < \infty \tag{3}$$

where $D > 0$ is the potential depth, $R > 0$ its radius and f ($f(0) = 1$) the 'potential form factor' (determining its shape) which is further assumed to be an appropriate analytic function of even powers of $x = r/R$ with $\mathrm{d}^2 f/\mathrm{d}x^2|_{x=0} < 0$. Potentials of this class include the well-known Gaussian potential: $V_G(r) = -D\,\mathrm{e}^{-r^2/R^2}$, the (reduced) Pöschl–Teller (PT) potential: $V_{PT}(r) = -D\cosh^{-2}(r/R)$ and others, which have been used in practice.

Application of the HVT technique to that class of potentials has led to (truncated) expansions of the quantities of interest, such as the energy eigenvalues E_{nl}, the ms radii of the particle orbits $\langle r^2\rangle_{nl}$ etc of the form [11]

$$E_{nl} = -Df_1(s) \qquad \langle r^2\rangle_{nl} = R^2 f_2(s) \qquad \langle\hat{T}\rangle_{nl} = -D\frac{s}{2}\frac{\partial f_1(s)}{\partial s} \tag{4}$$

where $f_1(s)$ and $f_2(s)$ are power series of the dimensionless quantity

$$s = [\hbar^2/(2\mu DR^2)]^{1/2} \tag{5}$$

which is assumed to be sufficiently small. The coefficients in those power series depend on the quantum numbers nl of the state and on the numbers:

$$d_k = \frac{1}{(2k)!}\frac{\mathrm{d}^{2k}}{\mathrm{d}x^{2k}} f(x)|_{x=0} \tag{6}$$

determined by the potential shape.

Use of the explicit expressions of the coefficients in the power series in (4) (see [11] and references therein) leads, after some algebra, to the following expressions for the quantities in (1) and (2) by keeping in them terms of order s^4:

$$\begin{aligned}\Delta E = E_{1\mathrm{p}} - E_{1\mathrm{s}} = 2D(-d_1)^{1/2}s\,\big\{1 - \tfrac{5}{2}(-d_1)^{1/2}d_1^{-2}d_2 s + \tfrac{5}{8}d_1^{-3}\left[18d_2^2 - 21d_1d_3\right]s^2 \\ + \tfrac{5}{64}(-d_1)^{1/2}d_1^{-5}\left[1008d_1^2d_4 - 2268\,d_1d_2d_3 + 1271\,d_2^3\right]s^3 + \cdots\big\}\end{aligned} \tag{7}$$

$$\langle r^2\rangle_{1\mathrm{s}} = \tfrac{3}{2}R^2(-d_1)^{-1/2}s\,\big\{1+\tfrac{5}{2}(-d_1)^{1/2}d_1^{-2}d_2s-\tfrac{5}{16}d_1^{-3}\big[55d_2^2-42d_1d_3\big]s^2 - \tfrac{45}{8}(-d_1)^{1/2}d_1^{-5}\big[14d_1^2d_4-42d_1d_2d_3+29d_2^3\big]s^3+\cdots\big\} \qquad (8)$$

$$\langle\hat{T}\rangle_{1\mathrm{s}} = \tfrac{3}{2}D(-d_1)^{1/2}s\,\big\{1-\tfrac{5}{2}(-d_1)^{1/2}d_1^{-2}d_2s+\tfrac{15}{16}d_1^{-3}\big[11d_2^2-14d_1d_3\big]s^2 + \tfrac{45}{16}(-d_1)^{1/2}d_1^{-5}\big[28d_1^2d_4-56d_1d_2d_3+29d_2^3\big]s^3+\cdots\big\}\,. \qquad (9)$$

It is evident that the meaningful quantities to 'assess the degree of saturation' of the inequalities are not C_1 and C_2, themselves, but rather the quantities $RC1$ and $RC2$, which are the ratios of C_1 and C_2 respectively, to ΔE:

$$RC1 = \frac{C_1}{E_{1\mathrm{p}}-E_{1\mathrm{s}}} \qquad \text{and} \qquad RC2 = \frac{C_2}{E_{1\mathrm{p}}-E_{1\mathrm{s}}}. \qquad (10)$$

These (dimensionless) quantities can be used directly to evaluate the 'percentage deviations' from equalities of inequalities (1*b*) and (2*b*) respectively, which express the difference between the two sides of each inequality with respect to their l.h.s. $(E_{1\mathrm{p}}-E_{1\mathrm{s}})$.

The expression of $RC1$ which is derived is the following:

$$RC1 \simeq RC1a = 1-(PQ)^{-1} \qquad (11)$$

where P and Q are the quantities in curly brackets in formulae (7) and (8), respectively (where, however, the higher terms denoted by dots had been neglected).

We may also write

$$RC1a \simeq RC1b = \tfrac{5}{16}d_2^2d_1^{-3}s^2\,\big\{1+\tfrac{3}{4}(-d_1)^{1/2}d_1^{-2}d_2^{-1}\,\big[31d_2^2-28d_1d_3\big]\,s+\vartheta(s^2)\big\}\,. \qquad (12)$$

On the other hand, for $RC2$ we have

$$RC2 \simeq RC2a = \tfrac{15}{16}d_2^2d_1^{-3}s^2\,\big\{1+\tfrac{1}{12}(-d_1)^{1/2}d_1^{-2}d_2^{-1} \times\big[227d_2^2-252d_1d_3\big]\,s+\vartheta(s^2)\big\}\big/P \qquad (13)$$

or

$$RC2a \simeq RC2b = \tfrac{15}{16}d_2^2d_1^{-3}s^2\,\big\{1+\tfrac{1}{12}(-d_1)^{1/2}d_1^{-2}d_2^{-1} \times\big[257d_2^2-252d_1d_3\big]\,s+\vartheta(s^2)\big\}. \qquad (14)$$

We may note that all the above expressions of $RC1$ and $RC2$ depend exclusively on the dimensionless parameter s and on the numbers d_k which determine the potential shape. We may also note from their (truncated) expansions in s (see $RC1b$ and $RC2b$) that they are of order s^2 and higher and therefore they are expected in general to be quite small. Thus, the correction terms C_1 and C_2 are of the order s^3 and higher (since ΔE is of order s and higher as is clear from (7)).

In figures 1 and 2, the absolute values of RC (that is of $RC1a$, $RC1b$, $RC2a$, $RC2b$) are displayed as functions of s, for small values of this parameter, in the case of the PT and the Gaussian potential, respectively. The percentage deviations from the respective equalities are quite small and increase with s. The condition of considering sufficiently small values of s is necessary in order that the pertinent formulae for $RC1$ and $RC2$ provide a reasonable estimate of those quantities, as one can also check by employing the more laborious task of solving numerically the Schrödinger equation to determine its eigenfunctions and eigenvalues and also calculating numerically the expectation values involved. The values of $RC1a$, $RC1b$, $RC2a$, $RC2b$ obtained with the approximate analytic formulae given in this paper are in fair agreement with the corresponding values of $RC1$ and $RC2$ obtained through the numerical solution of the Schrödinger equation, as long as s is very small.

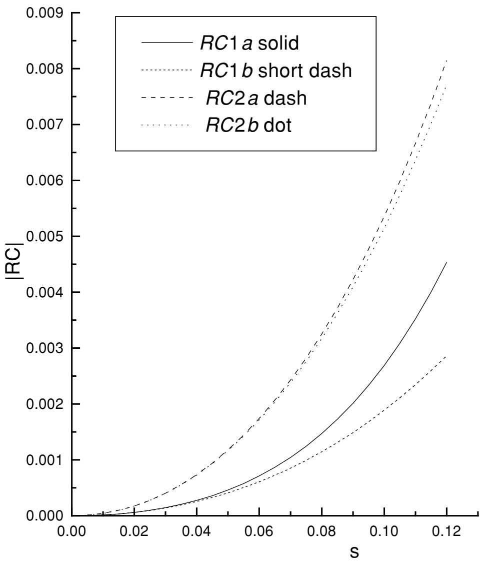

Figure 1. The variation of the quantities $RC1a$, $RC1b$, $RC2a$ and $RC2b$ (see text) with the dimensionless parameter s, for the (reduced) Pöschl–Teller potential.

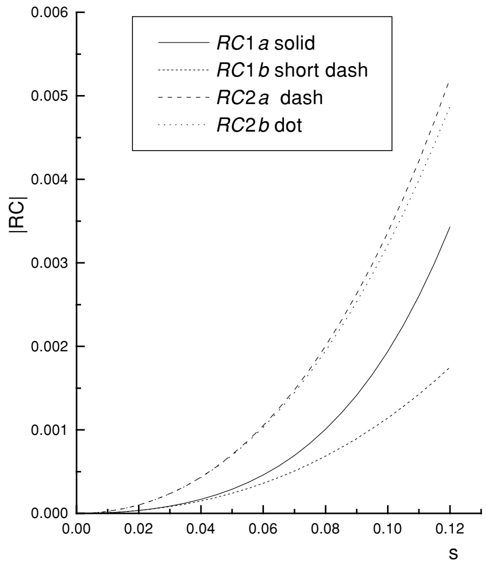

Figure 2. The same as in figure 1 for the Gaussian potential.

We may observe that for a given (small) value of s, the (absolute) values of $RC1$ are smaller than those of $RC2$ and therefore we may conclude that the first inequality 'saturates better' than the second inequality. Furthermore, both parameters $RC1$ and $RC2$ have smaller values for the Gaussian potential in comparison with the corresponding values for the PT and therefore we may also conclude that the saturation of the inequalities for the Gaussian potential is better.

Finally, in order to discuss the inequalities in connection with a specific physical problem, we consider the binding energy of a Λ particle in finite nuclei and the determination of the potential parameters by fitting to known experimental values of the two lowest energy levels for a number of hypernuclei [12]. We find that a very good fit is obtained by treating as fitting parameters the potential depth and the parameters a and r_0 in the expression of the potential radius $R = a + r_0 A_c^{1/3}$, where A_c is the mass number of the core nucleus. For the PT potential the best fit values are $D = 34.29$ MeV, $a = -1.371$ fm, $r_0 = 1.649$ fm, while for the Gaussian $D = 33.89$ MeV, $a = -1.241$ fm, $r_0 = 1.698$ fm. Using these values we can estimate $RC1$ and $RC2$ when s is sufficiently small. For example, in the case of ${}^{89}_{\Lambda}\mathrm{Y}$ where s is rather small we may estimate that for the PT potential ($s = 0.1204$) $RC1a = 0.0046$, $RC1b = 0.0029$. The value obtained by solving the Schrödinger equation numerically is 0.0036. Also $RC2a = 0.0082$, $RC2b = 0.0078$ (while the corresponding value from the Schrödinger equation is 0.0087). For the Gaussian potential ($s = 0.1145$) $RC1a = 0.0030$, $RC1b = 0.0016$. The value from the numerical solution of the Schrödinger equation is 0.0024. In addition, $RC2a = 0.0046$, $RC2b = 0.0044$ (while the corresponding value from the Schrödinger equation is 0.0058). We again realize that the saturation of (1b) is better than that of (2b).

Before ending, it would be pertinent to recall that other numerical techniques in studying our basic inequalities could also be used. In particular, an efficient numerical form of the HVT (such as the so-called renormalized hypervirial perturbation theory (renormalized HVPT))

[13] which does not halt at any term of the algebraic expansion, would be very appropriate. Such an approach has been extensively used in the literature in treating various problems (see e.g. [5, 14]). Two interesting applications of that method were made recently, where the method was also summarized. The first application [15] refers to the treatment of a non-linear Schrödinger equation with power-law potential terms and the other [16] to a Penning trap problem.

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