Quantum mechanical virial-like theorem for confined quantum systems

Neetik Mukherjee* and Amlan K. Roy†
Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur 741246, Nadia, West Bengal, India

(Received 31 December 2018; published 22 February 2019)

Confinement of atoms inside impenetrable (hard) and penetrable (soft) cavities has been studied for nearly eight decades. However, a unified virial theorem for such systems has not yet been found. Here we provide a general virial-like equation in terms of mean square and expectation values of potential and kinetic energy operators. It appears to be applicable in *both free and confined* situations. Apart from that, we have derived an equation using the time-independent Schrödinger equation, which can be treated as a sufficient condition for a given stationary quantum state. A change of boundary condition does not affect these virial equations. In the *hard* confining condition, the perturbing (confining potential) does not affect the expression; it merely shifts the boundary from infinity to a finite region. In the *soft* case, on the contrary, the final expression includes contributions from the perturbing term. These are demonstrated numerically for several representative enclosed systems like harmonic oscillators (one-dimensional and three-dimensional) and hydrogen atoms. Its applicability in various other confinements (including angular) has been discussed. In essence, a virial equation has been proposed for *free and confined* quantum systems, from simple arguments.

DOI: 10.1103/PhysRevA.99.022123

I. INTRODUCTION

Over the past 20 years confined quantum systems have emerged as a topic of considerable significance for physicists, chemists, and biologists [1]. Invention and advancement of contemporary experimental techniques have given the required insight about responses of matter under such constrained conditions. Furthermore, recent progress in nanoscience and nanotechnology has inspired extensive research activity to explore and acquire more thorough, in-depth understanding. Nowadays, various physical, chemical processes are carried out in spatially confined environments. They have profound applications in diverse areas of research, like condensed matter, semiconductor physics, astrophysics [2], nanotechnology, and quantum dots, wires, and wells [3]. In recent years, these models have also been employed to interpret trapping of atoms, molecules inside fullerene cages, zeolite cavities [1,3,4], etc.

A quantum particle under the influence of confinement displays many fascinating, distinctive changes in observable physical, chemical properties [5,6] from its corresponding *unconfined or free* counterpart. Many elegant reviews and monographs have been written on the subject. Usually, the Schrödinger equation (SE) cannot be solved *exactly*; therefore, one has to take recourse to approximate methods. The perturbative approach leads to an asymptotic series [7], and the standard linear variation method is fraught with the problem of proper boundary behavior, as familiar orthonormal basis sets do not vanish at finite boundaries. Thus linear combinations of such bases are explicitly inappropriate in representing their eigenstates. Recently for some central potentials (harmonic oscillator, H atom, pseudoharmonic oscillator, etc.) under hard confinement conditions, such an equation has been solved *exactly*. These eigenfunctions can then readily be used as an appropriate orthonormal basis set in other confined systems [8].

In 1937, the first model for a confined quantum system, a H atom trapped inside a *hard, impenetrable* barrier, was proposed to understand its behavior under extreme pressure [9]. With time this was found to be somehow restrictive for practical purposes, leading to the development of so-called *penetrable* barriers. For the sake of convenience, it may be appropriate to categorize different confining potentials, following Ref. [10], in two broad classes, namely, (i) a *penetrable* potential which is finitely bounded from above, whereas in an *impenetrable* case, it rises to infinity at large r, and (ii) a continuous potential will be termed as *smooth* while a *sharp* one possesses discontinuity. In the case of the *impenetrable*, *sharp* condition, the potential is modified by the addition of a term that disappears up to a certain distance from origin, rising to infinity thereafter. It is defined as $V = V(r)$ at $0 \leqslant r \leqslant r_c$, whereas $V = \infty$ at $r > r_c$ (r_c implies confinement radius). In this scenario, the Dirichlet boundary condition $R_{n,\ell}(0) = R_{n,\ell}(r_c) = 0$ is satisfied [1]. On the other hand, an *impenetrable, smooth* potential is defined as $V = V(r) + V_c(r)$, where $V_c(r)$ is the confining potential that becomes infinity at $r \to \infty$ and remains continuous otherwise [11,12]. Similarly, for the *penetrable, sharp* case the potential has the form $V = V(r)$ at $0 \leqslant r \leqslant r_c$ and $V = V_c(r)$ at $r > r_c$, where $V_c(r)$ is the confining potential [13]. Finally, in the *penetrable, smooth* case it becomes $V = V(r) + V_c(r)$ [14]. In recent years, various models have been proposed and investigated by many authors [3,15–18], particularly in the context

*neetik.mukherjee@iiserkol.ac.in
†Corresponding author: akroy@iiserkol.ac.in; akroy6k@gmail.com

of the H atom, maintaining these confinement conditions and revealing numerous striking features [1,3,19–21].

Extensive theoretical calculations have been made in the case of a confined harmonic oscillator (CHO) [one dimension (1D), 2D, 3D, and d dimensions] [8,22–26] and a confined hydrogen atom (CHA) inside an impenetrable cavity [3,23,27–36]. They offer many extraordinary features, especially relating to *simultaneous, incidental, interdimensional degeneracy* [25] in their energy spectra. The effects of contraction on ground and excited energy states, as well as other properties like hyperfine splitting constant, dipole shielding factor, nuclear magnetic screening constant, static and dynamic polarizability, etc., were explored [1,3,4]. A wide range of attractive analytical and numerical approaches including perturbation theory, the Padé approximation, the WKB method, the hypervirial theorem, the power-series solution, supersymmetric quantum mechanics, Lie algebra, Lagrange mesh, asymptotic iteration, the generalized pseudospectral method, etc., were invoked to solve the relevant eigenvalue problem [27–35]. Exact solutions [32] of CHAs are expressible in terms of Kummer's M function (confluent hypergeometric).

In quantum mechanics, stationary states of a bound system satisfy the virial theorem (VT). In fact, it is a necessary condition for a quantum stationary state to follow [37]. Historically the quantum mechanical VT was derived from analogy with a classical counterpart; for a nonrelativistic Hamiltonian, it offers a relation between expectation values of kinetic energy and directional derivatives of potential energy. In this regard, it is important to point out that a variationally optimized wave function also follows the VT. Hence, it becomes a necessary condition for an exact wave function. On the contrary, merely fulfilling this relation will not ensure a bound state. After some controversy, it is now generally accepted that the standard form of the VT does not ordinarily hold good in enclosed conditions; rather a modified form is invoked. Several attempts have been made to find an appropriate form of the VT in such systems [7,38,39]. Previously, some semiclassical strategies based on the Wilson-Sommerfeld rule and uncertainty principle were adopted to construct this in such systems [40]. In recent years, the standard form of the VT and the Hellmann-Feynman theorem were combined to design a virial-like expression for *penetrable and impenetrable* CHAs [10]; however, the mathematical form of the expression changes from system to system. Importantly, all these relations can only serve as necessary conditions for an exact state to follow. In this endeavor our primary objective is to propose a general virial-like expression for both *free and confined* conditions using the time-independent SE, the hyper-virial theorem (HVT) [41], along with mean square and expectation values of potential and kinetic energy operators. Apart from that, a relation involving the SE and the HVT has been derived, which can serve as a sufficient condition (only true for exact states) for a bound stationary state. A detailed derivation of these relations is given in Sec. II. Next in Sec. III, we proceed to verify the utility and applicability of these relations in the context of several representative confined systems. We begin with the oldest, most frequently used model of *hard* confinement, where the potential is trapped inside an infinite wall satisfying the *Dirichlet boundary condition*. In this category, at first, we discuss the typical and most prolific cases of CHO (1D and 3D) as well as a CHA. Later, this is extended to the so-called shell-confined H atom (SCHA), in order to understand the role of nodal structure in the confined condition. This can be potentially treated as a confined off-center model, needed to probe quantum wells and quantum dots. With time, a model for off-center quantum dot structures was also adopted, but within the framework of the *Newmann boundary condition*, a prominent example being the trapping of a H atom inside a *homogeneous, impenetrable* cavity (HICHA), which is analyzed next. It my be noted that, at $r_c \to 0$ this behaves similar to a CHA, while at $r_c \to \infty$ it resembles a free H-atom (FHA). In order to make these artificial atomic models more realistic, subsequently a finite wall was placed at a certain r_c; this has been widely used to study the properties of encapsulated atoms within a fullerene cage and a zeolite cavity. As an approximation to this, we explore the case of a H atom inside an *inhomogeneous, penetrable* spherical cavity (SPCHA). Apart from that, to incorporate the interaction of a particle with the environment, a *homogeneous, penetrable* confinement model was proposed—for this we considered a H atom under similar conditions (HPCHA). This will help us to determine the advantages of the presently derived relations in the pursuit of confined quantum systems. Section IV makes a few concluding remarks.

II. THEORETICAL FORMALISM

The time-independent nonrelativistic SE for a system may simply be written as

$$(\hat{T} + \hat{V})\psi_n(\tau) = \mathcal{E}_n\psi_n(\tau), \tag{1}$$

where $\hat{T}$ and $\hat{V}$ are the usual kinetic and potential energy operators of a given Hamiltonian and both are Hermitian, while τ is a generalized variable of coordinates. After some straightforward algebra (multiplying both sides by $\hat{T}$, integrating over the whole space, and rearranging), one gets

$$\langle \hat{T}^2\rangle_n + \langle \hat{T}\hat{V}\rangle_n = \mathcal{E}_n\langle \hat{T}\rangle_n. \tag{2}$$

Now, substitution of $\mathcal{E}_n$ by $\langle \hat{T}\rangle_n + \langle \hat{V}\rangle_n$ in Eq. (2) produces

$$\langle \hat{T}^2\rangle_n - \langle \hat{T}\rangle_n^2 = \langle \hat{V}\rangle_n\langle \hat{T}\rangle_n - \langle \hat{T}\hat{V}\rangle_n. \tag{3}$$

A similar consideration using $\hat{V}$ leads to the following equation:

$$\langle \hat{V}^2\rangle_n - \langle \hat{V}\rangle_n^2 = \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n - \langle \hat{V}\hat{T}\rangle_n. \tag{4}$$

Here, for a given Hamiltonian $\hat{H}$ the domains of $\hat{T}|\psi_n\rangle$ and $\hat{V}|\psi_n\rangle$ are the same as that of $\hat{H}$ [42]. Thus, from the Hypervirial theorem, it can be proved that $\langle \hat{T}\hat{V}\rangle_n = \langle \hat{V}\hat{T}\rangle_n$ [43]. Hence, from Eqs. (3) and (4), one obtains

$$\langle \hat{T}^2\rangle_n - \langle \hat{T}\rangle_n^2 = \langle \hat{V}^2\rangle_n - \langle \hat{V}\rangle_n^2, \tag{5a}$$

$$\begin{aligned}(\Delta\hat{T}_n)^2 &= \langle \hat{V}\rangle_n\langle \hat{T}\rangle_n - \langle \hat{T}\hat{V}\rangle_n = (\Delta\hat{V}_n)^2 \\ &= \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n - \langle \hat{V}\hat{T}\rangle_n.\end{aligned} \tag{5b}$$

This relation suggests that the magnitudes of error incurred in $\langle \hat{T}\rangle_n$ and $\langle \hat{V}\rangle_n$ are equal. Now, one can easily interpret the fact that $\mathcal{E}_n$ is a sum of two average quantities but still provides an exact result. This is due to the cancellation of errors between $\langle \hat{T}\rangle_n$ and $\langle \hat{V}\rangle_n$.

Interestingly, using the condition $\langle \hat{T}\hat{V}\rangle_n = \langle \hat{V}\hat{T}\rangle_n$ and exploiting Eqs. (3) and (4), one can obtain the following expression:

$$\langle \hat{T}^2\rangle_n = \mathcal{E}_n(\mathcal{E}_n - 2\langle \hat{V}\rangle_n) + \langle \hat{V}^2\rangle_n. \tag{6}$$

Thus, instead of performing the fourth-order derivative of $\psi_n(\tau)$, one can alternatively evaluate $\langle \hat{T}^2\rangle_n$ from a knowledge of $\mathcal{E}_n$, $\langle \hat{V}\rangle_n$, and $\langle \hat{V}^2\rangle_n$.

Now we wish to verify whether Eq. (5) is true for eigenstates only. Let us consider two functions having forms $\phi_1 = (\hat{T} - \langle \hat{T}\rangle_n)|\psi_n\rangle$ and $\phi_2 = (\hat{V} - \langle \hat{V}\rangle_n)|\psi_n\rangle$. Making use of the Schwartz inequality, it is possible to write

$$\begin{aligned} &\langle \phi_1|\phi_1\rangle\langle \phi_2|\phi_2\rangle \geqslant |\langle \phi_2|\phi_1\rangle|^2, \\ &(\Delta\hat{T}_n)^2(\Delta\hat{V}_n)^2 \geqslant |\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n|^2. \end{aligned} \tag{7}$$

This inequality becomes equality when ϕ_1 and ϕ_2 are linearly dependent. That implies

$$(\hat{T} - \langle \hat{T}\rangle_n)|\psi_n\rangle = \alpha(\hat{V} - \langle \hat{V}\rangle_n)|\psi_n\rangle, \tag{8}$$

where α is a number. Putting this back in the inequality and doing some algebraic rearrangement, we get

$$\begin{aligned} \alpha^2(\Delta\hat{T}_n)^2(\Delta\hat{V}_n)^2 &= |\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n|^2, \\ \alpha^2 &= \frac{|\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n|^2}{(\Delta\hat{T}_n)^2(\Delta\hat{V}_n)^2}. \end{aligned} \tag{9}$$

The choice of $\alpha^2 = 1$ yields the following expression:

$$\left(\Delta\hat{T}_n^2\right)(\Delta\hat{V}_n)^2 = |\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n|^2. \tag{10}$$

Here $\alpha^2 = 1$. Now, by left multiplying Eq. (8) by $\langle\psi_n|(T - \langle T\rangle_n)|$, followed by integration over the whole space and rearrangement, we get

$$(\Delta\hat{T}_n)^2 = (\Delta\hat{V}_n)^2 = |\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n|. \tag{11}$$

Equation (11) is valid for two values of α, namely, 1 or -1. When $\alpha = -1$,

$$\begin{aligned} (\hat{T} - \langle \hat{T}\rangle_n)|\psi_n\rangle &= -(\hat{V} - \langle \hat{V}\rangle_n)|\psi_n\rangle, \\ (\hat{T} + \hat{V})|\psi_n\rangle &= (\langle \hat{T}\rangle_n + \langle \hat{V}\rangle_n)|\psi_n\rangle, \end{aligned} \tag{12}$$

which is nothing but the SE, $\hat{H}|\psi_n\rangle = \mathcal{E}_n|\psi_n\rangle$. Whereas $\alpha = 1$ leads to

$$(\hat{T} - \hat{V})|\psi_n\rangle = \left(\langle \hat{T}\rangle_n - \langle \hat{T}\rangle_n\right)|\psi_n\rangle, \tag{13}$$

which does not concern us here.

This above discussion suggests that Eqs. (5a) and (11) provide a necessary condition for a stationary state and Eq. (5b) is a special case of it. Now, to verify the suitability of Eq. (5b), it is useful to study $\langle \hat{H}^2\rangle_n - \langle \hat{H}\rangle_n^2 = (\Delta\hat{H}_n)^2$, because only for eigenstates is it *zero*. Thus,

$$\begin{aligned} (\Delta\hat{H}_n)^2 = (\Delta\hat{T}_n)^2 + (\Delta\hat{V}_n)^2 + [\langle \hat{T}\hat{V}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n] \\ + [\langle \hat{V}\hat{T}\rangle_n - \langle \hat{T}\rangle_n\langle \hat{V}\rangle_n]. \end{aligned} \tag{14}$$

Now, putting the condition of Eq. (5b) in Eq. (14) one can obtain

$$(\Delta\hat{H}_n)^2 = 0. \tag{15}$$

This clearly states that, Eq. (5b) is a *sufficient* condition for an eigenfunction. Hence, once this relation is obeyed by ψ_n, it is an eigenfunction of that particular $\hat{H}$, but $(\Delta\hat{T}_n)^2 = (\Delta\hat{V}_n)^2$. Equation (5a) is a *necessary* condition for a quantum system, which is actually a virial-like expression. Now, it will be interesting to examine the applicability of Eq. (5) in the context of confined quantum systems, which we do next.

For our current purpose, without loss of generality, our relevant radial SE under the influence of confinement may be rewritten (atomic units are employed unless otherwise stated) as

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2r^2} + v(r) + v_c(r)\right]\psi_{n,\ell}(r) = \mathcal{E}_{n,\ell}\ \psi_{n,\ell}(r), \tag{16}$$

where $v(r)$ signifies the *unperturbed effective* potential (for example, in a many-electron system that may include effective electron-nuclear attraction and electron-electron repulsion), and our desired confinement inside a spherical cage is accomplished by invoking the potential $v_c(r)$, with $\hat{V} = v(r) + v_c(r)$. Thus in a confinement scenario, the validity of Eq. (5) can be checked by deriving the expressions of $\langle \hat{T}\hat{V}\rangle_{n,\ell}$, $\langle \hat{V}\hat{T}\rangle_{n,\ell}$, $\langle \hat{V}^2\rangle_{n,\ell}$, and $\langle \hat{V}\rangle_{n,\ell}$ (other integrals remain unchanged). Towards this end, Eq. (5) may be modified as follows:

$$(\Delta\hat{T}_{n,\ell})^2 = \langle \hat{T}^2\rangle_{n,\ell} - \langle \hat{T}\rangle_{n,\ell}^2, \tag{17}$$

$$\begin{aligned} (\Delta\hat{V}_{n,\ell})^2 &= \langle v(r)^2\rangle_{n,\ell} + \langle v(r)v_c(r)\rangle_{n,\ell} + \langle v_c(r)v(r)\rangle_{n,\ell} \\ &\quad + \langle v_c(r)^2\rangle_{n,\ell} - \langle v(r)\rangle_{n,\ell}^2 - \langle v_c(r)\rangle_{n,\ell}^2 \\ &\quad - 2\langle v(r)\rangle_{n,\ell}\langle v_c(r)\rangle_{n,\ell}, \end{aligned} \tag{18}$$

$$\begin{aligned} \langle \hat{T}\rangle_{n,\ell}\langle \hat{V}\rangle_{n,\ell} - \langle \hat{V}\hat{T}\rangle_{n,\ell} &= \langle \hat{T}\rangle_{n,\ell}\big[\langle v(r)\rangle_{n,\ell} + \langle v_c(r)\rangle_{n,\ell}\big] \\ &\quad - \langle \hat{T}v(r)\rangle_{n,\ell} - \langle \hat{T}v_c(r)\rangle_{n,\ell} \\ \langle \hat{T}\rangle_{n,\ell}\langle \hat{V}\rangle_{n,\ell} - \langle \hat{T}\hat{V}\rangle_{n,\ell} &= \langle \hat{T}\rangle_{n,\ell}\big[\langle v(r)\rangle_{n,\ell} + \langle v_c(r)\rangle_{n,\ell}\big] \\ &\quad - \langle v(r)\hat{T}\rangle_{n,\ell} - \langle v_c(r)\hat{T}\rangle_{n,\ell}. \end{aligned} \tag{19}$$

In what follows, we examine the abovementioned criteria for a number of important confining potentials, as mentioned in the Introduction, viz., (i) CHO in 1D and 3D, and (ii) a H atom encapsulated in five different confining environments, namely, CHA, SCHA, HICHA, SPCHA, and HPCHA. This offers us the opportunity to understand the effect of the boundary condition on derived relations. It may be recalled that, out of these seven different potentials, 1DCHO, 3DCHO, and CHA are exactly solvable. However, it is instructive to note that, in order to construct the exact wave function for a specific state, one needs to supply the energy eigenvalue, which is calculated using imaginary-time propagation [44–47] and a generalized pseudo-spectral [26,48–50] method, respectively, for 1D and 3D problems. Except for in a CHA, in all the remaining confining H atom cases, we have employed numerically calculated wave functions and energies through the GPS scheme. Now, we can use the relations in Eq. (5) to inspect the goodness of the numerical wave function.

III. RESULTS AND DISCUSSION

We now discuss the results under four broad categories, viz., (i) impenetrable, sharp; (ii) impenetrable, smooth; (iii) penetrable, sharp; and (iv) penetrable, smooth.

A. Impenetrable, sharp confinement

Under this condition, the desired confinement effect on $v(r)$ is imposed by invoking the following form of potential: $v_c(r) = +\infty$ for $r > r_c$, and 0 for $r \leqslant r_c$, where r_c signifies the radius of the box. Thus Eq. (16) needs to be solved under the Dirichlet boundary condition, $\psi_{n_r,l}(0) = \psi_{n_r,l}(r_c) = 0$. Four systems are included under this heading, namely, 1DCHO, 3DCHO, CHA, and SCHA, which are taken up one by one.

1. 1DCHO

The single-particle time-independent nonrelativistic SE in 1D is (α is force constant)

$$-\frac{1}{2}\frac{d^2\psi_n}{dx^2} + 4\alpha^2x^2\psi_n + v_c\psi_n = \mathcal{E}_n\psi_n, \tag{20}$$

where the confining potential is defined as $v_c = 0$ for $x < |x_c|$ and $v_c = \infty$ for $x \geqslant |x_c|$. Here x_c signifies the confinement length. Note that we consider only the *symmetric* case, while *asymmetric* confinement can also be worked out without any further complication and hence is omitted here. Equation (20) can be solved exactly using the boundary condition $\psi_n(-x_c) = \psi_n(x_c) = 0$ to produce the following analytical closed forms for *even and odd* states ($\alpha = \sqrt{1/8}$, for sake of convenience):

$$\psi_e(x) = N_e\ {}_1F_1\left[\left(\frac{1}{4} - \frac{\mathcal{E}_n}{4\sqrt{2}\alpha}\right), \frac{1}{2}, 2\sqrt{2}\alpha x^2\right]e^{-\sqrt{2}\alpha x^2},$$

$$\psi_o(x) = N_o x\ {}_1F_1\left[\left(\frac{3}{4} - \frac{\mathcal{E}_n}{4\sqrt{2}\alpha}\right), \frac{3}{2}, 2\sqrt{2}\alpha x^2\right]e^{-\sqrt{2}\alpha x^2}. \tag{21}$$

In this equation, N_e and N_o represent normalization constants for even and odd states, respectively, while $\mathcal{E}_n$, the energy of respective eigenstates, has been calculated accurately by an imaginary-time evolution method [47] and ${}_1F_1[a, b, x]$ denotes the confluent hypergeometric function. Now, the expectation values take the following forms:

$$\langle\hat{T}\hat{V}\rangle_n = \langle\hat{T}v(x)\rangle_n + \langle\hat{T}v_c\rangle_n = \langle\hat{T}v(x)\rangle_n. \tag{22}$$

One can make use of the property of the Reimann integral to simplify:

$$\langle\hat{T}v_c\rangle_n = \int_{-\infty}^{-x_c}\psi_n^*(x)\hat{T}v_c\psi_n(x)dx + \int_{-x_c}^{x_c}\psi_n^*(x)\hat{T}v_c\psi_n(x)dx + \int_{x_c}^{\infty}\psi_n^*(x)\hat{T}v_c\psi_n(x)dx = 0. \tag{23}$$

The first and third integrals become *zero* because $\psi_n(x) = 0$ when $x \geqslant |x_c|$, whereas the second integral becomes *zero* because $v_c = 0$ inside the box. Similarly,

$$\langle\hat{V}\hat{T}\rangle_n = \langle v(x)\hat{T}\rangle_n + \langle v_c\hat{T}\rangle_n = \langle v(x)\hat{T}\rangle_n, \tag{24}$$

$$\langle\hat{V}^2\rangle_n = \langle(v(x)^2\rangle_n + \langle v(x)v_c\rangle_n + \langle v_c v(x)\rangle_n + \langle v_c^2\rangle_n = \langle(v(x))^2\rangle_n, \tag{25}$$

$$\langle\hat{V}\rangle_n = \langle v(x)\rangle_n + \langle v_c\rangle_n = \langle v(x)\rangle_n. \tag{26}$$

Thus, for a 1DCHO, with the help of the above equations, Eq. (5) may be recast as

$$(\Delta\hat{T}_n)^2 = \left(\Delta\hat{V}_n\right)^2 = \langle\hat{T}\rangle_n\langle v(x)\rangle_n - \langle v(x)\hat{T}\rangle_n = \langle\hat{T}\rangle_n\langle v(x)\rangle_n - \langle\hat{T}v(x)\rangle_n. \tag{27}$$

Thus it is evident from Eq. (27) that v_c has no contribution to the desired expectation values. Hence the only difference between free and enclosed system is that, in the latter, the boundary has been reduced to a finite region from infinity. Numerical values of $\mathcal{E}_n$, $(\Delta\hat{T}_n)^2$, $(\Delta\hat{V}_n)^2$, $\langle T\rangle_n\langle V\rangle_n - \langle TV\rangle_n$, and $\langle T\rangle_n\langle V\rangle_n - \langle VT\rangle_n$ are produced in Table I for $n = 0$ and 1 states of a 1DCHO at six selected x_c values, namely, 0.1, 0.5, 1, 3, 5, and ∞, which cover a decent region of confinement. In all these six x_c, $\mathcal{E}_0$ and $\mathcal{E}_1$ remain in excellent agreement with available literature results as compared in Ref. [47] and hence are not repeated here. However, no direct reference could be found for the expectation values to tally. It is easily noticed that, in both confined and free (last column) conditions, Eq. (5) is obeyed, as all the expectation values offer identical results, which validates the applicability of our designed theorem in the case of a 1DCHO. Additionally, with an increase in x_c, both $(\Delta\hat{T})^2$ and $(\Delta\hat{V})^2$ increase, which presumably occurs as the wave function delocalizes with x_c. Consequently, the difference between mean square and average values of $\hat{T}$ and $\hat{V}$ tends to grow.

2. 3DCHO

The isotropic harmonic oscillator is defined by $v(r) = \frac{1}{2}\omega r^2$, where ω signifies the oscillation frequency. The *exact* generalized radial wave function of a 3DCHO is mathematically expressed as [25]

$$\psi_{n_r,\ell}(r) = N_{n_r,\ell}\ r^\ell\ {}_1F_1\left[\frac{1}{2}\left(\ell + \frac{3}{2} - \frac{\mathcal{E}_{n_r,\ell}}{\omega}\right), \left(\ell + \frac{3}{2}\right), \omega r^2\right]e^{-\frac{\omega}{2}r^2}. \tag{28}$$

Here $N_{n_r,\ell}$ signifies the normalization constant, and $\mathcal{E}_{n_r,\ell}$ corresponds to the energy of a given state characterized by quantum numbers n_r and ℓ. Note that the levels are designated by $n_r + 1$ and ℓ values, such that $n_r = \ell = 0$ and $n_r = \ell = 2$ correspond to $1s$ and $3d$ states, respectively. The radial quantum number n_r relates to n as $n = 2n_r + \ell$.

The relevant expectation values now take the following form:

$$\langle\hat{T}\hat{V}\rangle_{n_r,\ell} = \langle\hat{T}v(r)\rangle_{n_r,\ell} + \langle\hat{T}v_c(r)\rangle_{n_r,\ell} = \langle\hat{T}v(r)\rangle_{n_r,\ell}. \tag{29}$$

This occurs because $\langle\hat{T}v_c(r)\rangle_{n_r,\ell} = 0$, due to the wave function vanishing when $r \geqslant r_c$. A similar argument

TABLE I. $\mathcal{E}_n$, $(\Delta V_n)^2$, $(\Delta T_n)^2$, $\langle T\rangle_n\langle V\rangle_n - \langle TV\rangle_n$, and $\langle T\rangle_n\langle V\rangle_n - \langle VT\rangle_n$ values for $n=0$ and 1 states in a 1DCHO at six (0.1, 0.5, 1, 3, 5, and ∞) values of x_c. See text for detail.

n	Property	$x_c=0.1$	$x_c=0.5$	$x_c=1$	$x_c=3$	$x_c=5$	$x_c=\infty$
	$\mathcal{E}_0$ [a]	123.3707084678	4.9511293232	1.2984598320	0.5003910829	0.50000007	0.4999999999
	$(\Delta V_0)^2$	0.000000600468	0.0003747558	0.0058688193	0.1215456043	0.124999	0.1299999999
0	$(\Delta T_0)^2$	0.000000600466	0.0003747558	0.0058688193	0.1215456043	0.124999	0.1299999999
	$\langle T\rangle_0\langle V\rangle_0 - \langle TV\rangle_0$	0.000000600466	0.0003747558	0.0058688193	0.1215456043	0.124999	0.1299999999
	$\langle T\rangle_0\langle V\rangle_0 - \langle VT\rangle_0$	0.000000600466	0.0003747558	0.0058688193	0.1215456043	0.124999	0.1299999999
	$\mathcal{E}_1$ [b]	493.481633417	19.7745341792	5.0755820152	1.5060815272	1.5000000036	1.499999999
	$(\Delta V_1)^2$	0.00000085445	0.00053374630	0.0084865378	0.3353761814	0.3749997486	0.374999999
1	$(\Delta T_1)^2$	0.00000085434	0.00053374630	0.0084865378	0.3353761814	0.3749997486	0.374999999
	$\langle T\rangle_1\langle V\rangle_1 - \langle TV\rangle_1$	0.00000085434	0.00053374630	0.0084865378	0.3353761814	0.3749997486	0.374999999
	$\langle T\rangle_1\langle V\rangle_1 - \langle VT\rangle_1$	0.00000085434	0.00053374630	0.0084865378	0.3353761814	0.3749997486	0.374999999

[a]Literature results [47] of $\mathcal{E}_0$ for $x_c = 0.1$, 0.5, 1, 3, 5, and ∞ are 123.37070846785, 4.9511293232541, 1.2984598320321, 0.5003910829301, 0.5000000000768, and 0.5, respectively.

[b]Literature results [47] of $\mathcal{E}_1$ for $x_c = 0.1$, 0.5, 1, 3, 5, and ∞ are 493.48163341761, 19.774534179208, 5.0755820152268, 0.5060815272531, 1.5000000036719, and 1.5, respectively.

($\langle v_c(r)\hat{T}\rangle_{n_r,\ell}=0$) leads to the following relation:

$$\langle \hat{V}\hat{T}\rangle_{n_r,\ell} = \langle v(r)\hat{T}\rangle_{n_r,\ell} + \langle v_c(r)\hat{T}\rangle_{n_r,\ell} = \langle v(r)\hat{T}\rangle_{n_r,\ell}. \quad (30)$$

Then since $\langle v(r)v_c(r)\rangle_{n_r,\ell} = \langle v_c(r)v(r)\rangle_{n_r,\ell} = \langle v_c(r)^2\rangle_{n_r,\ell} = 0$, we can write

$$\langle \hat{V}^2\rangle_{n_r,\ell} = \langle v(r)^2\rangle_{n_r,\ell} + \langle v(r)v_c(r)\rangle_{n_r,\ell} + \langle v_c(r)v(r)\rangle_{n_r,\ell} + \langle v_c(r)^2\rangle_{n_r,\ell} = \langle v(r)^2\rangle_{n_r,\ell}. \quad (31)$$

And finally, one can derive (since $\langle v_c(r)\rangle_{n_r,\ell}=0$)

$$\langle \hat{V}\rangle_{n_r,\ell} = \langle v(r)\rangle_{n_r,\ell} + \langle v_c(r)\rangle_{n_r,\ell} = \langle v(r)\rangle_{n_r,\ell}. \quad (32)$$

Thus, for a 3DCHO, Eq. (5) can be recast as

$$\begin{aligned}\langle \hat{T}^2\rangle_{n_r,\ell} - \langle \hat{T}\rangle^2_{n_r,\ell} &= \langle \hat{V}^2\rangle_{n_r,\ell} - \langle \hat{V}\rangle^2_{n_r,\ell},\\ (\Delta\hat{T}_{n_r,\ell})^2 = (\Delta\hat{V}_{n_r,\ell})^2 &= \langle \hat{T}\rangle_{n_r,\ell}\langle v(r)\rangle_{n_r,\ell} - \langle v(r)\hat{T}\rangle_{n_r,\ell}\\ &= \langle \hat{T}\rangle_{n_r,\ell}\langle v(r)\rangle_{n_r,\ell} - \langle \hat{T}v(r)\rangle_{n_r,\ell}. \end{aligned} \quad (33)$$

This implies that, similar to a 1DCHO, here also the perturbing (confining) potential makes no contribution to the desired expectation values; only the boundary in the confined system gets shifted to r_c, from ∞ of the corresponding free counterpart. This clearly indicates the validity of Eq. (5) in a 3DCHO. As an illustration, Table II imprints numerically calculated expectation values, for three low-lying ($1s$, $1p$, and $2s$) states at six chosen values of confinement radius, i.e., 0.1, 0.5, 1, 2, 5, and ∞. This again establishes the utility of Eq. (5) for such potential in both confined and free systems, as evident from identical values of these quantities at all r_c values—the last column signifying the corresponding *unconstrained* system. Accurate energies are quoted from GPS results [26]. No literature is available for the average values considered here. Like the 1D case, here also $(\Delta\hat{T}_{n_r,\ell})^2$ and $(\Delta\hat{V}_{n_r,\ell})^2$ increase with r_c.

3. CHA

We begin with the *exact* wave function for a CHA, which assumes the following form [32]:

$$\psi_{n,\ell}(r) = N_{n,\ell}\left(2r\sqrt{-2\mathcal{E}_{n,\ell}}\right)^{\ell} {}_1F_1\left[\left(\ell+1-\frac{1}{\sqrt{-2\mathcal{E}_{n,\ell}}}\right),(2\ell+2),2r\sqrt{-2\mathcal{E}_{n,\ell}}\right]e^{-r\sqrt{-2\mathcal{E}_{n,\ell}}}, \quad (34)$$

with $N_{n,\ell}$ denoting the normalization constant and $\mathcal{E}_{n,\ell}$ corresponding to the energy of a state represented by quantum numbers n and ℓ. The pertinent expectation values can be simplified as

$$\langle \hat{T}\hat{V}\rangle_{n,\ell} = \langle \hat{T}v(r)\rangle_{n,\ell} + \langle \hat{T}v_c(r)\rangle_{n,\ell} = \langle \hat{T}v(r)\rangle_{n,\ell}. \quad (35)$$

In this instance, $\langle \hat{T}v_c(r)\rangle_{n,\ell}=0$, as the wave function vanishes for $r \geqslant r_c$. Use of the same argument, along with the fact that $\langle v_c(r)\hat{T}\rangle_{n,\ell}=0$, gives rise to

$$\langle \hat{V}\hat{T}\rangle_{n,\ell} = \langle v(r)\hat{T}\rangle_{n,\ell} + \langle v_c(r)\hat{T}\rangle_{n,\ell} = \langle v(r)\hat{T}\rangle_{n,\ell}. \quad (36)$$

Now since $\langle v(r)v_c(r)\rangle_{n,\ell} = \langle v_c(r)v(r)\rangle_{n,\ell} = \langle v_c(r)^2\rangle_{n,\ell} = 0$, one may write

$$\langle \hat{V}^2\rangle_{n,\ell} = \langle v(r)^2\rangle_{n,\ell} + \langle v(r)v_c(r)\rangle_{n,\ell} + \langle v_c(r)v(r)\rangle_{n,\ell} + \langle v_c(r)^2\rangle_{n,\ell} = \langle v(r)^2\rangle_{n,\ell}. \quad (37)$$

Again because $\langle v_c(r)\rangle_{n,\ell}=0$, it follows that

$$\langle \hat{V}\rangle_{n,\ell} = \langle v(r)\rangle_{n,\ell} + \langle v_c(r)\rangle_{n,\ell} = \langle v(r)\rangle_{n,\ell}. \quad (38)$$

Thus, like the previous two systems, for CHA also, Eq. (5) remains unchanged, i.e.,

$$\begin{aligned}\langle \hat{T}^2\rangle_{n,\ell} - \langle \hat{T}\rangle^2_{n,\ell} &= \langle \hat{V}^2\rangle_{n,\ell} - \langle \hat{V}\rangle^2_{n,\ell},\\ (\Delta\hat{T}_{n,\ell})^2 = (\Delta\hat{V}_{n,\ell})^2 &= \langle \hat{T}\rangle_{n,\ell}\langle v(r)\rangle_{n,\ell} - \langle v(r)\hat{T}\rangle_{n,\ell}\\ &= \langle \hat{T}\rangle_{n,\ell}\langle v(r)\rangle_{n,\ell} - \langle \hat{T}v(r)\rangle_{n,\ell}. \end{aligned} \quad (39)$$

TABLE II. $\mathcal{E}_{n_r,\ell}$, $(\Delta V_{n_r,\ell})^2$, $(\Delta T_{n_r,\ell})^2$, $\langle T\rangle_{n_r,\ell}\langle V\rangle_{n_r,\ell} - \langle TV\rangle_{n_r,\ell}$, and $\langle T\rangle_{n_r,\ell}\langle V\rangle_{n_r,\ell} - \langle VT\rangle_{n_r,l}$ for 1s, 1p, and 2s states in a 3DCHO at six specific r_c values, namely, 0.1, 0.5, 1, 2, 5, and ∞. See text for detail.

State	Property	$r_c = 0.1$	$r_c = 0.5$	$r_c = 1$	$r_c = 2$	$r_c = 5$	$r_c = \infty$
	$\mathcal{E}_{1,0}$[a]	493.4816334599	19.774534179	5.0755820153	1.7648164388	1.5000000003	1.499999999
	$(\Delta V_{1,0})^2$	0.00000085434	0.0005337463	0.0084865378	0.1211110138	0.3749999628	0.374999999
1s	$(\Delta T_{1,0})^2$	0.00000085434	0.0005337463	0.0084865378	0.1211110138	0.3749999628	0.374999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	0.00000085434	0.0005337463	0.0084865378	0.1211110138	0.3749999628	0.374999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	0.00000085434	0.0005337463	0.0084865378	0.1211110138	0.3749999628	0.374999999
	$\mathcal{E}_{1,1}$[b]	1009.53830080	40.428276496	10.282256939	3.246947098	2.5000000584	2.499999999
	$(\Delta V_{1,1})^2$	0.0000008424	0.00052642239	0.0084064867	0.129302864	0.6249963610	0.624999999
1p	$(\Delta T_{1,1})^2$	0.00000084238	0.00052642239	0.0084064867	0.129302864	0.6249963610	0.624999999
	$\langle T\rangle_{1,1}\langle V\rangle_{1,1} - \langle TV\rangle_{1,1}$	0.00000084238	0.00052642239	0.0084064867	0.129302864	0.6249963610	0.624999999
	$\langle T\rangle_{1,1}\langle V\rangle_{1,1} - \langle VT\rangle_{1,1}$	0.00000084238	0.00052642239	0.0084064867	0.129302864	0.6249963610	0.624999999
	$\mathcal{E}_{2,0}$[c]	1973.922483399	78.9969211469	19.8996965019	5.5846390792	3.5000122149	3.499999999
	$(\Delta V_{2,0})^2$	0.00000182	0.00113739969	0.01815844553	0.2779838025	1.6246856738	1.624999999
2s	$(\Delta T_{2,0})^2$	0.00000182	0.00113739969	0.01815844553	0.2779838025	1.6246856738	1.624999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	0.00000182	0.00113739969	0.01815844553	0.2779838025	1.6246856738	1.624999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	0.00000182	0.00113739969	0.01815844553	0.2779838025	1.6246856738	1.624999999

[a]Literature results [26] of $\mathcal{E}_{1,0}$ for $r_c = 0.1, 0.5, 1, 3, 5$, and ∞ are 493.48163346, 19.774534180, 5.0755820154, 1.7648164388, 1.5000000037, and 1.5, respectively.

[b]Literature results [26] of $\mathcal{E}_{1,1}$ for $r_c = 0.1, 0.5, 1, 3, 5$, and ∞ are 1009.5383008, 40.428276496, 10.282256939, 3.2469470987, 2.5000000584, and 2.5, respectively.

[c]Literature results [26] of $\mathcal{E}_{2,0}$ for $r_c = 0.1$, 0.5, 1, 3, 5, and ∞ are 1973.922483399, 78.996921147, 19.899696502, 5.5846390792, 3.500012215, and 3.5, respectively.

This equation implies that, a CHA satisfies the results given in Eq. (5); as before, v_c has no impact on it. It has only introduced the boundary in a finite range. Table III demonstrates sample values of $\mathcal{E}_{n,\ell}$, $(\Delta\hat{T}_{n,\ell})^2$, $(\Delta\hat{V}_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for the same low-lying (1s, 2s, and 2p) states of the previous table, in a CHA at the same six particular r_c values, namely, 0.1, 0.2, 0.5, 1, 5, and ∞. For the sake of completeness, accurate values of $\mathcal{E}_{n,\ell}$ are reproduced from Ref. [27]. Once again, no literature results could be found to compare the numerically calculated expectation values. In both confining and free (last column) conditions, these results complement the conclusion of Eq. (5). In passing, it is interesting to note that both $(\Delta\hat{T}_{n,\ell})^2$ and $(\Delta\hat{V}_{n,\ell})^2$ decrease with the rise in r_c.

4. SCHA

In this case, the desired confinement is accomplished by introducing the potential as follows: $v_c = \infty$, when $0 < r \leqslant r_a$, $r \geqslant r_b$ and $v_c = 0$ when $r_a < r < r_b$, where r_a and r_b signify the inner and outer radii, respectively. Expectation values of such a potential can then be simply worked out as follows:

$$\langle\hat{T}\hat{V}\rangle_{n,\ell} = \langle\hat{T}v(r)\rangle_{n,\ell} + \langle\hat{T}v_c(r)\rangle_{n,\ell} = \langle\hat{T}v(r)\rangle_{n,\ell}, \tag{40}$$

which upon application of the property of the Reimann integral provides

$$\begin{aligned}\langle\hat{T}v_c\rangle_{n,\ell} = &\int_0^{r_a} \psi^*_{n,\ell}(r)\hat{T}v_c\psi_{n,\ell}(r)r^2dr\\ &+ \int_{r_a}^{r_b} \psi^*_{n,\ell}(r)\hat{T}v_c\psi_{n,\ell}(r)r^2dr\\ &+ \int_{r_b}^{\infty} \psi^*_{n,\ell}(r)\hat{T}v_c\psi_{n,\ell}(r)r^2dr = 0.\end{aligned} \tag{41}$$

The first and third integrals contribute zero as the wave function vanishes in these two regions. On the contrary, in the $r_a < r < r_b$ region $v_c = 0$; thus the second integral disappears. The same argument can be used to write

$$\langle\hat{V}\hat{T}\rangle_{n,\ell} = \langle v(r)\hat{T}\rangle_{n,\ell} + \langle v_c(r)\hat{T}\rangle_{n,\ell} = \langle v(r)\hat{T}\rangle_{n,\ell}. \tag{42}$$

The second equality holds because $\langle v_c(r)\hat{T}\rangle_{n,\ell} = 0$. Likewise, $\langle\hat{V}^2\rangle_{n,\ell}$ may be expressed as

$$\begin{aligned}\langle\hat{V}^2\rangle_{n,\ell} = &\langle v(r)^2\rangle_{n,\ell} + \langle v(r)v_c(r)\rangle_{n,\ell} + \langle v_c(r)v(r)\rangle_{n,\ell}\\ &+ \langle v_c(r)^2\rangle_{n,\ell} = \langle v(r)^2\rangle_{n,\ell},\end{aligned} \tag{43}$$

since $\langle v(r)v_c(r)\rangle_{n,\ell} = \langle v_c(r)v(r)\rangle_{n,\ell} = \langle v_c(r)^2\rangle_{n,\ell} = 0$. Next, utilizing $\langle v_c(r)\rangle_{n,\ell} = 0$, we get

$$\langle\hat{V}\rangle_{n,\ell} = \langle v(r)\rangle_{n,\ell} + \langle v_c(r)\rangle_{n,\ell} = \langle v(r)\rangle_{n,\ell}. \tag{44}$$

Collecting all these facts, we can write the final expressions for a SCHA as

$$\begin{aligned}\langle\hat{T}^2\rangle_{n,\ell} - \langle\hat{T}\rangle^2_{n,\ell} &= \langle\hat{V}^2\rangle_{n,\ell} - \langle\hat{V}\rangle^2_{n,\ell},\\ (\Delta\hat{T}_{n,\ell})^2 = (\Delta\hat{V}_{n,\ell})^2 &= \langle\hat{T}\rangle_{n,\ell}\langle v(r)\rangle_{n,\ell} - \langle v(r)\hat{T}\rangle_{n,\ell}\\ &= \langle\hat{T}\rangle_{n,\ell}\langle v(r)\rangle_{n,\ell} - \langle\hat{T}v(r)\rangle_{n,\ell}.\end{aligned} \tag{45}$$

Equation (45) explains that, similar to the three previous confined cases, a SCHA satisfies the results given in Eq. (5). As before, the role of v_c is to incorporate the effect of a boundary on the wave function. As mentioned earlier, closed-form analytical solutions are unavailable in this case as yet; we have employed the GPS method to extract the eigenvalues and eigenfunctions of a definite state. Table IV produces the calculated values of various quantities for ground and two excited (1s, 2s, and 2p) states of a SCHA at five chosen sets of r_a and r_b values. The equality of four quantities at all shells

TABLE III. $\mathcal{E}_{n,\ell}$, $(\Delta V_{n,\ell})^2$, $(\Delta T_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ of 1s, 2s, and 2p states in CHA at six (0.1, 0.2, 0.5, 1, 5, ∞) r_c values. See text for detail.

State	Property	$r_c = 0.1$	$r_c = 0.2$	$r_c = 0.5$	$r_c = 1$	$r_c = 5$	$r_c = \infty$
1s	$\mathcal{E}_{1,0}$[a]	468.993038659	111.069858836	14.7479700303	2.3739908660	−0.4964170065	−0.499999999
	$(\Delta V_{1,0})^2$	308.872889980	80.3808359891	14.5396201848	4.4909017616	1.0176222756	0.9999999999
	$(\Delta T_{1,0})^2$	308.872889980	80.3808359891	14.5396201848	4.4909017616	1.0176222756	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	308.872889980	80.3808359891	14.5396201848	4.4909017616	1.0176222756	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	308.872889980	80.3808359891	14.5396201848	4.4909017616	1.0176222756	0.9999999999
2s	$\mathcal{E}_{n,l}$[b]	1942.720354554	477.8516723922	72.6720391904	16.5702560934	0.1412542037	−0.1249999999
	$(\Delta V_{2,0})^2$	925.842896028	236.7351455444	40.5134596945	11.3096437104	0.8156705939	0.1874999999
	$(\Delta T_{2,0})^2$	925.842896028	236.7351455444	40.5134596945	11.3096437104	0.8156705939	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	925.842896028	236.7351455444	40.5134596945	11.3096437104	0.8156705939	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	925.842896028	236.7351455444	40.5134596945	11.3096437104	0.8156705939	0.1874999999
2p	$\mathcal{E}_{2,1}$[c]	991.0075894411	243.10933211	36.6588758801	8.2231383161	0.0075939204	−0.124999999
	$(\Delta V_{2,1})^2$	47.98046148	12.14249373	2.01620344857	0.5370036884	0.0381647208	0.02083333333
	$(\Delta T_{2,1})^2$	47.98046148	12.14249373	2.01620344857	0.5370036884	0.0381647208	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle TV\rangle_{2,1}$	47.98046148	12.14249373	2.01620344857	0.5370036884	0.0381647208	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle VT\rangle_{2,1}$	47.98046148	12.14249373	2.01620344857	0.5370036884	0.0381647208	0.02083333333

[a]Literature results [27] of $\mathcal{E}_{1,0}$ for $r_c = 0.1$, 0.2, 0.5, 1, 5, and ∞ are 468.9930386595, 111.0698588367, 14.74797003035, 2.373990866100, −0.496417006591, and −0.5, respectively.

[b]Literature results [27] of $\mathcal{E}_{2,0}$ for $r_c = 0.1$, 0.2, 0.5, 1, and ∞ are 1942.720354554, 477.8516723922, 72.67203919047, 16.57025609346, and −0.125, respectively.

[c]Literature results [27] of $\mathcal{E}_{2,1}$ for $r_c = 0.1$, 0.2, 0.5, 1, and ∞ are 991.0075894412, 243.1093166600, 36.65887588018, 8.223138316165, and −0.125, respectively.

once again justifies the validity of the relations derived in Eq. (5). No literature is available to compare the computed expectation values.

B. Impenetrable, smooth/homogeneous confinement

One such potential, $v(r) = -\frac{1}{r} + \frac{1}{2}\omega r^2$, was first proposed in Ref. [51] to mimic the quantum-dot structure. Later, in 2012 [10], this was modified into a generalized form: $v(r) = -\frac{1}{r} + (\frac{r}{r_c})^k$ [($k > 1$ and real; $\frac{1}{2}\omega = (\frac{1}{r_c})^k$]. At a fixed r_c, the perturbing potential takes following form:

$$\lim_{k\to\infty}\left(\frac{r}{r_c}\right)^k = \begin{cases} 0 & \text{for} \quad r < r_c, \\ 1 & \text{for} \quad r = r_c, \\ \infty & \text{for} \quad r > r_c. \end{cases}$$

The required expectation values for this potential are then given by

$$\begin{aligned} \langle \hat{T}\hat{V}\rangle_{n,\ell} &= -\left\langle \hat{T}\left(\frac{1}{r}\right)\right\rangle_{n,\ell} + \left\langle \hat{T}\left(\frac{r}{r_c}\right)^k\right\rangle_{n,\ell}, \\ \langle \hat{V}\hat{T}\rangle_{n,\ell} &= -\left\langle \left(\frac{1}{r}\right)\hat{T}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^k\hat{T}\right\rangle_{n,\ell}, \end{aligned} \tag{46}$$

and

$$\begin{aligned} \langle \hat{V}^2\rangle_{n,\ell} &= \left\langle \frac{1}{r^2}\right\rangle_{n,\ell} - 2\left\langle \frac{r^{k-1}}{r_c^k}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^{2k}\right\rangle_{n,\ell}, \\ \langle V\rangle_{n,\ell} &= -\left\langle \frac{1}{r}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^{k}\right\rangle_{n,\ell}. \end{aligned} \tag{47}$$

Finally, we get the virial expression from Eq. (5) in following form:

$$\begin{aligned} \langle \hat{T}^2\rangle_{n,\ell} - \langle \hat{T}\rangle_{n,\ell}^2 &= (\Delta\hat{T}_{n,\ell})^2 = (\Delta\hat{V}_{n,\ell})^2 = \langle \hat{V}^2\rangle_{n,\ell} - \langle \hat{V}\rangle_{n,\ell}^2 \\ &= \left\langle \frac{1}{r^2}\right\rangle_{n,\ell} - 2\left\langle \frac{r^{k-1}}{r_c^k}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^{2k}\right\rangle_{n,\ell} \\ &\quad - \left\langle \frac{1}{r}\right\rangle_{n,\ell}^2 + 2\left\langle \frac{1}{r}\right\rangle_{n,\ell}\left\langle \left(\frac{r}{r_c}\right)^{k}\right\rangle_{n,\ell} - \left\langle \left(\frac{r}{r_c}\right)^{k}\right\rangle_{n,\ell}^2 \\ &= \langle \hat{T}\rangle_{n,\ell}\left(\left\langle -\frac{1}{r}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^{2}\right\rangle_{n,\ell}\right) \\ &\quad + \left\langle \left(\frac{1}{r}\right)\hat{T}\right\rangle_{n,\ell} - \left\langle \left(\frac{r}{r_c}\right)^{k}\hat{T}\right\rangle_{n,\ell} \\ &= \langle \hat{T}\rangle_{n,\ell}\left(\left\langle -\frac{1}{r}\right\rangle_{n,\ell} + \left\langle \left(\frac{r}{r_c}\right)^{2}\right\rangle_{n,\ell}\right) \\ &\quad + \left\langle \hat{T}\left(\frac{1}{r}\right)\right\rangle_{n,\ell} - \left\langle \hat{T}\left(\frac{r}{r_c}\right)^{k}\right\rangle_{n,\ell}. \end{aligned} \tag{48}$$

One striking difference from the previous impenetrable, sharp potentials is that here the perturbing potential contributes to the final form of expression. Now for the illustration, we choose $k = 2$. In this scenario (finite positive k), at very small r_c, the potential blows up sharply; at $r_c \to \infty$ it behaves as a free system; and at other definite r_c, it rises with r. Table V offers sample results for $\mathcal{E}_{n,\ell}$ and related quantities of Eq. (5), for 1s, 2s, and 2p states of a HICHA at six specific r_c values, viz., 0.1, 0.2, 0.5, 1, 5, and ∞. Energies for these states at $r_c = 1$ could be compared with the known

TABLE IV. $\mathcal{E}_{n,\ell}$, $(\Delta V_{n,\ell})^2$, $(\Delta T_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for 1s, 2s, and 2p states in a SCHA at five sets of (r_a, r_b) values. See text for detail.

State	Property	$r_a = 0.1,\ r_b = 0.5$	$r_a = 0.2,\ r_b = 1$	$r_a = 0.5,\ r_b = 2$	$r_a = 1,\ r_b = 5$	$r_a = 2,\ r_b = 8$
	$\mathcal{E}_{1,0}$	27.27172629	5.92023765	1.34445210	−0.05806114	−0.07992493
	$(\Delta V_{1,0})^2$	1.01266084	0.25766775	0.04408223	0.011743288	0.0030965826
1s	$(\Delta T_{1,0})^2$	1.01266084	0.25766775	0.04408223	0.011743288	0.0030965826
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	1.01266084	0.25766777	0.04408222	0.011743282	0.0030965824
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	1.01266084	0.25766777	0.04408222	0.011743282	0.0030965824
	$\mathcal{E}_{2,0}$	119.52182029	28.91900480	7.87809191	0.85031117	0.325553290
	$(\Delta V_{2,0})^2$	2.31747169	0.58308875	0.097543493	0.02432941	0.00630949665
2s	$(\Delta T_{2,0})^2$	2.31747169	0.58308875	0.097543493	0.02432941	0.00630949665
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	2.31747169	0.58308875	0.097543493	0.02432941	0.00630949665
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	2.31747169	0.58308875	0.097543493	0.02432941	0.00630949665
	$\mathcal{E}_{2,1}$	40.49778250	9.26352721	2.09854297	0.088632364	−0.028352228
	$(\Delta V_{2,1})^2$	0.86315456	0.21982576	0.040223458	0.010141187	0.0028634216
2p	$(\Delta T_{2,1})^2$	0.86315456	0.21982576	0.040223458	0.010141187	0.0028634216
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle TV\rangle_{2,1}$	0.86315456	0.21982576	0.040223458	0.010141187	0.0028634216
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle VT\rangle_{2,1}$	0.86315456	0.21982576	0.040223458	0.010141187	0.0028634216

literature values [51], which show reasonable agreement. The other computed quantities could not be compared due to a lack of reference values. Clearly, similar to the previous cases, these results also establish the applicability of our proposed virial-like expressions in a HICHA.

C. Penetrable, sharp confinement

In this context, we have chosen the following potential, first introduced in 1979 [13],

$$v(r) = \begin{cases} -\frac{1}{r} & \text{for} \quad r < r_c, \\ V_0 & \text{for} \quad r \geqslant r_c, \end{cases}$$

where V_0 is a positive constant. The expectation values in this case, are given as follows:

$$\begin{aligned}\langle \hat{T}\hat{V}\rangle_{n,\ell} &= \langle \hat{T}v(r)\rangle_{n,\ell} = -\int_0^{r_c} \psi^*_{n,\ell}(r)\hat{T}\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad + V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\hat{T}\psi_{n,\ell}(r)\, r^2 dr,\ \langle \hat{V}\hat{T}\rangle_{n,\ell} \\ &= \langle v(r)\hat{T}\rangle_{n,\ell} = -\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\hat{T}\psi_{n,\ell}(r)\, r^2 dr \\ &\quad + V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\hat{T}\psi_{n,\ell}(r)\, r^2 dr, \end{aligned} \tag{49}$$

where the property of the Reimann integral has been used. One can further write

$$\begin{aligned}\langle \hat{V}^2\rangle_{n,\ell} &= \int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r^2}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad + V_0^2\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad - 2\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad \times V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr,\end{aligned}$$

$$\begin{aligned}\langle V\rangle_{n,\ell} &= -\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad + V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr.\end{aligned} \tag{50}$$

After some algebra, we eventually obtain the following expressions:

$$\begin{aligned}\langle \hat{T}^2\rangle_{n,\ell} - \langle \hat{T}\rangle^2_{n,\ell} &= (\Delta\hat{T}_{n,\ell})^2 = (\Delta\hat{V}_{n,\ell})^2 \\ &= \langle \hat{V}^2\rangle_{n,\ell} - \langle \hat{V}\rangle^2_{n,\ell} \\ &= \int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r^2}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad + V_0^2\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad - 2\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad \times V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr \\ &\quad - \left[-\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \right. \\ &\quad \left. + V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr\right]^2 \\ &= \langle \hat{T}\rangle_{n,\ell}\left[-\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr \right. \\ &\quad \left. + V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr\right] \\ &\quad + \int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\hat{T}\psi_{n,\ell}(r)\, r^2 dr \\ &\quad - V_0\int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\hat{T}\psi_{n,\ell}(r)\, r^2 dr \\ &= \langle \hat{T}\rangle_{n,\ell}\left[-\int_0^{r_c} \psi^*_{n,\ell}(r)\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr\right.\end{aligned}$$

TABLE V. $\mathcal{E}_{n,\ell}$, $(\Delta V_{n,\ell})^2$, $(\Delta T_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for $1s$, $2s$, and $2p$ states in a HICHA at six chosen r_c values, namely, 0.1, 0.2, 0.5, 1, 5, and ∞. See text for detail.

State	Property	$r_c = 0.1$	$r_c = 0.2$	$r_c = 0.5$	$r_c = 1$	$r_c = 5$	$r_c = \infty$
	$\mathcal{E}_{1,0}$	16.80524705	7.43767694	2.16863754	0.593771218[a]	−0.404345971	−0.499999999
	$(\Delta V_{1,0})^2$	13.2294032	7.3539601	3.6335903	2.30437841	1.1794853	0.9999999999
$1s$	$(\Delta T_{1,0})^2$	13.2294032	7.3539601	3.6335903	2.30437841	1.1794853	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	13.2294032	7.3539601	3.6335903	2.30437841	1.1794853	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	13.2294032	7.3539601	3.6335903	2.30437841	1.1794853	0.9999999999
	$\mathcal{E}_{2,0}$	45.89969929	22.186822249	8.25704419	3.771224646[a]	0.434727738	−0.1249999999
	$(\Delta V_{2,0})^2$	18.4752785	9.8452409	4.4513850	2.5360027	0.78733209	0.1874999999
$2s$	$(\Delta T_{2,0})^2$	18.4752785	9.8452409	4.4513850	2.5360027	0.78733209	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	18.4752785	9.8452409	4.4513850	2.5360027	0.78733209	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	18.4752785	9.8452409	4.4513850	2.5360027	0.78733209	0.1874999999
	$\mathcal{E}_{2,1}$	32.48998926	15.64056055	5.76850468	2.60273839[a]	0.265263485	−0.124999999
	$(\Delta V_{2,1})^2$	1.5579056	0.8086356	0.3486783	0.1899865	0.05526280	0.02083333333
$2p$	$(\Delta T_{2,1})^2$	1.5579056	0.8086356	0.3486783	0.1899865	0.05526280	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle TV\rangle_{2,1}$	1.5579056	0.8086356	0.3486783	0.1899865	0.05526280	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle VT\rangle_{2,1}$	1.5579056	0.8086356	0.3486783	0.1899865	0.05526280	0.02083333333

[a]Literature results [51] of $\mathcal{E}_{n,\ell}$ for $1s$, $2s$, and $2p$ states at $r_c = 1$ are 0.594, 3.771, 2.603, respectively.

$$+ V_0 \int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\psi_{n,\ell}(r)\, r^2 dr\Bigg]$$
$$+ \int_0^{r_c} \psi^*_{n,\ell}(r)\hat{T}\left(\frac{1}{r}\right)\psi_{n,\ell}(r)\, r^2 dr$$
$$- V_0 \int_{r_c}^{\infty} \psi^*_{n,\ell}(r)\hat{T}\psi_{n,\ell}(r)\, r^2 dr. \quad (51)$$

Thus, analogous to a HICHA, here also the perturbing term V_0 contributes to the expectation values. Table VI presents specimen energies ($\mathcal{E}_{n,\ell}$), along with respective expectation values for $1s$, $2s$, and $2p$ states of a SPCHA at six arbitrary sets of $\{V_0, r_c\}$. We are aware of only one work for ground-state energy, which is duly quoted; this produces reasonably good agreement. These results further demonstrate the validity of this virial-like expression for a SPCHA.

D. Penetrable, smooth/homogeneous confinement

One example of such a potential is $v(r) = -\frac{1}{r} + v_{p,h}(r)$, where $v_{p,h}(r) = U_0/e^{w(1-\frac{r}{r_c})} + 1$ (U_0 and w both are positive and real). Its importance and utility was first discussed in Ref. [15] in the context of explaining the interactions present in artificial atoms. The relevant expressions can be written as

$$\langle\hat{T}\hat{V}\rangle_{n,\ell} = -\left\langle\hat{T}\left(\frac{1}{r}\right)\right\rangle_{n,\ell} + \langle\hat{T}v_{p,h}(r)\rangle_{n,\ell},$$
$$\langle\hat{V}\hat{T}\rangle_{n,\ell} = -\left\langle\left(\frac{1}{r}\right)\hat{T}\right\rangle_{n,\ell} + \langle v_{p,h}(r)\hat{T}\rangle_{n,\ell}, \quad (52)$$

and

$$\langle\hat{V}^2\rangle_{n,\ell} = \left\langle\frac{1}{r^2}\right\rangle_{n,\ell} - 2\left\langle\left(\frac{1}{r}\right)v_{p,h}(r)\right\rangle_{n,\ell} + \left\langle v^2_{p,h}(r)\right\rangle_{n,\ell},$$
$$\langle V\rangle_{n,\ell} = -\left\langle\frac{1}{r}\right\rangle_{n,\ell} + \left\langle v_{p,h}(r)\right\rangle_{n,\ell}. \quad (53)$$

Eventually we arrive at the following expression after some algebra:

$$\langle\hat{T}^2\rangle_{n,\ell} - \langle\hat{T}\rangle^2_{n,\ell} = (\Delta\hat{T}_{n,\ell})^2 = (\Delta\hat{V}_{n,\ell})^2 = \langle\hat{V}^2\rangle_{n,\ell} - \langle\hat{V}\rangle^2_{n,\ell}$$
$$= \left\langle\frac{1}{r^2}\right\rangle_{n,\ell} - 2\left\langle\left(\frac{1}{r}\right)v_{p,h}(r)\right\rangle_{n,\ell} + \left\langle v^2_{p,h}(r)\right\rangle_{n,\ell}$$
$$- \left(-\left\langle\frac{1}{r}\right\rangle_{n,\ell} + \langle v_{p,h}(r)\rangle_{n,\ell}\right)^2$$
$$= \langle\hat{T}\rangle_{n,\ell}\left(-\left\langle\frac{1}{r}\right\rangle_{n,\ell} + \langle v_{p,h}(r)\rangle_{n,\ell}\right)$$
$$+ \left\langle\left(\frac{1}{r}\right)\hat{T}\right\rangle_{n,\ell} - \langle v_{p,h}(r)\hat{T}\rangle_{n,\ell}$$
$$= \langle\hat{T}\rangle_{n,\ell}\left(-\left\langle\frac{1}{r}\right\rangle_{n,\ell} + \langle v_{p,h}(r)\rangle_{n,\ell}\right)$$
$$+ \left\langle\hat{T}\left(\frac{1}{r}\right)\right\rangle_{n,\ell} - \langle\hat{T}v_{p,h}(r)\rangle_{n,\ell}. \quad (54)$$

Thus we notice that, similar to a HICHA and a SPCHA, here also the perturbing term $v_{p,h}(r)$ remains in the final expression.

In order to explain the result for a HPCHA, we have taken $w = 1000$ and $U_0 = 10$ as potential parameters. Table VII reports the calculation of $\mathcal{E}_{n,\ell}$, $(\Delta\hat{T}_{n,\ell})^2$, $(\Delta\hat{V}_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for $1s$, $2s$, and $2p$ states at six chosen r_c values, namely, 0.1, 0.2, 0.5, 1, 5, and ∞. The last column clearly implies that at $r_c \to \infty$ and $U \to 0$ this system merges to a FHA. These results, like the previous cases, demonstrate that relation (5) is valid for a HPCHA as well. Ground-state energies at all these r_c values are compared with the available literature results. No further comparison could be made due to a lack of data.

TABLE VI. $\mathcal{E}_{n,\ell}$, $(\Delta V_{n,\ell})^2$, $(\Delta T_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for 1s, 2s, and 2p states in a SPCHA at six sets of $\{V_0, r_c\}$. See text for detail.

State	Property	$V_0 = 0$ $r_c = 5.77827$	$V_0 = 0$ $r_c = 4.87924$	$V_0 = 1$ $r_c = 5.72824$	$V_0 = 4$ $r_c = 5.75669$	$V_0 = 10$ $r_c = 5.49360$	$V_0 = \infty$ $r_c = 5.80119$
	$\mathcal{E}_{1,0}$[a]	– 0.9998090	– 0.9990142	– 0.999186	– 0.998703	– 0.997682	– 0.998302
	$(\Delta V_{1,0})^2$	1.000433	1.003194	1.00266	1.00447	1.00848	1.0047
1s	$(\Delta T_{1,0})^2$	1.000433	1.003194	1.00266	1.00447	1.00848	1.0047
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	1.000433	1.003194	1.00266	1.00447	1.00848	1.0047
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	1.000433	1.003194	1.00266	1.00447	1.00848	1.0047
	$\mathcal{E}_{2,0}$	– 0.1578690	– 0.0909114	– 0.035144	0.0128918	0.0818295	0.0434530
	$(\Delta V_{2,0})^2$	0.355830	0.412397	0.56205	0.64650	0.774448	0.60752
2s	$(\Delta T_{2,0})^2$	0.355830	0.412397	0.56205	0.64650	0.774448	0.60752
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	0.355830	0.412397	0.56205	0.64650	0.774448	0.60752
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	0.355830	0.412397	0.56205	0.64650	0.774448	0.60752
	$\mathcal{E}_{2,1}$	– 0.1996605	– 0.1587620	– 0.1406809	– 0.1172265	– 0.0832120	– 0.1022024
	$(\Delta V_{2,1})^2$	0.032028	0.0413657	0.046701	0.0637238	0.094861	0.0316629
2p	$(\Delta T_{2,1})^2$	0.032028	0.0413657	0.046701	0.0637238	0.094861	0.0316629
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle TV\rangle_{2,1}$	0.032028	0.0413657	0.046701	0.0637238	0.094861	0.0316629
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle VT\rangle_{2,1}$	0.032028	0.0413657	0.046701	0.0637238	0.094861	0.0316629

[a]Literature results [13] of the 1s state at these six $\{V_0, r_c\}$ pairs are −0.9998, −0.9990, −0.9994, −0.9990, −0.9980, and −0.9980, respectively.

IV. FUTURE AND OUTLOOK

A virial-like relation $[(\Delta\hat{T}_n)^2 = (\Delta\hat{V}_n)^2]$ has been proposed for *free* and *confined* quantum systems, by invoking the SE and the HVT. This can be used as an essential condition for an exact quantum system. Besides this, Eq. (5b) in its complete form has been found to be a sufficient condition for these bound, stationary states. Generalized expressions have been derived for impenetrable, penetrable, and shell-confined quantum systems along with the sharp and smooth situations. The change in boundary condition does not influence the form of these relations. Their applicability has been tested and verified by doing pilot calculations on quantum harmonic oscillator and H atom—a total of seven different confining potentials, as well as the respective free systems. In all cases these conditions have been satisfied. Under the impenetrable, sharp (hard) confinement condition the perturbing term does not survive in the final expression. However in impenetrable-smooth, penetrable-sharp, and penetrable-smooth cases it occurs in the eventual form. It is worth mentioning that these relations are applicable in other coordinate systems, such as ellipsoidal, parabolic, cylindrical, spheroidal, etc., as well as in angular confinement. There are several open questions that may lead to important conclusions and that require further scrutiny, such as the use of these sufficient conditions in the

TABLE VII. $\mathcal{E}_{n,\ell}$, $(\Delta V_{n,\ell})^2$, $(\Delta T_{n,\ell})^2$, $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle TV\rangle_{n,\ell}$, and $\langle T\rangle_{n,\ell}\langle V\rangle_{n,\ell} - \langle VT\rangle_{n,\ell}$ for 1s, 2s, and 2p states in a HPCHA at six select r_c values, namely, 0.1, 0.2, 0.5, 1, 5, and ∞, having $U = 10$ and $w = 1000$. The last column indicates values at $r_c = \infty$ and $U = 0$. See text for detail.

State	Property	$r_c = 0.1$	$r_c = 0.2$	$r_c = 0.5$	$r_c = 1$	$r_c = 5$	$r_c = \infty$, $U = 0$
	$\mathcal{E}_{1,0}$[a]	9.4871580	9.35868	5.25360	1.1528598	– 0.4973688	– 0.499999999
	$(\Delta V_{1,0})^2$	1.15378	2.4119	6.6390	3.25938	1.0133575	0.9999999999
1s	$(\Delta T_{1,0})^2$	1.15378	2.4119	6.6390	3.25938	1.0133575	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle TV\rangle_{1,0}$	1.15378	2.4119	6.6390	3.25938	1.0133575	0.9999999999
	$\langle T\rangle_{1,0}\langle V\rangle_{1,0} - \langle VT\rangle_{1,0}$	1.15378	2.4119	6.6390	3.25938	1.0133575	0.9999999999
	$\mathcal{E}_{2,0}$	9.8734148	9.8593719	9.7728942	9.029792	0.10745905	– 0.1249999999
	$(\Delta V_{2,0})^2$	0.20807	0.346874	0.153805	5.11808	0.7615043	0.1874999999
2s	$(\Delta T_{2,0})^2$	0.20807	0.346874	0.153805	5.11808	0.7615043	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle TV\rangle_{2,0}$	0.20807	0.346874	0.153805	5.11808	0.7615043	0.1874999999
	$\langle T\rangle_{2,0}\langle V\rangle_{2,0} - \langle VT\rangle_{2,0}$	0.20807	0.346874	0.153805	5.11808	0.7615043	0.1874999999
	$\mathcal{E}_{2,1}$	9.8749992211	9.87497532482	9.869939026	4.980371	– 0.011992	– 0.124999999
	$(\Delta V_{2,1})^2$	0.02083685	0.0209243374	0.04006099	0.36608	0.03609	0.02083333333
2p	$(\Delta T_{2,1})^2$	0.02083685	0.0209243374	0.04006099	0.36608	0.03609	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle TV\rangle_{2,1}$	0.02083685	0.0209243374	0.04006099	0.36608	0.03609	0.02083333333
	$\langle T\rangle_{2,1}\langle V\rangle_{2,1} - \langle VT\rangle_{2,1}$	0.02083685	0.0209243374	0.04006099	0.36608	0.03609	0.02083333333

[a]Literature results [15] of $\mathcal{E}_{1,0}$ for $r_c = 0.1$, 0.2, 0.5, 1.0, 5.0, and ∞ are 9.4973, 9.3620, 5.2456, 1.1761, −0.4947, and −0.5000, respectively.

context of determining optimized wave functions for various quantum systems, in both ground and excited states. Importantly, one can perform unconstrained optimization (without employing the orthogonality criteria) of trial states by adopting this condition. A parallel inspection in many-electron systems would be highly desirable.

ACKNOWLEDGMENTS

Financial support from the DST, SERB (New Delhi, India; Sanction Order No. EMR/2014/000838), is gratefully acknowledged. The authors acknowledge valuable discussion with Prof. A. K. Nanda.

[1] J. R. Sabin, E. Brändas, and S. A. Cruz (Editors), *The Theory of Confined Quantum Systems*, Parts I and II, Advances in Quantum Chemistry Vols. 57 and 58 (Academic Press, San Diego, 2009).
[2] H. Pang, W.-S. Dai, and M. Xie, J. Phys. A **44**, 365001 (2011).
[3] K. D. Sen (Editor), *Electronic Structure of Quantum Confined Atoms and Molecules* (Springer, Cham, Switzerland, 2014).
[4] K. D. Sen (Editor), *Statistical Complexity: Applications in Electronic Structure* (Springer, Dordrecht, 2012).
[5] N. Aquino and R. A. Rojas, Eur. J. Phys. **37**, 015401 (2016).
[6] R. M. Yu, L. R. Zan, L. G. Jiao, and Y. K. Ho, Few-Body Syst. **58**, 152 (2017).
[7] F. M. Fernàndez and E. A. Castro, Int. J. Quantum Chem. **21**, 741 (1982).
[8] A. Ghosal, N. Mukherjee, and A. K. Roy, Ann. Phys. (Berlin) **528**, 796 (2016).
[9] A. Michels, J. de Boer, and A. Bijl, Physica **4**, 981 (1937).
[10] J. Katriel and H. E. Montgomery, Jr., J. Chem. Phys. **137**, 114109 (2012).
[11] C. Zicovich-Wilson, J. H. Planelles, and W. Jaskólski, Int. J. Quantum Chem. **50**, 429 (1994).
[12] S. H. Patil and Y. P. Varshni, *The Theory of Confined Quantum Systems*, Part I, Advances in Quantum Chemistry Vol. 57 (Academic Press, 2009), pp. 1–24.
[13] E. Lee-Koo and S. Rubinstein, J. Chem. Phys. **71**, 351 (1979).
[14] J. Adamowski, M. Sobkowicz, B. Szafran, and S. Bednarek, Phys. Rev. B **62**, 4234 (2000).
[15] N. Aquino, A. Flores-Riveros, and J. F. Rivas-Silva, Phys. Lett. A **377**, 2062 (2013).
[16] K. D. Sen, J. Chem. Phys. **123**, 074110 (2005).
[17] J. M. Randazzo and C. A. Rios, J. Phys. B **49**, 235003 (2016).
[18] R. Cabrera-Trujillo, R. Méndez-Fragoso, and S. A. Cruz, J. Phys. B **49**, 015005 (2016).
[19] L. Stevanovićć, J. Phys. B **43**, 165002 (2010).
[20] H. E. Montgomery, Jr. and K. D. Sen, Phys. Lett. A **376**, 1992 (2012).
[21] R. Cabrera-Trujillo and S. A. Cruz, Phys. Rev. A **87**, 012502 (2013).
[22] N. Aquino, J. Phys. A **30**, 2403 (1997).
[23] N. Sobrino-Coll, D. Puertas-Centeno, N. M. Tamme, I. V. Toranzo, and J. S. Dehesa, J. Stat. Mech.:Theory Exp. (2017) 083102.
[24] G. Campoy, N. Aquino, and V. D. Granados, J. Phys. A **35**, 4903 (2002).
[25] H. E. Montgomery, Jr., N. A. Aquino, and K. D. Sen, Int. J. Quantum Chem. **107**, 798 (2007)
[26] A. K. Roy, Mod. Phys. Lett. A **29**, 1450104 (2014).
[27] A. K. Roy, Int. J. Quantum Chem. **115**, 937 (2015).
[28] S. Goldman and C. Joslin, J. Phys. Chem. **96**, 6021 (1992).
[29] N. Aquino A., Int. J. Quantum Chem. **54**, 107 (1995).
[30] J. Garza, R. Vargas, and A. Vela, Phys. Rev. E **58**, 3949 (1998).
[31] C. Laughlin, B. L. Burrows, and M. Cohen, J. Phys. B **35**, 701 (2002).
[32] B. L. Burrows and M. Cohen, Int. J. Quantum Chem. **106**, 478 (2006).
[33] N. Aquino, G. Campoy, and H. E. Montgomery, Jr., Int. J. Quantum Chem. **107**, 1548 (2007).
[34] D. Baye and K. D. Sen, Phys. Rev. E **78**, 026701 (2008).
[35] H. Ciftci, R. L. Hall, and N. Saad, Int. J. Quantum Chem. **109**, 931 (2009).
[36] D. Puertas-Centeno, N. M. Tamme, I. V. Toranzo, and J. S. Dehesa, J. Math. Phys. **58**, 103302 (2017).
[37] P.-O. Löwdin, J. Mol. Spectrosc. **3**, 46 (1959).
[38] T. L. Cotrell and S. Paterson, Philos. Mag. **42**, 391 (1951).
[39] W. Byers-Brown, J. Chem. Phys. **28**, 522 (1958).
[40] S. Mukhopadhyay and K. Bhattacharyya, Int. J. Quantum Chem. **101**, 27 (2005).
[41] J. O. Hirschfelder, J. Chem. Phys. **33**, 1462 (1960).
[42] K. D. Sen, V. I. Pupyshev, and H. E. Montgomery, Jr., *The Theory of Confined Quantum Systems*, Part I, Advances in Quantum Chemistry Vol. 57 (Academic Press, San Diego, 2009), pp. 25–77.
[43] S. T. Epstein and J. O. Hirschfelder, Phys. Rev. **123**, 1495 (1961).
[44] A. K. Roy, N. Gupta, and B. M. Deb, Phys. Rev. A **65**, 012109 (2001).
[45] N. Gupta, A. K. Roy, and B. M. Deb, Pramana **59**, 575 (2002).
[46] A. Wadehra, A. K. Roy, and B. M. Deb, Int. J. Quantum Chem. **91**, 597 (2003).
[47] A. K. Roy, Mod. Phys. Lett. A **30**, 1550176 (2015).
[48] A. K. Roy, J. Phys. G: Nucl. Part. Phys. **30**, 269 (2004).
[49] A. K. Roy, Int. J. Quantum Chem. **113**, 1503 (2013); **114**, 383 (2014).
[50] A. K. Roy, Mod. Phys. Lett. A **29**, 1450042 (2014).
[51] S. H. Patil and Y. P. Varshni, Can. J. Phys. **82**, 917 (2004).