On the Hylleraas Coordinates

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(Dated: January 27, 2022)

Abstract

The Hylleraas coordinates $s = r_1 + r_2$, $t = r_1 - r_2$, $u = |r_1 - r_2|$ are the natural coordinates for the determination of properties of the Helium atom, the positive ions of its isoelectronic sequence, and the negative Hydrogen ion. In this paper, we derive a new expression for integrals representing properties such as the energy, normalization and expectation of arbitrary operators, as written in the $(s, t, u)$ coordinates. The expression derived is valid for both finite and infinite space. The integrals for the various properties are comprised in each case of two components $A$ and $B$. The contribution of these components to the volume of integration and the normalization of a wave function for finite space, and in variational calculations of the ground state energy of the Helium atom confined in a finite volume is demonstrated by example. We prove that when the integration space is infinite, the expression for the energy and other properties employed by Hylleraas corresponds only to that of integral $A$. We further prove that for the approximate variational wave functions employed by Hylleraas and other authors, the contribution of the term $B$ vanishes. This contribution also vanishes for the exact wave function. It is interesting to note that the component $B$ to the integral is not mentioned in the literature. A principle purpose of the paper, therefore, is to point out the existence of this term.

PACS numbers:
I. INTRODUCTION

The Schrödinger equation [1] for the Helium atom, or the positive ions of its isoelectronic sequence, or of the negative Hydrogen ion, is

\[ \hat{H} \Psi = E \Psi, \]

where the Hamiltonian \( \hat{H} \) is

\[ \hat{H} = -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \]

where \( r_1, r_2 \) are the coordinates of the two electrons, \( r_{12} \) is the distance between them (see Fig.1), \( Z \) the charge of the nucleus, and \( \Psi \) and \( E \) the eigenfunction and eigenenergy of the system. As noted by Hylleraas [2], the Schrödinger equation in this instance is not a six-dimensional but rather a three-dimensional eigenvalue problem. The natural coordinates of the system are \( r_1, r_2, \) and \( r_{12} \) forming the triangle \( (r_1, r_2, r_{12}) \). The other three angle variables which determine the orientation of the triangle in space, because of the symmetry of the system, are arbitrary and can be integrated over. Equivalently, the system is uniquely described by the coordinates \( r_1, r_2, \) and \( \theta_{12} \), the angle between the vectors \( r_1 \) and \( r_2 \).

As is well known, there is no closed-form analytical solution to the two-electron eigenvalue problem. Hence, the energy is most accurately obtained by variational minimization of the energy functional \( E[\Psi] \) defined as

\[ E[\psi] = \frac{\int \psi \hat{H} \psi d\tau}{\int \psi^2 d\tau}, \]

with respect to the parameters in the wave function. In performing such variational calculations, Hylleraas further introduced the ‘elliptical’ coordinates

\[ s = r_1 + r_2, \ t = r_1 - r_2, \ u = r_{12}. \]

Then assuming approximate wave functions dependent on these coordinates, he applied the variational principle to obtain the energy. There has been similar work employing these \((s, t, u)\) coordinates over the past decades [3, 4, 5, 6, 7, 8].

In this paper, we investigate integrals of the form \( \int f d\tau \) appearing in Eq. (3) in the elliptical coordinates \((s, t, u)\) for both finite and infinite space. We have discovered another
way of writing the integrals in these coordinates that differs from the commonly employed one in the literature. In section II we derive the integral to be a sum of two contributions $A$ and $B$ valid for both finite and infinite space. This is a natural separation of the integration domain. We demonstrate the correctness of our derivation by three examples for finite space as described in section III. These examples correspond to (a) volume of integration, (b) normalization of a wave function, and (c) variational calculations of the ground state energy of the Helium atom confined to a finite volume. In section IV, we prove for the case when the space is infinite that the energy and normalization integrals employed by Hylleraas and others corresponds \\textit{only} to that of integral $A$. We further prove that for the approximate wave functions employed by these authors, the contribution of $B$ vanishes. As the asymptotic structure of the exact wave function is known to also decay exponentially, once again the contribution of integral $B$ for infinite space vanishes for the true wave function. We summarize our results and conclusions in section V.

II. INTEGRALS IN $(s, t, u)$ COORDINATES

Let us first focus on the volume element $d\tau$ of Eq.(3). Employing the symmetry of the system, $d\tau$ can be rewritten as

$$d\tau = dr_1 dr_2 = J(r_1, r_2, \theta_{12}) dr_1 dr_2 d\theta_{12},$$

where $J(r_1, r_2, \theta_{12})$ is the Jacobian of the coordinate transformation. By fixing $r_1$ first, carry out the integral of $r_2$ with respect to $r_1$ to arrive at (see Fig.1)

$$\int d\tau = \int dr_1 r_2^2 dr_2 \sin \theta_{12} d\theta_{12} d\phi_{12} = 2\pi \int dr_1 r_2^2 dr_2 \sin \theta_{12} d\theta_{12}. \tag{6}$$

Next, by integrating over $r_1$, we note there is no dependence on the Euler angles, so that Eq.(6) reduces to

$$\int d\tau = 8\pi^2 \int r_1^2 r_2^2 dr_1 dr_2 \sin \theta_{12} d\theta_{12}. \tag{7}$$

We now introduce the new variable $u$, the distance between $r_1$ and $r_2$:

$$u^2 = r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}. \tag{8}$$
During the previous integration steps, if \( r_1 \) and \( r_2 \) are fixed first, then

\[
u \, du = r_1 r_2 \sin \theta_{12} d\theta_{12}, \tag{9}\]

so that (for the case of infinite volume)

\[
\int d\tau = 8\pi^2 \int_0^\infty \int_0^\infty r_1^2 r_2^2 dr_1 dr_2 \int_0^\pi \sin \theta_{12} d\theta_{12} = 8\pi^2 \int_0^\infty \int_0^\infty r_1 r_2 dr_1 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} udu. \tag{10}\]

Eq. (10) appears in the work of Hylleraas\[2\].

Let us next confine the two electrons in some finite volume of space such that \( 0 \leq r_1 \leq R \) and \( 0 \leq r_2 \leq R \). The reason we choose the same \( R \) is because of the symmetry between the two electrons. The limit \( R \rightarrow \infty \) then leads to the infinite space integral. For the elliptical coordinates \( s \) and \( t \) of Eq. (4), it is easy to show that

\[
dr_1 dr_2 = \frac{1}{2} ds dt, \quad r_1 r_2 = \frac{1}{4} (s^2 - t^2). \tag{11}\]
Therefore, for any integrand \( f \), which is a function of \((s, t, u)\), we have from Eqs.(10) and (11) that the integral in terms of the new coordinates \((s, t, u)\) is

\[
\int f d\tau = 8\pi^2 \int_0^R \int_0^R r_1 r_2 dr_1 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} uf(s, t, u) du = 8\pi^2 \int \int \frac{1}{S_t^2} ds dt \int_{|t|}^s f(s, t, u) \frac{s^2-t^2}{4} u du.
\]

(12)

Here \( S' \) denotes the integration domain in the new coordinates \((s, t)\). This domain has changed from \( S : [0 \leq r_1 \leq R, 0 \leq r_2 \leq R] \) as shown in Fig.2 to \( S' : [0 \leq s \leq 2R; -R \leq t \leq R] \).

The function \( f(s, t, u) \) could be \( \psi \hat{H} \psi \) or \( \psi^2 \). As stated by Bethe [10]: “The exact symmetry requirement [of the wave function] then takes the simple form that \( \psi \) be an even function of \( t \) for parahelium, an odd function of \( t \) for ortho-helium. Since the Hamiltonian is an even function of \( t \) and since the integrals in Eq.(3) contain two factors, the contribution to the integral from \( -t \) is identical with that from \( +t \). We therefore restrict ourselves to positive values of \( t \) in the integrals and multiply the volume element by a factor of 2”. With that in
FIG. 3: The domain $S'$ of integration of the Hylleraas coordinates $s$ and $t$.

mind, Eq. (12) can be rewritten as

$$\int f d\tau = 2\pi^2 \int \int_{S'} dsdt \int_{|t|}^{s} f(s,t,u)(s^2 - t^2)udu$$

$$= 2\pi^2 \int_{0}^{R} ds \int_{0}^{s} dt \int_{t}^{s} f(s,t,u)(s^2 - t^2)udu$$

$$+ 2\pi^2 \int_{R}^{2R} ds \int_{0}^{2R-s} dt \int_{t}^{s} f(s,t,u)(s^2 - t^2)udu. \quad (13)$$

Now we can see from equation (13) that the integral has two components. For convenience, let us denote them as $A$ and $B$ where

$$A = 2\pi^2 \int_{0}^{R} ds \int_{0}^{s} dt \int_{t}^{s} f(s,t,u)(s^2 - t^2)udu, \quad (14)$$

and

$$B = 2\pi^2 \int_{R}^{2R} ds \int_{0}^{2R-s} dt \int_{t}^{s} f(s,t,u)(s^2 - t^2)udu. \quad (15)$$

We next give examples to demonstrate the correctness of this separation of the volume
III. EXAMPLES

(a) Volume of integration

We first consider the volume of integration by choosing \( f(s, t, u) = 1 \). The result should be the square of the volume of a sphere with radius \( R \). Indeed, one easier way to determine this is by employing Eq.(7)

\[
\int d\tau = 8\pi^2 \cdot 2\left(\frac{R^3}{3}\right)^2 = \left(\frac{4\pi R^3}{3}\right)^2.
\]

On the other hand, we can carry out the integral via its components derived in Eq.(13). On using the following integrals

\[
\int_{t}^{s} (s^2 - t^2) u du = \frac{(s^2 - t^2)^2}{2}, \tag{17}
\]

\[
\int_{0}^{R} ds \int_{0}^{s} du \frac{(s^2 - t^2)^2}{2} = \frac{2R^6}{45}, \tag{18}
\]

\[
\int_{R}^{2R} ds \int_{0}^{2R-s} du \frac{(s^2 - t^2)^2}{2} = \frac{38R^6}{45}, \tag{19}
\]

we also have

\[
\int d\tau = A + B = 2\pi^2 \left(\frac{2R^6}{45} + \frac{38R^6}{45}\right) = \left(\frac{4\pi R^3}{3}\right)^2. \tag{20}
\]

The agreement of the two ways to obtain the volume demonstrates that the new way of expressing the integrals within the \((s, t, u)\) coordinates as defined by Eq.(13) is correct.

(b) Normalization

Let us next consider the normalization of the trial wave function

\[
\psi = Ce^{-\alpha s}, \tag{21}
\]

where \( \alpha \) is a variational parameter, \( C \) is the normalization constant. Then in spherical polar coordinates for a finite volume of radius \( R \), the normalization integral is

\[
1 = \int \psi^2 d\tau = C^2 (4\pi \int_{0}^{R} e^{-2\alpha r^2} dr)^2
\]

\[
= \frac{C^2 \pi^2}{\alpha^6} \left[1 - e^{-2\alpha R(1 + 2\alpha R + 2\alpha^2 R^2)}\right]^2. \tag{22}
\]
For \( R \to \infty \), \( C = \frac{\alpha^3}{\pi} \), the well known result.

In the \((s,t,u)\) coordinates, the contribution from \( A \) of Eq.(14) is

\[
A = \int_A \psi^2 d\tau = 2\pi^2 C^2 \int_0^R dse^{-2\alpha s} \int_0^s dt \int_t^s duu(s^2 - t^2)
\]

\[
A = \frac{C^2\pi^2}{\alpha^6}[1 - \frac{e^{-2\alpha R}}{15}(15 + 30\alpha R + 30\alpha^2 R^2 + 20\alpha^3 R^3 + 10\alpha^4 R^4 + 4\alpha^5 R^5)]. (23)
\]

The contribution to normalization from \( B \) of Eq.(15) is

\[
B = \int_B \psi^2 d\tau = 2\pi^2 C^2 \int_R^{2R} dse^{-2\alpha s} \int_0^{2R-s} dt \int_t^{2R-s} duu(s^2 - t^2)
\]

\[
B = \frac{C^2\pi^2}{\alpha^6}[e^{-4\alpha R}(1 + 2\alpha R + 2\alpha^2 R^2)^2
\]

\[-e^{-2\alpha R}\frac{15 + 30\alpha R + 30\alpha^2 R^2 - 20\alpha^3 R^3 - 10\alpha^4 R^4 - 4\alpha^5 R^5}]. (26)
\]

It is easily verified that the sum of \( A \) and \( B \) of Eq.(24) and Eq.(26) are equivalent to that of Eq.(22). This again demonstrates the correctness of the two integrals derived.

(c) Variational Calculations

In the final example, we consider the Helium atom confined within shells of volume of integration corresponding to \( R = 2.0, 3.0, 4.0 \), and \( 5.0 \) \( \text{a.u.} \). We determine variationally the ground state energy of the atom thus confined. The approximate wave function we employ is that of Eq.(21), which then does not satisfy the boundary condition of vanishing at the surface. The total energy of Eq.(3) is determined in both spherical polar coordinates as well as via Eq.(14) and Eq.(15) of contributions \( A \) and \( B \). A point to note is that the commonly employed expression for the integrand of the kinetic energy in \((s,t,u)\) coordinates is valid only for infinite space and assumes that the wave function vanishes there. However, since the volume of integration is finite, there is a contribution to the kinetic energy from the surface of the volume as the wave function does not vanish on the surface (see the Appendix for details). The analytical expression for the kinetic energy contributions from integrals \( A \) and \( B \) and the surface contribution as well as those for the total energy are given in the Appendix. The various numerical contributions of the kinetic energy \( T \), external \( E_{\text{ext}} \) and electron-interaction \( E_{\text{ee}} \) potential energies are listed in Table I. The well known \[10\] variational result for \textit{infinite} space quoted to six significant figures is \( E = -2.84765 \) \( \text{a.u.} \)
TABLE I: The variationally determined ground state energy of the Helium atom and of the corresponding kinetic energy $T$, external $E_{\text{ext}}$ and electron-interaction $E_{\text{ee}}$ potential energy components as a function of the radius $R$ of the volume of integration in (a.u.). The contribution from the integrals $A$ and $B$ for each energy component as well as the surface contribution to the kinetic energy are quoted as are the energy minimized values of the variational parameter $\alpha$.

| $R$ | $\alpha$ | $T$ | $E_{\text{ext}}$ | $E_{\text{ee}}$ | $E$ |
|-----|----------|-----|-----------------|----------------|-----|
|     | A | B | S | A | B | A | B |
| 2.0 | 1.652 | 1.91327 | 0.81583 | 0.16747 | -5.64802 | -1.16273 | -0.88250 | 0.20120 | -2.83048 |
| 3.0 | 1.687 | 2.68121 | 0.16476 | 0.01175 | -6.59864 | -0.16328 | 1.03104 | 0.02713 | -2.84603 |
| 4.0 | 1.688 | 2.82820 | 0.02114 | 0.00071 | -6.73641 | -0.01643 | 1.05256 | 0.00267 | -2.84756 |
| 5.0 | 1.688 | 2.84729 | 0.00205 | 0.00004 | -6.75073 | -0.00131 | 1.05480 | 0.00021 | -2.84765 |

for $\alpha = 27/16$. For each value of $R$, the sum of the contributions from integrals $A$ and $B$ for the separate kinetic plus surface $S$ contribution, external, and electron-interaction energy components is the same as those obtained in spherical polar coordinates.

Note there is a contribution to each component of the energy from both integral $A$ and $B$ for each value of $R$. Due to the exponential decay of the wave function, the contribution from $B$ diminishes but always is finite even at $R = 5.0$ (a.u.). Observe that at $R = 5.0$ (a.u.), the total energy is the same as the well known result to six significant figures. However, the contribution of $B$ becomes negligible in the $R \to \infty$ limit. Thus, it is only in this limit that the integral corresponding to $B$ can be ignored. The variational results once again prove the correctness of the derivations for the two integrals $A$ and $B$.

IV. COMPARISON WITH THE HYLLERAAS INTEGRAL

In this section, we compare our new way of writing the integral with that of Hylleraas. As noted previously, Eq. (10) appears in the work of Hylleraas. Following this equation,
and without any further detail, he then writes the integral for the energy and normalization for when the space is infinite as

$$\int f d\tau = 2\pi^2 \int_0^\infty ds \int_0^s du \int_0^u dt \ u \ (s^2 - t^2) \ f(s, t, u).$$  \tag{27}$$

Observe that in this integral, the integration over the variable $t$ is performed before that of the variable $u$. (We note that in all subsequent literature employing these elliptical coordinates, it is the Hylleraas expression that is employed.) This order of integration is surprising because the variable $u$ depends on the variables $s$ and $t$. Hence, it is natural to perform the integral over $u$ prior to that of $t$ and $s$ as in our expression Eq. (13). The derivation of Eq. (13) is a consequence of our attempt to understand how Hylleraas arrived at his expression of Eq. (27). For a comparison of Eqs. (13) and (27), we take the $R \rightarrow \infty$ limit of Eq. (13). The two results ought to be equivalent. However, we find that it is only $\lim_{R \rightarrow \infty} A$ (see Eq. (14)) that is equivalent to Eq. (27) of Hylleraas. For $R \rightarrow \infty$

$$A|_{R \rightarrow \infty} = 2\pi^2 \int_0^\infty ds \int_0^s dt \int_t^u du \ u \ (s^2 - t^2) \ f(s, t, u).$$  \tag{28}$$

As shown by Fig. 4, in Eq. (27), for each $u$ with $0 \leq u \leq s$, we have $0 \leq t \leq u$, the area swept is the upper shaded triangle. On the other hand, in Eq. (28), for each $t$ with $0 \leq t \leq s$, we have $t \leq u \leq s$, so that the area is the same as in Eq. (27). Therefore, for any integrand, the integrals of Eq. (27) and (28) are the same. Thus, the Hylleraas integral is the same as that of $A$ for $R \rightarrow \infty$. The difference in the order of integration between the expression of Hylleraas and of our derivation is of critical significance for work on the Helium atom to be published elsewhere.

Let us now turn to Eq. (15) and examine the integral $B$ in the same limit. As we have shown earlier, in finite space, the contribution of $B$ plays an important role. When $R \rightarrow \infty$, we have

$$B|_{R \rightarrow \infty} = 2\pi^2 \lim_{R \rightarrow \infty} \int_R^{2R} ds \int_0^{2R-s} dt \int_t^s f(s, t, u)(s^2 - t^2) \ u \ du$$  \tag{29}$$

$$= \lim_{R \rightarrow \infty} 2\pi^2 \int_R^{2R} h(R, s) ds$$  \tag{30}$$

It is only when the function $h(R, s)$ decays in a manner such that $\lim_{R \rightarrow \infty} B$ vanishes that the Hylleraas expression corresponds to the exact value of the integral $\int f d\tau$. Thus, for
example, if one assumes as in all prior literature, that $h(R, s)$ decays exponentially, and is of the form

$$h(R, s) = g(R)e^{-\alpha s} \sum_{l \geq 0} s^l,$$

then since for any non-negative polynomial of $s$,

$$\lim_{R \to \infty} \int_{2R}^{R} ds e^{-\alpha s} s^l = 0,$$

we have $B|_{R \to \infty} = 0$. However, if the dependence on the coordinate $s$ contains terms of the form $s^p$ with $p \geq -1$ or is multiplied by some power of $\ln s$, the contribution of $B$ could be nonzero. For example, the integral $\int_{R}^{2R} h(s) ds$ for $h(s) = 1/s$ is $\ln 2$ irrespective of how large $R$ is. As noted above, for the form of approximate wave functions employed in the literature, the contribution of $B$ always vanishes in the limit as $R \to \infty$. It also vanishes for the exact wave function whose asymptotic decay is known to be $r^{\beta}e^{-\alpha r}$, where $(1 + \beta) = (Z - N + 1)/\alpha$, and $\alpha = \sqrt{2I}$, with $I$ being the ionization potential.

It is interesting that the contribution of the integral $B$ to the integral $\int f d\tau$ is not mentioned at all in the literature. One would imagine that in spite of the fact that the contribution of $B$ vanishes for the choice of a particular approximate wave function, mention of this term pointing out its lack of contribution would appear somewhere. But this is
not the case. Hence, one principal purpose of this paper is to note the existence of this term.

V. CONCLUSION

In this paper we have derived a new expression for integrals representing the energy, normalization, or other expectation values when written in the Hylleraas \((s, t, u)\) coordinates, i.e. \(\int f(s, t, u)d\tau\). The expression derived for the integral is valid for both finite and infinite space. The integrals for the various properties are comprised in each case of two components \(A\) and \(B\). The contribution of these components to the volume of integration, the normalization of a wave function, and in variational calculations of the energy, for finite space is demonstrated by example. We prove that when the space of integration is infinite, the expression used by Hylleraas and others corresponds only to that of integral \(A\). In the literature, the form of the approximate wave functions are such that the integrands for the energy and normalization are usually of the form \(e^{-\alpha s} \sum_{l,m,n} h_l(s)t^m u^n; h_l(s) = s^l \text{ or } (lns)^l\) [7, 11], etc. We show that for such wave functions the contribution of \(B\) vanishes. The contribution of integral \(B\) also vanishes for the exact wave function. Thus, in calculations of the integral \(\int f(s, t, u)d\tau\) when the space considered is infinite, one may ignore the contribution of the component \(B\) by choosing an appropriate decay of the approximate wave function. Nevertheless, we reiterate that from a rigorous mathematical perspective, the integral \(\int f(s, t, u)d\tau\) is composed of two components \(A\) and \(B\).

APPENDIX

For the wave function of Eq.(21), the contribution to the total energy from integral \(A\) is

\[
E_A = 2\pi^2 \int_0^R ds \int_0^s dt \int_u^s du [u(s^2 - t^2)(\frac{d\psi}{ds})^2 - 4ZsuC^2 e^{-2\alpha s} + (s^2 - t^2)C^2 e^{-2\alpha s}]\), \quad (A.1)
\]

where the first, second, and third terms correspond respectively to the kinetic, external, and electron-interaction energies. (The surface contribution to the kinetic energy is discussed
Thus,\[
E_A = \frac{\pi^2 C^2}{8\alpha^5} \left[ -(27 - 8\alpha) - \frac{1}{15} \{ e^{-2\alpha R} [-405 - 30(-4 + 27R)\alpha - 30R(-8 + 27R)\alpha^2 \\
- 60R^2(-4 + 9R)\alpha^3 + 10(16 - 27R)R^3\alpha^4 + 80R^4\alpha^5 + 32R^5\alpha^6]) \} \right]. \quad (A.2)
\]

The contribution from integral $B$ is
\[
E_B = 2\pi^2 \int_0^{2R} ds \int_0^{2R-s} dt \int_t^s du [u(s^2 - t^2) (\frac{\partial \psi}{\partial s})^2 - 4ZsuC^2 e^{-2\alpha s} \\
+ (s^2 - t^2)C^2 e^{-2\alpha s})] \quad (A.3)
\]
\[
= \frac{\pi^2 C^2}{8\alpha^5} e^{-4\alpha R} \left[ -21 - 4(-2 + 21R)\alpha + 8(4 - 17R)R\alpha^2 - 32R^2(-2 + 3R)\alpha^3 \\
+ 64R^3\alpha^4 + 32R^4\alpha^5 \right] \\
+ \frac{\pi^2 C^2}{120\alpha^5} e^{-2\alpha R} \left[ 315 + 30(-4 + 21R)\alpha + 30R(-8 + 5R)\alpha^2 - 60R^2(4 + 9R)\alpha^3 \\
+ 10(16 - 27R)R^3\alpha^4 + 80R^4\alpha^5 + 32R^5\alpha^6 \right]. \quad (A.4)
\]

The kinetic energy is
\[
T = -\int \psi \nabla^2 \psi d\tau = \int (\nabla_1 \psi) \cdot (\nabla_1 \psi) d\tau - \int \nabla \cdot (\psi \nabla_1 \psi) d\tau. \quad (A.5)
\]

The first term of Eq. (A.5) corresponds to the first terms in Eqs. (A.1) and (A.3) for the total energy for integrals $A$ and $B$, respectively. This contribution is
\[
T_A + T_B = \alpha^2. \quad (A.6)
\]

The surface contribution to the kinetic energy is
\[
T_s = \int \nabla \cdot (\psi \nabla_1 \psi) d\tau = \int (\nabla_1 \cdot (e^{-\alpha r_1} \nabla_1 e^{-\alpha r_1})) dr_1 \\
= -\int (e^{-\alpha r_1} \nabla_1 e^{-\alpha r_1}) \cdot dS_1 \quad (A.7)
\]
\[
= 4\pi CR^2 \alpha e^{-2\alpha R} \frac{4\alpha^4 R^2 e^{-2\alpha R}}{(1 - e^{-2\alpha R}(1 + 2\alpha R + 2R^2\alpha^2))}. \quad (A.8)
\]

In spherical polar coordinates, the kinetic energy $T$ in a volume of radius $R$ is
\[
T = -\int \psi \nabla^2 \psi d\tau = 16\pi^2 C^2 \int_0^R \int_0^R e^{-2\alpha (r_1 + r_2)}(\alpha^2 - \frac{2\alpha}{r_1})r_1^2 r_2^2 dr_1 dr_2, \quad (A.9)
\]
so that
\[
T = \frac{\alpha^2 [1 + e^{-2\alpha R}(-1 - 2\alpha R + 2\alpha^2 R^2)]}{[1 - e^{-2\alpha R}(1 + 2\alpha R + 2\alpha^2 R^2)]}. \quad (A.10)
\]

The sum of Eqs. (A.6) and (A.8) equals Eq. (A.10).
ACKNOWLEDGMENTS

This work was supported in part by the Research Foundation of CUNY. L. M. was supported in part by NSF through CREST, and by a “Research Centers in Minority Institutions” award, RR-03037, from the National Center for Research Resources, National Institutes of Health. We thank Professors J. B. Krieger and Hong-Yi Fan for their comments on the manuscript.

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