Energy and information analysis for confined H atom in harmonic environment

Neetik Mukherjee, Amlan K. Roy

Department of Chemical Sciences
Indian Institute of Science Education and Research Kolkata,
Mohanpur-741246, Nadia, West Bengal, India
E-mail: akroy@iiserkol.ac.in, akroy6k@gmail.com

Abstract. Over the past two decades, constrained quantum systems have arisen to be a field of considerable importance in physical, chemical and biological sciences. In this work, we have investigated the behavior of a confined H atom inside a harmonic environment: 

\[ V(r) = -\frac{1}{r} + \left( \frac{r}{r_c} \right)^2. \]

The eigenvalue equation is solved using a generalized Legendre pseudospectral method, which offers an optimal, non-uniform spatial discretization. By means of a symmetrization technique and a non-linear mapping, a symmetric eigenvalue equation is obtained. A detailed energy analysis reveals that (a) for all the states, energy values decrease with growth in confinement radius, \( r_c \) (b) for fixed number of nodes, it grows with rise in \( l \), and (c) at a fixed \( n \), it decreases with progress in \( l \). Interestingly, the energy arrangement of various quantum states is found to be very different from that in a free H atom. A general rule has been proposed to understand the energy ordering pattern. Furthermore, we have analyzed some information-based quantities like Shannon information entropy, Fisher information and Onicescu energy, in position and momentum spaces for this soft, impenetrable stressed system. These are examined with respect to \( r_c \) as well as \( n, l \) quantum numbers. Additionally, the Compton profile and Compton entropy have also been explored here.

1. Introduction

Study of quantum systems in tight environment has become a subject of much topical interest in the last two decades. It has potential application in numerous branches in science including mineralogy. Various allotropes of carbon are formed due to high pressure exerted on it naturally [1]. Several studies reveal that, under such conditions a particle shows drastic variations in its physical and chemical properties. In chemical perspective, a particle under extreme condition shows changes in coordination number, ionization potential, electron affinity, binding energy [1, 2] etc.

The very first model for confined H atom confined inside a hard, impenetrable wall was investigated in 1937. This was designed to mimic the extreme pressure environment [3]. However in order to incorporate the variable pressure condition, the so-called penetrable barrier model would be more desirable. It is very useful to classify various confining potentials into two broad categories [4, 5], and they are: (i) a penetrable potential which is finitely enclosed from above, while in an impenetrable situation, it rises to infinity at finite value of \( r \) (ii) a continuous potential will be considered as smooth whereas a sharp one reflects discontinuity. In impenetrable, sharp situation, the potential is adjusted by incorporation of a term that remains ineffective up to
a certain distance from origin, and rising to infinity thereafter. It has the form \( V = V(r) \) at \( 0 \leq r \leq r_c \), whereas \( V = \infty \) at \( r > r_c \) (\( r_c \) is the confinement radius). Here, the Dirichlet boundary condition \( R_{n,\ell}(0) = R_{n,\ell}(r_c) = 0 \) is maintained \([6]\). However, an impenetrable, smooth potential is expressed as \( V = V(r) + V_c(r) \), and \( V_c(r) \) implies the confining potential that leads to infinity at \( r \to \infty \), and remains continuous elsewhere \([7, 8]\). On the contrary, for penetrable, sharp case the potential takes the form: \( V = V(r) \) at \( 0 \leq r \leq r_c \) and \( V = V_c(r) \) at \( r > r_c \) \([9]\). Finally, in the penetrable, smooth condition it becomes, \( V = V(r) + V_c(r) \) \([10, 11]\). In last two years, several models were designed and investigated by a large number of researchers, especially in H atom, trapped under these confinement conditions, uncovering several interesting features \([3, 12, 13]\).

Information-based uncertainty measures like Shannon (S), Rényi entropy (R), Fisher information (I), Onicescu energy (E) are the functionals of density. Hence, once the density becomes available, one can calculate these measures \([6, 13]\). In either position or momentum spaces, they guide us to interpret various properties like ionization potential, electron affinity, localization properties, entanglement, molecular reactivity \([14, 15]\), and so on.

Here our objective is to deal with an important model system, given by a H atom confined inside a smooth, impenetrable potential, which has the form as, \( v(r) = -\frac{1}{r} + \left(\frac{r}{r_c}\right)^k \) \((k > 1\) and real; \(\frac{1}{2}\omega = \left(\frac{1}{r_c}\right)^k\)). At a given \( r_c \), the potential has the following characteristic form,

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

Further, this potential can be treated as a bridge between a) H atom under an impenetrable wall and b) free H atom. Here we restrict ourselves to \( k = 2 \), signifying a harmonic barrier. The perturbing harmonic term provides a homogeneous impenetrable environment to H atom; therefore we denote it by the short form HICHA (Homogeneous Impenetrable Confined H Atom). Akin to other confined systems, in this occasion also the effect of confinement relaxes with rise in \( r_c \). It is one of the very few initial models used to mimic quantum-dot systems. This study will point out the impact of a continuous but impenetrable barrier on H atom. The eigenfunctions and eigenvalues for such a system have been computed by adopting a numerical strategy \([7, 8]\).

However, we have derived a new rule about the ordering in energies. It is noteworthy to mention that, in \([7, 8]\), the authors have varied the force constant \((k)\). Actually the force constant is inversely proportional to the square of \( r_c \). Here instead of using \( k \), we have chosen \( r_c \) as confinement parameter. Apart from that, the information analysis for this type of system are yet to be published. Therefore, we aim to perform an energy and information analysis for various states of HICHA using a generalized pseudo-spectral method (GPS). A detailed study reveals the influence of harmonic perturbation on a Coulombic system. Additionally, we have also studied the information entropy for the Compton profile of this system. This will highlight the effect of confinement on its kinetic energy dissipation pattern. In Section 2 we provide a brief description about the GPS method as well as the information measures. Section 3 offers the result and discussion and finally we conclude in Section 4.

### 2. Methodology

All the HICHA calculations in this work, were done by using the GPS method employing Legendre polynomial. It furnishes accurate eigenvalues and eigenfunctions at various \( r_c \) values. By providing an optimal, non-uniform spatial grid, it transforms to a symmetric eigenvalue problem. This can easily be solved by exploiting available standard diagonalization library. It has been applied to a series of model and real systems, in both free and confined conditions, \([16, 17, 18, 19]\). Of late, this has also provided excellent quality results in certain radial
confinement [20, 21, 22, 23] studies in several Coulombic systems, including many electron atoms [24].

2.1. Solution of eigenvalue equation under Dirichlet boundary condition

This method approximates an exact wave function \( f(x) \) defined in the period \([-1, 1]\) by the polynomial \( f_N(x) \) of order \( N \),

\[
f(x) \equiv f_N(x) = \sum_{j=0}^{N} f(x_j)g_j(x).
\]

It ensures that the approximation be exact at the collocation points \( x_j \),

\[
f_N(x_j) = f(x_j).
\]

As stated before, here we have employed Legendre polynomials, where \( x_0 = -1, x_N = 1 \), while \( x_j (j = 1, ..., N - 1) \) are defined by the roots of first derivative of Legendre polynomial \( P_N(x) \), with respect to \( x \), namely,

\[
P'_N(x_j) = 0.
\]

In Eq. (1), \( g_j(x) \) are termed as cardinal functions, which are given by,

\[
g_j(x) = -\frac{1}{N(N+1)P_N(x_j)} \frac{(1-x^2)P'_N(x)}{(x-x_j)},
\]

fulfilling the property that, \( g_j(x_j') = \delta_{j,j'} \).

To solve the radial Schrödinger equation (SE) for a central potential using finite-difference methods, it needs a significantly larger number of points in an equal-spacing grid arrangement. However, in GPS method, this is alleviated by (i) a mapping of the semi-infinite domain \( r \in [0, \infty] \) onto a finite domain \( x \in [-1, 1] \) via a suitable transformation \( r = r(x) \). Utilizing useful algebraic non-linear mapping,

\[
r = r(x) = L \frac{(1+x)}{(1-x+\alpha)},
\]

where \( (L, \alpha = \frac{2L}{r_{\text{max}}}) \) denote two used mapping parameters, plus a symmetrization process,

\[
\psi(r(x)) = \sqrt{r'(x)f(x)},
\]

gives rise to the modified Hamiltonian, as follows,

\[
\hat{H}(x) = -\frac{1}{2} \frac{d^2}{dx^2} \frac{1}{r(x)} V(r(x)) + V_m(x),
\]

where

\[
V_m(x) = \frac{3(r'')^2 - 2r'''r'}{8(r')^4}.
\]

This turns out to be an eigenvalue problem of symmetric matrices. The used mapping in Eq. (5) is such that \( V_m(x) = 0 \). Eventually, we obtain the following discrete set of coupled equations,

\[
\sum_{j=0}^{N} \left[ -\frac{1}{2} D^{(2)}_{j,j'} + \delta_{j,j'} V(r(x_j)) + \delta_{j,j'} V_m(r(x_j)) \right] A_j = E A_{j'}, \quad J = 1, ..., N - 1,
\]
\[ A_j = R'(x_j)f(x_j)[P_N(x_j)]^{-1} = [r'(x_j)]^{1/2}\psi(r(x_j))[P_N(x_j)]^{-1}. \] (10)

Here, \( D^{(2)}_{j,j'} \) signifies symmetrized second derivative of cardinal function with respect to \( r \),

\[ D^{(2)}_{j,j'} = [r'(x_j')][r'(x_j)]^{-1} - [r'(x_j)][r'(x_j')^{-1}, \quad j = j', \]

\[ d^{(2)}_{j,j'} = \begin{cases} \frac{N+1}{6(1-x_j^2)}, & j = j', \\ \frac{1}{(x_j - x_j')^2}, & j \neq j'. \end{cases} \] (12)

The symmetric eigenvalue problem can be easily and efficiently solved for eigenvalues and eigenfunctions using standard library routines.

2.2. Calculation of Information entropy

Here, pilot calculations are performed in both \( r \) and \( p \)-spaces. The position-space density has been constructed from \( \psi(r,\theta,\phi) \), the position-space wave function, obtained by the above discussed method. Subsequently \( \psi(p) \) is to be achieved from following equation,

\[ \psi_n(r)_l(r)(p) = \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^{\pi} \int_0^{2\pi} \psi_n(r)_l(r) \Theta_{l,m}(\theta) \Phi_m(\phi) e^{ipr\cos\theta} r^2 \sin\theta \, dr \, d\theta \, d\phi. \] (13)

Note that, \( \psi(p) \) requires to be normalized. One can then define normalized \( r \)- and \( p \)-space densities as, \( \rho(r) = |\psi_{n,l,m}(r)|^2 \) and \( \Pi(p) = |\psi_{n,l,m}(p)|^2 \). Then, the Compton density, \( J(q) \) can be extracted by adopting the following formula [25],

\[ J(q) = \frac{1}{2} \int_0^\infty \left( \frac{I(p)}{p} \right) dp. \] (14)

\( I(p) \) is the radial momentum density distribution and \( q \) is the projection of target electron momentum upon the scattering vector. The Compton profile can be used to calculate the momentum moments, \( \langle p^n \rangle \). They are connected to the spherically averaged Compton density as,

\[ \langle \frac{1}{p} \rangle = 2J(0), \quad \langle p^n \rangle = 2(n+1) \int_0^\infty q^n J(q) dq \quad (4 \geq n \geq 0) \] (15)

Shannon entropy (S) is the arithmetic mean and Rényi entropy (R) is the geometric mean of uncertainty. Whereas, Onicescu energy (E) is the expectation value of density. These three quantities are expressed in the following mathematical form respectively,

\[ S[\rho] = - \int \rho(\tau) \ln \rho(\tau) d\tau \]

\[ R^\alpha[\rho(\tau)] = \frac{1}{(1 - \alpha)} \ln (\rho(\tau)^{\alpha-1}), \quad 0 < \alpha < \infty, \quad \alpha \neq 1. \] (16)

\[ E = \langle \rho \rangle = \exp \left( R^2[\rho] \right), \quad \langle \rho \rangle = \int \rho^2(\tau) \, d\tau. \]
Figure 1. Variation of energy in HICHA for first six states (1s, 2s, 2p, 3s, 3p, 3d) with changes in \( r_c \). For more details, consult text.

Table 1. Energy values HICHA for \( n = 1 - 10 \) and \( l = 0 - 9 \) states at \( r_c = 0.1 \).

| \( n \) | \( l = 0 \) | \( l = 1 \) | \( l = 2 \) | \( l = 3 \) | \( l = 4 \) | \( l = 5 \) | \( l = 6 \) | \( l = 7 \) | \( l = 8 \) | \( l = 9 \) |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 1      | 16.805 | -      | -      | -      | -      | -      | -      | -      | -      | -      |
| 2      | 45.899 | 32.4899| -      | -      | -      | -      | -      | -      | -      | -      |
| 3      | 74.600 | 61.0729| 47.218 | -      | -      | -      | -      | -      | -      | -      |
| 4      | 103.157| 89.5561| 75.669 | 61.6913| -      | -      | -      | -      | -      | -      |
| 5      | 131.639| 117.987| 104.078| 90.0856| 76.0521| -      | -      | -      | -      | -      |
| 6      | 160.077| 146.386| 132.460| 118.457| 104.415| 90.3526| -      | -      | -      | -      |
| 7      | 188.486| 174.765| 160.824| 146.812| 132.765| 118.697| 104.616| -      | -      | -      |
| 8      | 216.875| 203.128| 189.176| 175.157| 161.105| 147.033| 132.949| 118.855| -      | -      |
| 9      | 245.248| 231.480| 217.519| 203.494| 189.438| 175.363| 161.275| 147.179| 133.077| -      |
| 10     | 273.609| 259.824| 245.854| 231.824| 217.764| 203.686| 189.597| 175.499| 161.395| 147.286|

3. Result and Discussion

At the onset, it is important to mention a few points for a smooth discussion. Throughout the calculation we have opted \(|m| = 0\). Here, net \( S, R, E, I \) in \( r \) and \( p \) spaces are divided into radial and angular contributions. It is needless to mention that at \( r_c \to \infty \) all the results correspond to the respective free H atom (FHA) values. Reference results for energies in HICHA are very scarce. Only a few literature results are available [7, 8]. Our current results have been verified to be consistently superior for the entire range of \( r_c \) for low- and high-lying states as well.

Figure 1 imprints the variation of energy for \( n \leq 3 \) states of HICHA with changes in \( r_c \). In all these six cases \( \epsilon_n \) decreases very sharply at smaller \( r_c \) region. It is interesting to note that, unlike FHA, in HICHA \( \epsilon_n \) depends on both \( n, l \) quantum numbers. Table I shows the \( \epsilon_n \) values for \( n = 1 - 10 \) and \( l = 0 - 9 \) states at \( r_c = 0.1 \). These results indicate that, at very low \( r_c \) region, when \( \Delta n = i \) and \( \Delta l \geq (2i + 1) \) (\( i \) is a positive integer) then lower \( (n, l) \) state has higher energy compared to a higher \( (n, l) \) state. Therefore, at the small \( r_c \) region \( \epsilon_n(3s) > \epsilon_n(4f) \) and \( \epsilon_n(4s) > \epsilon_n(5f) > \epsilon_n(5g) \) and so on.

Now the three panels (a)-(c) in Fig. 2 portray the variation of \( S_r, S_p \) and \( S_l \) for the same
six states of Fig. 1 with increase in $r_c$ respectively. Left and middle panels suggest that, $S_r$ increases and $S_p$ decreases with growth in $r_c$. This indicates that, with the advancement of $r_c$, effect of confinement relaxes. At a fixed $n$, $S_r$ falls off with rise in $l$. However, at a constant $l$, it increases with rise in $n$. The right panel suggests that, in all these six cases $S_l(S_r + S_p = S_t)$ obeys the lower bound value given by $S_t \geq 3(1 + \ln \pi)$.

To gain further insight, Fig. 3 displays $R^\alpha_r, R^\beta_p$ in (a), (b) panels respectively, for first six states as functions of $r_c$. One notices that, $R^\alpha_r$ ($\alpha = 0.6$) increases and $R^\beta_p$ ($\beta = 3$) decreases with acceleration in $r_c$. Like $S$, at a given $n$, $R^\alpha_r$ abates with rise in $l$. However, at a constant $l$, it increases with progress in $n$. These observations reinforce the conclusion drawn in Fig. 2.

Next, Fig. 4 shows the variation of $E_r, E_p$ for the same six states with changes in $r_c$. As usual $E$ imprints a reverse nature with respect to $S$. Panels (a), (b) suggest that, $E_r$ decays and $E_p$ advances with growth in $r_c$. However, the dependence of $E$ on $n, l$ is not clear from panel (a).

Figure 5 now records the variation of $I_r, I_p$ for the same six states with increase in $r_c$ in panels (a), (b) respectively. They exhibit that, $I_r$ increases and $I_p$ decreases with advancement in $r_c$. Like $E_r$ here also, one cannot determine the influence of $n, l$ quantum numbers on $I_r$.

Table 2 offers the $S, E, I$ values in ground state at eight different $r_c$ values namely,
Figure 4. Plots of $E_r$, $E_p$ against $r_c$ for first six states of HICHA, in (a) and (b).

Figure 5. Plots of $I_r$, $I_p$ against $r_c$ for first six states of HICHA, in (a) and (b).

0.1, 0.2, 0.5, 1, 2, 5, 8, $\infty$. These results complement the conclusion drawn from Figs. 2, 4 and 5. To the best of our knowledge, no such literature is available for comparison.

In Figure 6, panel (a) delineates the Compton profile for the 1s state of HICHA at four different $r_c$ values namely 0.1, 2, 5 and 8. It suggests that, with increase in $r_c$ the sharpness of the Compton density distribution increases. Therefore, with increase of confinement, kinetic energy dissipation decelerates. This can further be examined by studying $S$ and $E$ of the system. Thus, panel (b) depicts the variation of Compton Shannon entropy ($S_c$), Compton Onicescu energy ($E_c$) and $\langle \frac{1}{2p} \rangle$ with alterations in $r_c$. One finds that, $S_c$ decreases and $E_c$ as well as $\langle \frac{1}{2p} \rangle$ increase with progress in $r_c$. This decrease in $S_c$ and increase in $E_c$ suggest that the dissipation in kinetic energy enhances with relaxation in confinement.
Table 2. Values of $S_r$, $S_p$, $E_r$, $E_p$, $I_r$, $I_p$ for HICHA ($n = 1, l = 0$) at eight representative $r_c$’s.

| $r_c$ | $S_r$ | $S_p$ | $E_r$ | $E_p$ | $I_r$ | $I_p$ |
|-------|-------|-------|-------|-------|-------|-------|
| 0.1   | -0.91566109 | 7.35307032 | 4.131779628 | 0.0010422175 | 94.710796 | 0.381792129 |
| 0.2   | 0.052768647 | 6.38756548 | 1.599164401 | 0.0027729332 | 49.8541421 | 0.72903709 |
| 0.5   | 1.276107967 | 5.17221865 | 0.489826968 | 0.0096225321 | 22.3087069 | 1.65240877 |
| 1     | 2.130332820 | 4.3296668 | 0.218575181 | 0.0231665955 | 12.8509181 | 2.93351472 |
| 2     | 2.882449058 | 3.5967152 | 0.110132418 | 0.05088542 | 8.02939092 | 4.88465544 |
| 5     | 3.626749943 | 2.888923 | 0.058459157 | 0.113903221 | 5.1989752 | 8.18387106 |
| 8     | 3.865631044 | 2.669252 | 0.048526927 | 1.6068696 | 4.57764692 | 9.71697608 |
| $\infty$ | 4.144729885 | -2.1483865112 | 0.0397887358 | 0.2089749413 | 4.0000000 | 12.0000000 |

Figure 6. Plots of (a) Compton density for $n = 1, l = 0$ state in HICHA at four selected $r_c$ values namely 0.1, 2, 5, 8, and (b) $S_c$, $E_c$, $\langle \frac{1}{2p} \rangle$ with change in $r_c$.

4. Conclusion
The SE for HICHA cannot be solved exactly. Here we have made a systematic analysis of bound-state energies within a GPS method. Information measures such as, $S, R, I, E$ are investigated for HICHA, in conjugate $r$ and $p$ spaces. Interestingly a new energy distribution rule has been found for such systems. Apart from that, we have also examined the influence of confinement on the Compton profile of the ground state using these information theoretic measures.

In HICHA, unlike FHA, energy depends on both $n$ and $l$ quantum numbers. But in both cases energy decreases with growth in $r_c$. Like CHA, here also $S_r$, $R_r^c$ increase and $I_r$, $E_r$ decrease with rise in $r_c$. Similarly, in $p$ space we observe reverse trend. Additionally, $S$ has been successfully used to understand the effect of confinement on Compton profile.

Overall, we have presented an elaborate study of information measures in a soft impenetrable confinement. Further, it enlightened us about the effectiveness of $R, S, E, I$ in the context of HICHA. These may be interesting to study the statistical complexity measures in a HICHA. Multiple polarizability for such quantum-dot systems is highly desirable. Similar analysis can also be extended for H atom trapped in supramolecular cavity. In future, this idea may
be extended to investigate the effect of confined environment on many-electron atomic and molecular systems.

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References
[1] W. Grochala, R. Hoffmann, J. Feng and N. W. Ashcroft, Angew. Chem. Int. Ed. 46 (20), 3620-3642 (2007).
[2] R. J. Hemley, Annu. Rev. Phys. Chem. 51, 763-800 (2000).
[3] K. D. Sen (Ed.), Electronic Structure of Quantum Confined Atoms and Molecules, (Springer, Switzerland, 2014).
[4] J. Katriel and H. E. Montgomery Jr., J. Chem. Phys. 137 (11), 114109 (2012).
[5] N. Mukherjee and A. K. Roy, Phys. Rev. A 99 (2), 022125 (2019).
[6] N. Mukherjee and A. K. Roy, Int. J. Quant. Chem. 118 (14), e25596 (2018).
[7] S. H. Patil and Y. P. Varshni, Can. J. Phys. 82 (11), 917-930 (2004).
[8] S. H. Patil and Y. P. Varshni, in The Theory of Confined Quantum Systems Part I, Advances in Quantum Chemistry, Vol. 57 (Academic Press, 2009) pp. 1-24.
[9] E. Lee-Koo and S. Rubinstein, J. Chem. Phys. 71 (1), 351-257 (1979).
[10] R. Cabrera-Trujillo and J. Oddershede, Adv. Quant. Chem., 77, 295-315 (2017).
[11] R. Cabrera-Trujillo, J. Phys. B, 50 (15), 155006 (2017).
[12] S. Majumdar, N. Mukherjee and A. K. Roy, Chem. Phys. Lett. 687, 322-329 (2017).
[13] N. Mukherjee, S. Majumdar and A. K. Roy, Chem. Phys. Lett. 691, 449-455 (2018).
[14] S. Noorizadeh and E. Shakerzadah, Phys. Chem. Chem. Phys., 12, 4742-4749 (2010).
[15] N. L. Guevara, R. P. Sagar and R. O. Esquivel, Phys. Rev. A, 67 (1), 012507, (2003).
[16] A. K. Roy and A. F. Jalbout, Chem. Phys. Lett. 445 (4), 355-360 (2007).
[17] A. K. Roy, A. F. Jalbout and E. I. Proynov, Int. J. Quant. Chem. 108, 827-836 (2008).
[18] A. K. Roy, Int. J. Quant. Chem. 113 (10), 1503-1510 (2013).
[19] A. K. Roy, Int. J. Quant. Chem. 114 (6), 383-391 (2014).
[20] K. D. Sen and A. K. Roy, Phys. Lett. A 357 (2), 112-119 (2006).
[21] A. K. Roy, Mod. Phys. Lett. A 29 (9), 1450042 (2014).
[22] A. K. Roy, Int. J. Quant. Chem. 115 (15), 937-947 (2015).
[23] A. K. Roy, Int. J. Quant. Chem. 116 (12), 953-960 (2016).
[24] S. Majumdar and A. K. Roy, Quant. Rep. 2, 189-207 (2020).
[25] W. E. Duncanson and C. A. Coulson, Proc. Phys. Soc. 57 (3), 1926-1948 (1945).