N-dimensional electron in a spherical potential: the large-N limit

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(Dated: October 9, 2018)

Abstract

We show that the energy levels predicted by a $1/N$-expansion method for an N-dimensional Hydrogen atom in a spherical potential are always lower than the exact energy levels but monotonically converge towards their exact eigenstates for higher ordered corrections. The technique allows a systematic approach for quantum many body problems in a confined potential and explains the remarkable agreement of such approximate theories when compared with the exact numerical spectrum.

Keywords: $1/N$-expansion, hyperspherical coordinates.

PACS: 03.65.-w, 73.21.La

A fundamental theoretical problem in the realm of many body physics concerns the technical difficulty in making precise theoretical evaluations of physical observations, even more so in problems involving quantum systems. In most cases, this is compounded by the practical difficulty in establishing a suitable approximation scheme that conjoins simplicity with effectiveness. An interesting observation in connection suggests that an increase in the number of degrees of freedom often simplifies the theoretical analysis. A perturbative approach requires at least one dimensionless parameter and if we couple this fact with the previous statement, it effectively implies that as we go on increasing the dimensionality of this parameter, the perturbation analysis becomes more and more simple. Often it is found that a problem of inherently quantum mechanical origin can be mapped on to a classical phase space in the $N \to \infty$
limit thereby reducing a quantum problem to a classical one \cite{4}. In other words, one then has a limit where quantum interference effects simply die out paving the way for a simple classical analysis. The excited states for such a system can be obtained as an expansion in $1/N$ around the minimum of the effective classical potential $V_{\text{eff}}$. Such an approach is not at all uncommon in statistical physics \cite{5, 6} in problems which allow for at least a minimum. In many of those cases, the large-N limit has been fruitfully utilized in dealing with equilibrium as well as non-equilibrium problems in classical critical phenomena \cite{7}. In quantum mechanics too, $1/N$ expansion method has a long precedence. Detailed accounts of related applications can be obtained from review articles like the one due to Chatterjee \cite{8, 9, 10, 11} as also from more informal narratives like \cite{1, 4}. The versatility and flexibility of this technique has allowed it to be used in a range of diverse topics, starting from field theoretic studies in high energy physics \cite{12, 15} to problems on earthquake dynamics \cite{13} as well as on problems in colloidal physics \cite{14}.

In this brief report, we shall use the $1/N$-expansion method to study the problem of an N-dimensional Hydrogen atom confined in a Harmonic oscillator potential. Although the model is nothing new \cite{10}, however our objective here is. We intend to study the efficacy of this expansion method by calculating the energy eigenvalues and showing that to each order of correction, the large-N expansion method always predicts a slightly lower potential as compared to the exact eigenvalue obtained numerically. This is remarkable since this implies a certain monotonicity in these perturbation corrections which tells us that the corrections are always positive, a fact that has often been tacitly assumed in related calculations \cite{16, 17}. We argue that this is the underlying reason which makes this method more dynamic compared to standard perturbation technique which is limited strictly to a weak-coupling regime. In a following work, we build on this principle and analytically solve for the three-body problem of interacting electrons using an exact Coulomb potential \cite{18}.

In the first paper of the paper, we do a rehash of the N-dimensional quantum mechanics for a single electron in a spherical confining potential and then defining the potential in the relative frame of reference, we go on to solve the stationary state problem using the $1/N$-expansion method. As already stated, we then proceed to calculate the energy corrections due to this method
for both ground and excited states and show that all higher ordered corrections have a steady monotonicity that ensures a large-N eigenstate below its exact (meaning experimental) counterpart.

Taking cues from standard literature [8, 10], we begin with the Hamiltonian for the center of mass of an N-dimensional electron in a spherical potential

\[ H = \frac{\vec{p}^2}{2m_e} + V_N(\vec{r}) \] (1)

Using standardized units \( \hbar = m_e = 1 \) (h=Plank’s constant and \( m_e \)=mass of the electron), the Hamiltonian can be rewritten as

\[ H = -\frac{1}{2} \nabla_N^2 + V_N(\vec{r}) \] (2)

where terms have their usual meaning. The potential being radial \( V_N(\vec{r}) = V_N(r) \) and this gives the eigenvalue equation

\[ H\psi(\vec{r}) = \left[-\frac{1}{2} \nabla_N^2 + V_N(\vec{r})\right] \psi(\vec{r}) = E\psi(\vec{r}) \] (3)

For a system with spherical symmetry, the curvilinear coordinates can be written as follows (generalisation of the treatment available in [10])

\[
x_1 = r \cos \theta_1 \sin \theta_2 \sin \theta_3 \ldots \sin \theta_{N-1}
\]

\[
x_2 = r \sin \theta_1 \sin \theta_2 \sin \theta_3 \ldots \sin \theta_{N-1}
\]

\[
x_3 = r \sin \theta_2 \sin \theta_3 \sin \theta_4 \ldots \sin \theta_{N-1}
\]

\[
\vdots
\]

\[
x_k = r \cos \theta_k - 1 \sin \theta_k \sin \theta_{k+1} \ldots \sin \theta_{N-1}
\]

\[
x_{N-1} = r \cos \theta_{N-2} \sin \theta_{N-1}
\]

\[
x_N = r \cos \theta_{N-1}
\] (4)

where \( r \) is the radial distance and \( \theta_k (k < N - 1) \) are the angles defining the hyper-spherical space, \( \theta_{N-1} \) being the azimuthal angle. \( \psi(\vec{r}) \) is the eigenfunction of this system. The above definition can now be used to obtain the radial equation of motion [10]

\[
\begin{aligned}
\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} + \frac{l(l+N-2)}{2r^2} + V_N(r)\right] R(r) &= ER(r)
\end{aligned}
\] (5)

where \( l \)'s are the angular quantum numbers and \( R(r) \) is the radial wave function. Using the transformation \( u(r) = r^{(N-1)/2} R(r) \), we can now absorb the first
derivative in eqn. (6). The reconstructed radial equation of motion is now given by

\[-\frac{1}{2} \frac{d^2 R}{dr^2} + \kappa^2 \left[ \frac{1 - \frac{1}{\kappa}}{8r^2} + \frac{V_N(r)}{\kappa^2} \right] u(r) = Eu(r)\]

(6)

In the above, we have used \( \kappa = N + 2l \).

At this point, the meaning of the large-N limit turns out to be pretty obvious. It means that \( \kappa \to \infty \) (since \( N \) is large) encompasses the idea of a stationarity limit for a very heavy classical particle of effective mass \( \kappa^2 \) where the particle is localized at the point \( r = r_0 \), the point \( r_0 \) in turn defining the minimum of the classical potential \( V_{\text{eff}} = \frac{1}{8r^2} + \frac{V_N(r)}{\kappa^2} \). The ground state energy of such a localized system is given by \( E_\infty = \kappa^2 V_{\text{eff}}(r_0) \).

We now consider a specific form for the potential function \( V_N(r) \) and proceed to calculate the higher order corrections in the large-N limit. The model we choose for the purpose is an oscillator with anharmonic fluctuations. The reason for this choice has been accentuated by the observation that such a description, albeit simple, yet is able to reproduce a good estimate for the energy eigenstates \( \kappa \) when compared with numerical \( \kappa \) as well as with experimental \( \kappa \) result. For a simple harmonic oscillator \( V_N(r) = \frac{1}{2} \omega^2 r^2 \) which gives \( r_0 = \sqrt{\frac{\omega^2}{2\kappa}} \), \( V_{\text{eff}} = |\frac{\omega^2}{2r}| \) and eventually \( E_\infty = |\frac{3\omega^2}{2}| \).

One can now add quantum fluctuations and study the behavior of the system close to the classical minimum \( r_0 \). We go beyond this description in the sense that we consider a finite sized electron instead of a fixed mass and consider fluctuations around the classical stable minimum. To do this we revoke the original radial equation eq. (6) prior to the large-N limit being imposed on it. Using the \( 1/N \) expansion technique, we now embark on a stepwise evaluation of the energy eigenvalues due to the quantum fluctuations close to the classical minimum. We define the eigenvalue problem as follows

\[ [H_0 + \tilde{V}(r)]\psi(\vec{r}) = E\psi(\vec{r}) \]

(7)

The ground state eigenvalue equation \( H_0 \psi(\vec{r}) = E_0 \psi(\vec{r}) \) has already been defined through equation (3) \( E_0 = \frac{3\omega^2}{2} \) while \( \tilde{V}(r) \) is the part of the Hamiltonian that contributes to the quantum fluctuations. Taylor’s expansion allows this perturbation Hamiltonian to be represented as

\[ \tilde{V} = \tilde{V}(r_0) + (r - r_0) \tilde{V}'(r_0) + \frac{(r - r_0)^2}{2!} \tilde{V}''(r_0) + ... \]

(8)

where the primes denote derivatives with respect to \( r \). Before proceeding any further, we make a variable transformation from \( r \to x \) where \( x = \frac{\sqrt{2}}{r_0}(r - r_0) \) and transform eq. (7) likewise. In the translated
coordinate system, the complete eigenvalue equation is given by

\[- \frac{1}{2} \frac{d^2 u}{dx^2} + k[(1 - \frac{4}{k} + \frac{3}{k^2})(1 - 2 \frac{x}{\sqrt{k}} + 3 \frac{x^2}{k})
- 4 \frac{x^3}{k^{3/2}} + ... + r_0^2 \{\hat{V}(r_0) + r_0 V'(r_0)(1 + \frac{x}{\sqrt{k}})
+ \frac{r_0^2}{2} \hat{V}''(r_0)(1 + \frac{x^2}{k} + 2 \frac{x}{\sqrt{k}})\}u(x)\]

\[= (E_k) r_0^2 u(x)\]

In the analysis of the above equation we consider all terms up to \(O(r^2)\) and evaluate coefficients for increasing powers of \(x\) starting with \(x^0\). A little rearranging now allows us to rewrite the eigenvalue equation in terms of the variable \(x\) as follows

\[[H_0 + \hat{V}(x)]\psi(x) = \lambda \psi(x)\]  \(\text{(10)}\)

where

\[H_0 = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \omega^2 x^2 + \epsilon_0\]

\[\hat{V}(x) = \frac{1}{\sqrt{k}}(\epsilon_1 x + \epsilon_3 x^3) + \frac{1}{k}(\epsilon_2 x^2 + \epsilon_4 x^4)\]

\[+ \frac{1}{k^{3/2}}(\delta_1 x + \delta_3 x^3 + \delta_5 x^5)\]  \(\text{(11)}\)

where \(\lambda = (E_k) r_0^2\) and for a harmonic oscillator potential the constants \(\epsilon_k\) and \(\delta_k\) are given by

\[\epsilon_0 = \frac{k}{8} - \frac{1}{2} + \frac{3}{8k} + \frac{k^2}{64}\]

\[\epsilon_1 = 1, \ \epsilon_2 = -3/2, \ \epsilon_3 = \frac{1}{6} r_0^5 \hat{V}'''(r_0) - \text{...} (12)\]

Higher-ordered parameters like \(\epsilon_3\) have non-zero values for anharmonic oscillations.

The above description allows us to re-frame an effective classical potential \(V_{\text{eff}}\) in the large-N limit but now including higher-ordered fluctuations. It has the form

\[V_{\text{eff}}(R) = -\frac{1}{2} \frac{\omega^2}{k} R^2 + \frac{\epsilon_0}{k} + \frac{1}{k} V(R)\]  \(\text{(13)}\)

where \(V(R)\) represents some oscillator potential having a minimum at \(R_0\), a point which can be obtained from the relation

\[\frac{\partial}{\partial R} V_{\text{eff}}(R)|_{R=R_0} = 0\]  \(\text{(14)}\)

Defining the potential as in eq. \(\text{(11)}\) and then applying the optimization criterion as in eq. \(\text{(14)}\), we arrive at the quadratic equation

\[3\epsilon_3 R_0^2 - \sqrt{k\omega^2} R_0 + \epsilon_1 = 0\]  \(\text{(15)}\)

which gives the solution \(R_0^{(\pm)} = \frac{\sqrt{k\omega^2} \pm \sqrt{k\omega^4 - 12\epsilon_1 \epsilon_3}}{6\epsilon_3}\). To check the stability at the point \(R = R_0\), we evaluate the second derivatives and find that the two roots of eq. \(\text{(15)}\) satisfy the relation

\[\frac{\partial^2}{\partial R^2} V_{\text{eff}}(R)|_{R=R_0^{(\pm)}} = -\frac{\omega^2}{k} + \frac{6\epsilon_3}{k^{3/2}} \left(\frac{\sqrt{k\omega^2} \pm \sqrt{k\omega^4 - 12\epsilon_1 \epsilon_3}}{6\epsilon_3}\right)\]  \(\text{(16)}\)

The above result implies that the minima are subject to the restriction \(k\omega^4 \geq 12\epsilon_1 \epsilon_3\).
An idea of the exactitude of this analysis can be had from an evaluation of the parameters using a simple harmonic oscillator potential. This gives $\epsilon_3 = -1/2$, thereby naturally validating the restriction. The conclusion remains unchanged even after adding higher ordered anharmonic terms to the potential. To leading order in expansions, we now have the large-N expanded energy eigenvalue for the ground state as follows

$$E = \frac{k \omega^2}{2 r_0^2} R_0^2 + \sqrt{k} \frac{\epsilon_3}{r_0^2} R_0 (\epsilon_1 + \epsilon_3 R_0^2) + \frac{\epsilon_0}{k}$$

(17)

where $r_0^2 = \frac{k}{2\omega}$. The above expression for energy conclusively proves that even in the presence of fluctuations, large-N expansion gives positive corrections to energy, monotonically approaching the exact value as one scales up the order. We have checked for a range of such higher ordered fluctuations and have found the previous conclusion sacrosanct. A point of some interest here would be the variation of such an approximated energy with respect to the strength $\omega$ of the anharmonic oscillation for a fixed dimension, $N=3$ say. Fig. 1 shows this variation and evidently tells us that there is a minimum in the curve much as we would expect it to be. The minimum also signifies the fact that the results of the large-N approximation would be best valid close to the minimum, that is between $\omega = 0.4 - 0.5$ as per Fig. 1.

As a suggestive example, we might look at the next higher modification in the potential which gives rise to the following cubic equation

$$4\epsilon_4 R_0^3 + 3\sqrt{k}\epsilon_3 R_0^2 + (2\epsilon_2 - k\omega^2) R_0 + \sqrt{k}\epsilon_1 = 0$$

(18)

Once again, the above equation can be solved analytically using Cardan’s method and it is rather an easy algebraic exercise to show that the energy corrections are still
positive.

To conclude, we have shown using a perturbed anharmonic oscillator potential that a large-N expansion method provides an effective approximation scheme in tackling quantum mechanical problems. This is evident, since the order of corrections as suggested by this method monotonically converges towards the semi-classical limit as \( N \to \infty \). The results offer favorable comparisons with numerical and experimental data and might be used in more complicated quantum many body problems involving exact interaction potentials.

The author acknowledges helpful discussions with A. Chatterjee and is grateful to the Marie Curie Foundation, fellowship MIFI-CT-2005-008608, for research support.

[1] E. Witten, Phys. Today, July, 38 (1980).
[2] K. G. Wilson, Phys. Rev. D 7, 2911 (1973).
[3] G. t’ Hooft, Nucl. Phys. 72, 461 (1974).
[4] L. G. Yaffe, Phys. Today, August, 50 (1983).
[5] T. H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952); H. E. Stanley, Phys. Rev. 176, 718 (1968).
[6] Y. Sakamoto, H. Mukaida and C. Itoi, Phys. Rev. B72, 144405 (2005).
[7] S. K. Ma in Phase Transitions and Critical Phenomena, vol. 6, Edtd. Academic (New York), 1976.
[8] M. Moshe and J. Zinn-Justin, Phys. Reps. 385, 69 (2003).
[9] O. Aharony, S. S. Gubser, J. Maldacena et al, Phys. Reps. 323, 184 (2000).
[10] A. Chatterjee, Phys. Reps. 186, 249 (1990).
[11] T. D. Cohen, Rev. Mod. Phys. 68, 599 (1996).
[12] F. Canfora, Nucl. Phys. B 731, 389 (2005).
[13] O. V. Lunina, Y. Mart and A. S. Gladkov, J. Geodyn. 40, 216 (2005).
[14] P. Wette, H. J. Schope and T. Palberg, J. Chem. Phys. 123, 174902 (2005).
[15] P. Kovtun, M. Unsal and L. G. Yaffe, Phys. Rev. D 72, 105006 (2005); S. Bellucci, C. Sochichiu, Nucl. Phys. B 726, 233 (2005).
[16] M. El-Said, Phys. Rev. B 61, 13026 (2000).
[17] R. M. G. Garcia-Castellan, W. S. Choe and Y. C. Lee, Phys. Rev. B 57, 9792 (1998).
[18] Amit K Chattopadhyay, unpublished.
[19] G. Arfken in *Mathematical Methods for Physicists*, Academic Press (1985).

[20] N. F. Johnson and M. C. Payne, Phys. Rev. Lett. **67**, 1157 (1991).

[21] P. A. Maksym and T. T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990).

[22] Ch. Sikorski and U. Merkt, Phys. Rev. Lett. **62**, 2164 (1989).