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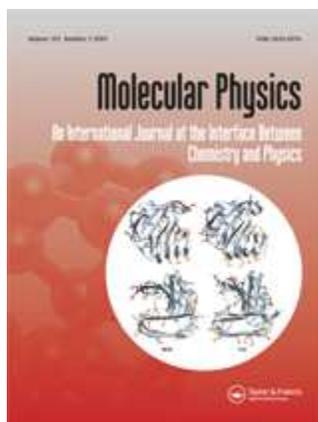
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Exact solutions for shell-confined hydrogen-like atoms: polarizabilities and Shannon entropies

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Abstract

An idealized model to treat the effect of spherically confining the electron in a hydrogen-like atom is studied, where the potential is infinite in all space except for a spherical shell. The exact solution of the Schrödinger equation is obtained in terms of two independent solutions of the Kummer equations. It is found that in some cases it is necessary to use the standard KummerM function and a non-standard second solution. In other cases we may use the KummerU function and in a limiting case the two standard solutions of Bessel's equation. The effect of an imposed dipole field on the shell is treated using the first-order perturbation equation from which the polarizability can be calculated. In addition the exact wavefunction is used to calculate the Shannon entropies of both position and momentum and it is shown that these measures give insight into the form of the wavefunction.

Key words: shell confined, polarizabilities, Shannon entropies.

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1 Introduction

In the present work we extend an earlier exact treatment of confined hydrogen-like atoms. The model consists of the conventional Coulomb potential restricted to a finite radial interval $R_1 < r < R_2$. In previous work [1,2,3] we adopted the traditional model with $R_1 = 0$; the present extension introduces non-trivial changes in the mathematical treatment of an exactly soluble problem.

We observe that this model was suggested (but not actually treated) in a calculation of the Shannon information entropy of confined atoms [4]. This entropy has been advocated as a particularly useful measure of the quality and properties of the wavefunction and has been the subject of much recent work [4-9].

In the following section we solve Schrödinger's equation in terms of confluent hypergeometric functions. It turns out that the standard choice of solutions is not always appropriate. In later sections we use the resulting solutions in calculations of dipole polarizabilities and Shannon entropies.

2 Solutions of the Schrödinger equation

We extend the notations of our earlier work with

$$H_0 = -\frac{1}{2}\nabla^2 + V_0(r; R_1, R_2) \quad (1)$$

where

$$V_0(r; R_1, R_2) = -\frac{Z}{r}, \quad R_1 \leq r \leq R_2, \quad \infty \text{ otherwise} \quad (2)$$

(a natural generalization of the conventional unconfined hydrogen-like Hamiltonian). The exact solutions are expressed conveniently in the form

$$\psi_0 = N_0 r^l Y_{lm}(\theta, \Phi) \exp(-\alpha r) f(c, d, 2\alpha r), \quad E_0 = -\frac{\alpha^2}{2} \quad (3)$$

where N_0 is a normalization constant, Y_{lm} is the usual spherical harmonic and the parameter α must be determined numerically from the boundary conditions. Here

$$c = (l+1) - \frac{Z}{\alpha}, \quad d = 2(l+1) \quad (4)$$

The function $f(c, d, 2\alpha r)$ satisfies the same second-order differential equation studied previously [1,2], but with *two-point finite* boundary conditions

$$f(c, d, 2\alpha R_1) = f(c, d, 2\alpha R_2) = 0 \quad (5)$$

Specifically, for fixed c and d , we have to solve:

$$L(c, d, x)y(x) = [xD^2 + (d-x)D - c]y(x) = 0 \quad (6)$$

where

$$x = 2\alpha r, \quad D = \frac{d}{dx}, \quad f(c, d, 2\alpha r) = y(x) \quad (7)$$

Equation (6) defines the Kummer functions and to satisfy both boundary conditions (5) we need to use two *independent* solutions. We have chosen one of

these as the usual Kummer M function, which is finite at $x = 0$ and has the series expansion :

$$M(c, d, x) = 1 + \frac{c}{d}x + \frac{c(c+1)}{d(d+1)}\frac{x^2}{2!} + \dots + \frac{(c)_n}{(d)_n}\frac{x^n}{n!} + \dots \quad (8)$$

where we have used the Pochhammer symbol $(a)_n = \Gamma(a+n)/\Gamma(a)$ The second series solution of Kummer's equation can be written in many ways. The standard form

$$x^{1-d}M(1+c-d, 2-d, x) \quad (9)$$

is singular when as in our case, $d = n + 1$ and n is a positive integer. A particular linear combination of (9) and $M(c, d, x)$, denoted by $U(c, d, x)$ [10] is often used as the second solution. A limiting form of this removes the singularity for positive integers n but it is not universally linearly independent of $M(c, d, x)$ since $c = l + 1 - Z/\alpha$ may be zero or a negative integer in the form $c = -m$. If in addition n is a positive integer $U(c, d, x)$ becomes a multiple of $M(c, d, x)$ [11] and an alternative second, independent solution, is required. Clearly for a fixed positive integer d there is an accumulation of such values of α as m increases and the energy, E_0 approaches 0. Even for formally unproblematic values of α in the region $0 < \alpha < 1$, the numerical computations become increasingly unstable and it is necessary to find an alternative form for the second independent solution. We now introduce formally a general linearly independent second solution $W(c, d, x)$ and write

$$f(c, d, 2\alpha r) = aM(c, d, 2\alpha r) + bW(c, d, 2\alpha r) \quad (10)$$

The boundary conditions on ψ_0 imply that we need to solve the pair of equations

$$aM(c, d, 2\alpha R_1) + bW(c, d, 2\alpha R_1) = 0 \quad (11)$$

$$aM(c, d, 2\alpha R_2) + bW(c, d, 2\alpha R_2) = 0 \quad (12)$$

To obtain non-zero solutions for a and b we need to solve

$$M(c, d, 2\alpha R_1)W(c, d, 2\alpha R_2) - M(c, d, 2\alpha R_2)W(c, d, 2\alpha R_1) = 0 \quad (13)$$

This is an equation for α and once this parameter is determined the ratio a/b may be determined from either (11) or (12). Note it is impractical to choose $W(c, d, x) = U(c, d, x)$, with $0 < \alpha < 1$, for the reasons outlined above. To obtain a second independent solution we follow the standard procedure for a series solution where one or more of the coefficients are singular (see for example Piaggio [12]). In this case we form the function

$$Q = x^s M(c + 2s + n, n + 1 + 2s, x) \quad (14)$$

which is obtained from (9) by replacing $1 - d$ by the variable s and writing $d = n + 1$ where n is a positive integer; it reduces to (9) with $s = 1 - d = -n$. This is the solution of

$$L(c, 1 - 2s - n, x)Q = 0, \quad L(c, d, x) \equiv xD^2 + (d - x)D - c \quad (15)$$

The operator $L(c, d, x)$ and more details of the solutions of the Kummer equation are considered in the appendix. Note $L(c, 1 - 2s - n, x)$ reduces to $L(c, 1 + n, x) =$

$L(c, d, x)$ when $s = -n$, but Q is singular for this choice of s . To deal with this we replace Q by $P = (s + n)Q$ and then

$$L(c, n + 1, x)P = (s + n)L(c, 1 - 2s - n, x)Q + 2(s + n)^2 DQ = 2(s + n)^2 DQ \quad (16)$$

This shows that P is a solution when $s = -n$ and since $(s + n)$ occurs quadratically we also have

$$\lim_{s \rightarrow -n} \left\{ L(c, d, x) \frac{\partial P}{\partial s} \right\} = 2 \lim_{s \rightarrow -n} \left\{ \frac{\partial((s + n)^2 DQ)}{\partial s} \right\} = 0 \quad (17)$$

and we may deduce that when $s = -n$ another solution is

$$N(c, d, x) = \lim_{s \rightarrow -n} \frac{\partial(s + n)Q}{\partial s} \quad (18)$$

and we may choose $W(c, d, x) = N(c, d, x)$ as an independent second solution. The solution $W(c, d, x) = P(c, d, x)$ is not independent of $M(c, d, x)$; further details are deferred to the appendix.

The functions $M(c, d, x)$ and $W(c, d, x)$ are calculated using the mathematical package MAPLE and in the tables below we list the energies E_0 for selected values of R_1 and R_2 . In table 1 we use $R_1 = 0.5$, $Z = 1$ with R_2 in the interval 2.9...17 and these lead to negative ground state ($l = 0$) energies decreasing with R_2 . Similarly in table 2 we use $R_1 = 2$, $Z = 1$, $R_2 = 7..20$ and again obtain negative ground state energies; we note that in the case $R_1 = 2$ as $R_2 \rightarrow \infty$ this solution approaches the 2s state for an *unconfined* hydrogen-like atom. In table 3 we again use $R_1 = 2$, $Z = 1$ but for the first excited $l = 0$ state and for the larger values of R_2 the energies are small and negative, but eventually they become positive and increase sharply. This is similar to the behaviour in our earlier work where the confinement was purely spherical ($R_1 = 0$ for some R_2) [1,3]. To deal with the case of positive energy we may replace α by $i\beta$ (β real) and solve (13), equating both real and imaginary parts to zero simultaneously. The resulting energy is given by $E_0 = \beta^2/2$. In the calculations in table 3, to find the value of R_2 for which $E_0 = \alpha = 0$ we use a similar analysis to that given in [1]. We multiply H_0 by r to obtain

$$(r^2 D_r^2 + 2(l + 1)r D_r + 2Zr)f = 0 \quad (19)$$

where $D_r = d/dr$. Using the substitutions

$$r = \frac{x^2}{8Z}, \quad p = -(2l + 1), \quad f = x^p y \quad (20)$$

leads to the canonical Bessel equation of order p :

$$(xD^2 + xD + (x^2 - p^2))y = 0 \quad (21)$$

so that the two independent solutions are the Bessel functions, $J_p(x)$, $Y_p(x)$. The analogue of (13) in the case $l = 0$ is

$$J_1(x_1)Y_1(x_2) - J_1(x_2)Y_1(x_1) = 0 \quad (22)$$

where $x_1 = \sqrt{8R_1}$ and $x_2 = \sqrt{8R_2}$. For $R_1 = 2$, $Z = 1$ and $\alpha = 0$ this is an equation for R_2 and can be used to find the position of the zero energy for the first excited s-state; this is given in table 3.

All of the calculations presented in the tables are for $l = 0$, but it is easy to extend to higher values. For example for the case $l = 1, R_1 = 0.2, R_2 = 30$ we obtain an energy of -0.1248 , which is close to the $2p$ energy of atomic hydrogen (-0.125); this is to be expected when R_1 is small and R_2 is large. Similarly for $l = 1, R_1 = 6, R_2 = 30$ we obtain -0.0554 . Since $R_1 = 6$ corresponds to the node of the $3p$ state for atomic hydrogen, as expected, this is close to the corresponding energy ($-1/18$). In the intermediate range of R_1 , with parameters $l = 1, R_1 = 0.2, R_2 = 30$ we obtain the lowest p-state energy -0.1140 lying between the hydrogen $2p$ and $3p$ energies.

3 Polarizabilities

As in our earlier treatment of (one-sided) confinement [2] we treat the dipole polarizability of s-states. This has been the subject of much interest over many years [13-16]. It turns out that the present model involves more extensive analysis. With the field-free solution written as in (3) the first order equation

$$(H_0 - E_0)\psi_1 = -rcos(\theta)\psi_0 \quad (23)$$

may be used to calculate the second-order energy and hence the polarizability with the first-order equation expressed in the form

$$\psi_1 = N_1 rcos(\theta)exp(-x/2)F(x) \quad (24)$$

In the following analysis it is convenient to express $f(c, d, x)$ of (7) in the form

$$f(c, d, x) = AM(c, d, x) + BU(c, d, x); \quad (25)$$

this allows direct use of the standard recurrence relations for $M(c, d, x)$ and $U(c, d, x)$. We emphasize that this is legitimate so long as we do not have the degenerate case where $U(c, d, x)$ is a multiple of $M(c, d, x)$. (In section 1 we needed to use (18) rather than $U(c, d, x)$ to avoid the solutions of (13), arising from the degenerate cases, that lead to unacceptable wavefunctions which did not satisfy (11) and (12)). Given α from (13) we can find A and B from either of the two equations:

$$f(c, d, x_1) = 0 \quad \text{or} \quad f(c, d, x_2) = 0 \quad (26)$$

The explicit solution for $F(x)$ of (24) is obtained from

$$L(c+1, d+2, x)F(x) = \mu x(AM(c, d, x) + BU(c, d, x)), \quad \mu = \frac{1}{2\alpha^2} \quad (27)$$

is now derived analogously to the earlier $F(x)$ in [2]. In the present case $F(x)$ naturally contains superpositions of both the KummerM and KummerU functions in the form

$$F(x) = \sum_{k=0, k \neq 2}^4 (A_k M(c-1+k, d+2, x) + B_k U(c-1+k, d+2, x)) + \frac{\partial}{\partial c} (A_2 M(c+1, d+2, x) + B_2 U(c+1, d+2, x)) \quad (28)$$

The coefficients are given by

$$\begin{aligned}
 A_0 &= \frac{(c-1)(c-3)(c-4)}{6}, \quad B_0 = 1 \\
 A_1 &= -2\frac{(c-1)(c-2)(c-3)}{3}, \quad B_1 = -4(c-1) \\
 A_2 &= c(c-1)(c-2), \quad B_2 = 6c(c-1) \\
 A_3 &= -2\frac{(c+1)c(c-1)}{3}, \quad B_3 = -4(c-1)c(c+1) \\
 A_4 &= \frac{(c+2)(c+1)c}{6}, \quad B_4 = (c-1)c(c+1)(c+2)
 \end{aligned} \tag{29}$$

We note that if $\alpha = 0$ so that the solution is expressed in terms of Bessel functions, or such that $N(c, d, x)$ needs to be used instead of $U(c, d, x)$, then it is necessary to consider an alternative form for ψ_1 or use a limiting process. However this will only occur for a discrete set of α in the interval $0 \leq \alpha \leq 1$.

4 Shannon Entropies

The Shannon entropy of the electron density in coordinate space is defined by

$$S_{\mathbf{r}} = - \int \rho(\mathbf{r}) \ln(\rho(\mathbf{r})) d\mathbf{r} \tag{30}$$

where $\rho(\mathbf{r}) = |\psi_0|^2$ and ψ_0 is the normalized wavefunction. As the electron density function, $\rho(\mathbf{r})$ becomes more de-localized $S_{\mathbf{r}}$ increases and conversely for localized electron densities $S_{\mathbf{r}}$ increases. This is analogous to the usual information theory entropy

$$- \sum_i p_i \ln(p_i) \geq 0 \tag{31}$$

for a discrete distribution $\{p_i\}$ which is a maximum for a uniform distribution and zero when one of the p_i is unity and the others all zero. There is one important difference and that is that $S_{\mathbf{r}}$ may be negative. This property of $S_{\mathbf{r}}$ may be illustrated using a one dimensional model where

$$\rho_{\mathbf{r}}(\mathbf{r}) = \rho(x) = \sqrt{\frac{a}{\pi}} \exp(-ax^2) \tag{32}$$

and $S_{\mathbf{r}}$ may be calculated exactly as

$$S_{\mathbf{r}} = \frac{1}{2} (1 + \ln(\frac{a}{\pi})) \tag{33}$$

As $a \rightarrow \infty$, $S_{\mathbf{r}} \rightarrow -\infty$ and as $a \rightarrow 0$, $S_{\mathbf{r}} \rightarrow \infty$. In this paper we consider $l = 0$ so that although we have a 3-dimensional example, $\rho_{\mathbf{r}}(\mathbf{r}) = \rho(r)$ a one-dimensional radial electron density.

The corresponding Shannon entropy for the momentum is given by

$$S_{\mathbf{p}} = - \int \gamma(\mathbf{p}) \ln(\gamma(\mathbf{p})) d\mathbf{p} \tag{34}$$

with $\gamma(\mathbf{p}) = |\phi_0|^2$ where ϕ_0 is the normalized momentum wavefunction obtained from a Fourier transform of ψ_0

$$\int \psi_0 \exp(i(\mathbf{p} \cdot \mathbf{r})) d\mathbf{r} \quad (35)$$

These entropies (or uncertainties) provide a measure of information about the probability distributions in the coordinate space and momentum space respectively. An uncertainty principle [9] has been derived for these entropies which for a single electron in 3 dimensions takes the form

$$S_T = S_{\mathbf{r}} + S_{\mathbf{p}} \geq 3(1 + \ln(\pi)) \approx 6.4342 \quad (36)$$

One of the earliest applications was the use of S_T to measure the quality of approximate wavefunctions [8] but more recently it has been related to various chemical properties that can be obtained from the wavefunction. (For a comprehensive list of these applications see [5]). Here we concentrate on the *separate* entropies to measure the wavefunction properties and shape. We use the example of calculations given in table 1 and since $l = 0$ we have $Y_{lm}(\theta, \Phi) = 1$ and (30) becomes

$$S_{\mathbf{r}} = -4\pi \int_0^\infty r^2 |\psi_0|^2 \ln(|\psi_0|^2) dr \quad (37)$$

The results are given in table 4 and we see a steady decrease in $S_{\mathbf{r}}$ as the system becomes more confined and the uncertainty in position decreases. To obtain ϕ_0 corresponding to ψ_0 we may fix the direction of \mathbf{p} in (35) to be the z-axis and obtain

$$2\pi \int_{R_1}^{R_2} \int_0^\pi r^2 \psi_0 \exp(-ipr \cos(\theta)) \sin(\theta) d\theta dr = 4\pi \int_{R_1}^{R_2} r^2 \psi_0 \text{sinc}(pr) dr \quad (38)$$

which only depends on the variable p. The Shannon entropies are defined for normalized wavefunctions and we may normalize ϕ_0 so that

$$\int |\phi_0|^2 d\mathbf{p} = 1 \quad (39)$$

and consequently ϕ_0 can be expressed in the form

$$\phi_0 = N_p \int_{R_1}^{R_2} r^2 \psi_0 \text{sinc}(pr) dr \quad (40)$$

where N_p is a normalization constant and the momentum entropy becomes

$$S_{\mathbf{p}} = -4\pi \int_0^\infty p^2 |\phi_0|^2 \ln(|\phi_0|^2) dp \quad (41)$$

Both (37) and (41) are easily calculated using standard numerical integration techniques and the values are given in table 4. At first sight the uncertainty principle (36) would seem to imply that as $S_{\mathbf{r}}$ decreases then $S_{\mathbf{p}}$ should increase. This is certainly the case for the very large and very small values of R_2 but in the intermediate region $S_{\mathbf{p}}$ decreases (and in fact becomes small and negative). This

behaviour mirrors the form of the wavefunction which localized near $r = R_2$ for large R_2 , localized near $r = R_1$ for small R_2 but has a bimodal shape in the intermediate region. (see figures 1,2 and 3; the wavefunctions are arbitrarily normalized). In the bimodal situation the spread of the coordinate wavefunction is large even though it is increasingly confined. Thus, from the standard Heisenberg uncertainty principle, the momentum spread is narrow and this manifests itself in S_p . The two entropy measures therefore give information about the shape of the wavefunctions whereas the sum, S_T essentially mirrors S_r .

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Appendix A: Solutions of Kummer's equation

We require two *linearly independent* solutions of the Kummer differential equation

$$L(c, d, x)f(x) = 0 \quad (\text{A1})$$

where we denote the second-order linear operator $L(c, d, x)$:

$$L(c, d, x) = xD^2 + (d - x)D - c, \quad D = \frac{d}{dx} \quad (\text{A2})$$

The standard (Frobenius) method of solution for $f(x)$ is to *assume* a convergent infinite series

$$f(x) = x^s F(x; s), \quad F(x; s) = \sum_{k=0}^{\infty} a_k(s) x^k \quad (\text{A3})$$

which yields on substitution into (A1)

$$L(c, d, x)f(x) = a_0(s)s(s + d - 1)x^{s-1} \quad (\text{A4})$$

provided that the higher-order expansion coefficients $a_k(s)$ satisfy the recurrence relations

$$a_{k+1}(s) = \frac{(s + k + c)}{(s + k + d)(s + k + 1)} a_k(s) \quad (\text{A5})$$

Assuming a_0 is non-zero, we generally have two linearly independent solutions to (A1) provided that the indicial equation

$$s(s + d - 1) = 0 \quad (\text{A6})$$

has *distinct* roots. Unless $d = 1$ the distinct roots are $s = 0$, $s = 1 - d$ and the two convergent series solutions are usually denoted by (we adopt the notations of Abramowitz and Stegun [10])

$$f_1(x) = M(c, d, x) \quad (\text{A7})$$

and

$$f_2(x) = x^{1-d} M(c + 1 - d, 2 - d, x) \quad (\text{A8})$$

where $M(c,d,x)$ denotes the Kummer function regular at $x = 0$:

$$M(c, d, x) = \sum_{k=0}^{\infty} \frac{c_k x^k}{d_k k!} \quad (\text{A9})$$

and we have used the Pockhammer symbol

$$c_k = c(c+1)\dots(c+k-1) = \frac{\Gamma(c+k)}{\Gamma(c)} \quad (\text{A10})$$

Clearly when $d = 1$, we have identically $f_1(x) = f_2(x)$, and we must derive a second solution by other means. Moreover, whenever d is zero or a negative integer in (A7) or $d > 1$ in (A8), a zero factor in some of the denominators in (A9) invalidates the form of series solution. The procedure for finding the second solution is similar in all cases but for definiteness, we now apply the procedure of Piaggio to the case $d = n + 1$ where n is a positive integer, so that $s = 0$ gives a finite solution, but $s = -n$ does not. In such a case, Piaggio rewrites the zero-order expansion coefficient, $a_0(-n)$, in the form

$$a_0(-n) = (s+n)b_0(-n) \quad (\text{A11})$$

but now assumes $b_0(-n)$ is non-zero, so that the n leading coefficients of the series $F(x; -n)$ vanish:

$$a_0(-n) = a_1(-n) = \dots = a_{n-1}(-n) = 0 \quad (\text{A12})$$

while the effect of the zero multiplier, $(s+n)$ on all higher-order coefficients is to cancel the zero term in each denominator. We follow Piaggio's procedure, writing the solution more generally

$$f(x) = (s+n)x^s F(x) \quad (\text{A13})$$

and obtain formally

$$L(c, d, x)[(s+n)x^s F(x)] = (s+n)x^s [L(c+s, n+1+2s) + \frac{s(s+n)}{x}] F(x) \quad (\text{A14})$$

By definition of the KummerM function,

$$L(c+s, d+2s, x)M(c+s, d+2s, x) = 0 \quad (\text{A15})$$

so that a solution, $F(x)$, of (A14) is given by a multiple of

$$M(c+s, n+1+2s, x) = 1 + \frac{(c+s)}{(n+1+2s)}x + \frac{(c+s)(c+s+1)}{(n+1+2s)(n+2+2s)}\frac{x^2}{2} + \dots \quad (\text{A16})$$

since the right hand side of (A14) is zero when $s = -n$, so long as $(s+n)F(x)$ is finite. It will be necessary to evaluate the limit of the product $(s+n)F(x)$ as $s \rightarrow -n$, in order to obtain the well-defined result:

$$f_2(x) = \lim_{s \rightarrow -n} \{x^s [(s+n)M(c+s, n+1+2s, x)]\}$$

$$= \frac{(c-n) \cdot (c-1)}{(1-n)(2-n) \cdot (-1)} \frac{1}{n!} \left(1 + \frac{c}{n+1}x + \dots\right) = kM(c, n+1, x) \quad (\text{A17})$$

which is a finite *multiple* of the solution $f_1(x)$ (with $s = 0$). Moreover, the presence of the *quadratic* factor $(s+n)^2$ on the right-hand side of (A14) implies that, provided the limit as $s \rightarrow -n$ exists, a third solution of (A1) is obtained by *first* taking partial derivatives with respect to s and *then* proceeding to the limit $s \rightarrow -n$: formally, this result may be written

$$f_3(x) = \lim_{s \rightarrow -n} \frac{\partial}{\partial s} [x^s (s+n) M(c+s, n+1+2s, x)] = N(c, n+1, x) \quad (\text{A18})$$

and we emphasize that this function, $N(c, n+1, x)$ is *not* necessarily identical with the second Kummer solution usually denoted by $U(c, n+1, x)$ (see [10]). However the three functions $M(c, n+1, x)$, $N(c, n+1, x)$ and $U(c, n+1, x)$ cannot be linearly independent, since they all satisfy the *second-order* differential equation (A1).

We note that, on account of the derivative of x^s , (A18) generally contains a term proportional to $\ln(x)M(c, n+1, x)$, which is linearly independent of $M(c, n+1, x)$. The solution of (A18) may be identified with (18) in the main text.

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Table 1 Ground state energies where $R_1 = 0.5$ for various R_2

R_1	R_2	E_0
0.5	17	-0.398906
0.5	15	-0.344312
0.5	13	-0.327935
0.5	11	-0.320705
0.5	9	-0.313823
0.5	7	-0.302277
0.5	5	-0.264904
0.5	3	-0.029066
0.5	2.9	-0.005937

Table 2 Ground state energies where $R_1 = 2$ for various R_2

R_1	R_2	E_0
2	20	-0.124986
2	13	-0.122945
2	12	-0.121104
2	11	-0.117727
2	10	-0.111565
2	9	-0.100268
2	8	-0.079198
2	7	-0.038704

Table 3 First excited state energies where $R_1 = 2$ for various R_2 ; the results include the zero energy and one positive energy.

R_1	R_2	E_0
2	20	-0.047672
2	17	-0.037193
2	16	-0.030875
2	15	-0.022229
2	14	-0.010407
2	13.171086	0
2	12	0.272603

Table 4 The position, momentum and total entropies for the states in table 1.

R_1	R_2	S_r	S_p	S_T
0.5	17	9.2542	0.4697	9.7239
0.5	15	9.0095	0.4131	9.4226
0.5	13	8.9015	-0.3029	8.5986
0.5	11	8.2187	-0.9717	7.2470
0.5	9	6.9682	-0.3132	6.6550
0.5	7	6.1373	0.3985	6.5358
0.5	5	5.3598	1.282	6.6418
0.5	3	4.0696	2.779	6.8486
0.5	2.9	3.9741	2.862	6.8361

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Figure Captions

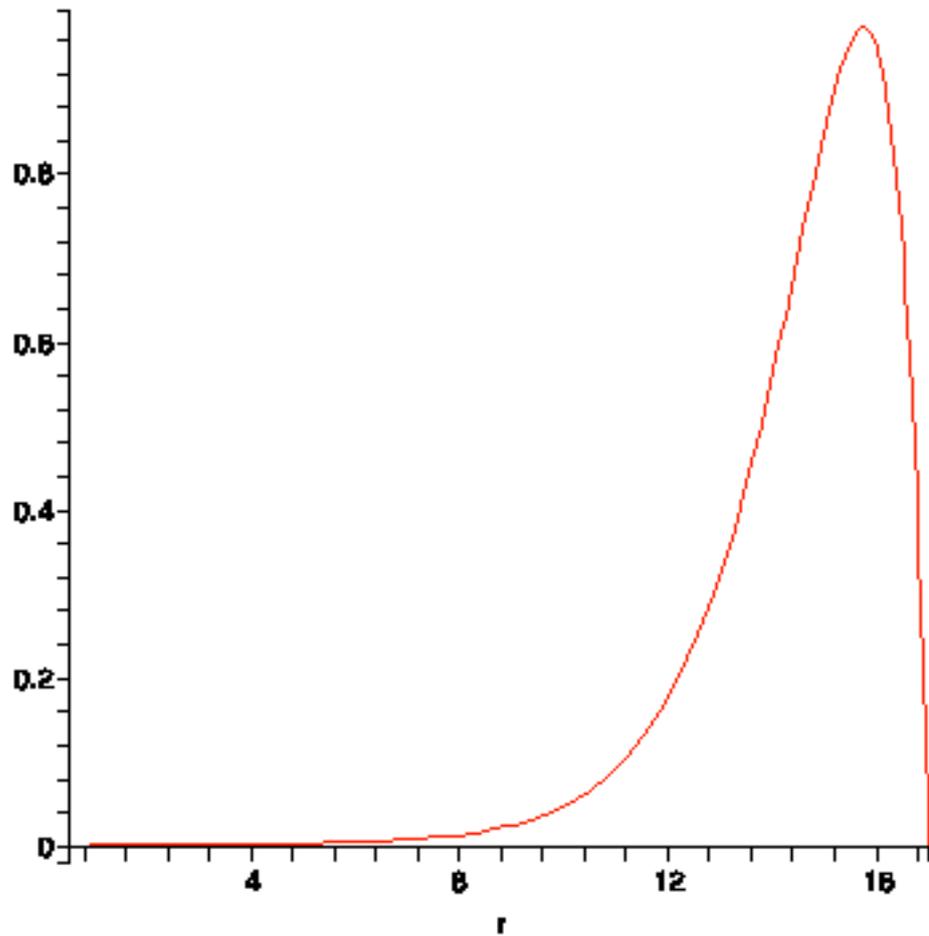
Figure 1: the ground state wavefunction for $\mathbf{R}_1 = 0.5$ and $\mathbf{R}_2 = 17$

Figure 2: the ground state wavefunction for $\mathbf{R}_1 = 0.5$ and $\mathbf{R}_2 = 2.9$

Figure 3: the ground state wavefunction for $\mathbf{R}_1 = 0.5$ and $\mathbf{R}_2 = 13$

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Figure 1: the ground state wavefunction for $R_1 = 0.5$ and $R_2 = 17$



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Figure 2: the ground state wavefunction for $R_1 = 0.5$ and $R_2 = 2.9$

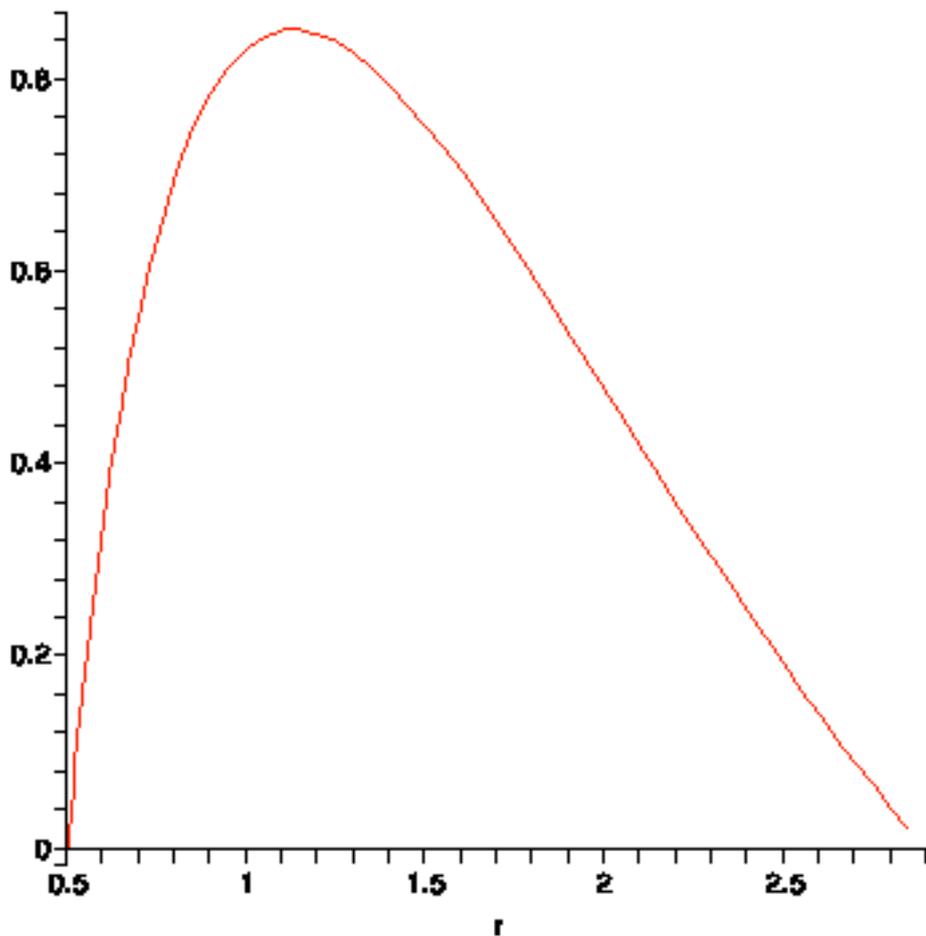
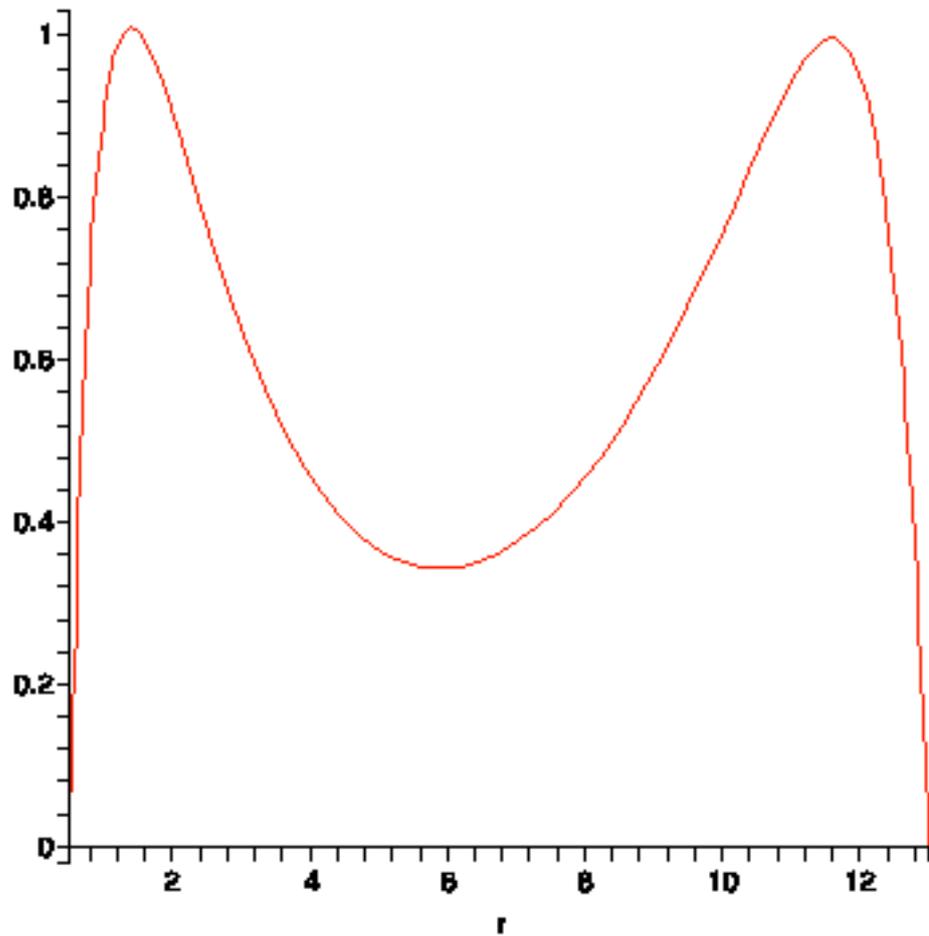
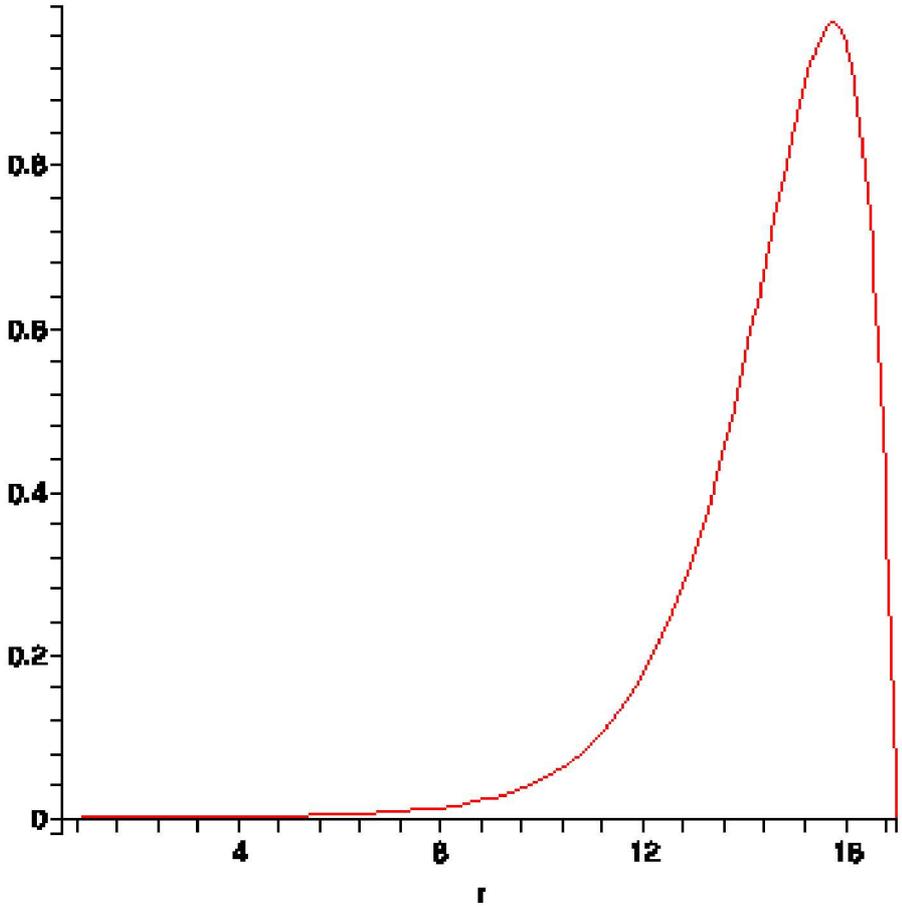
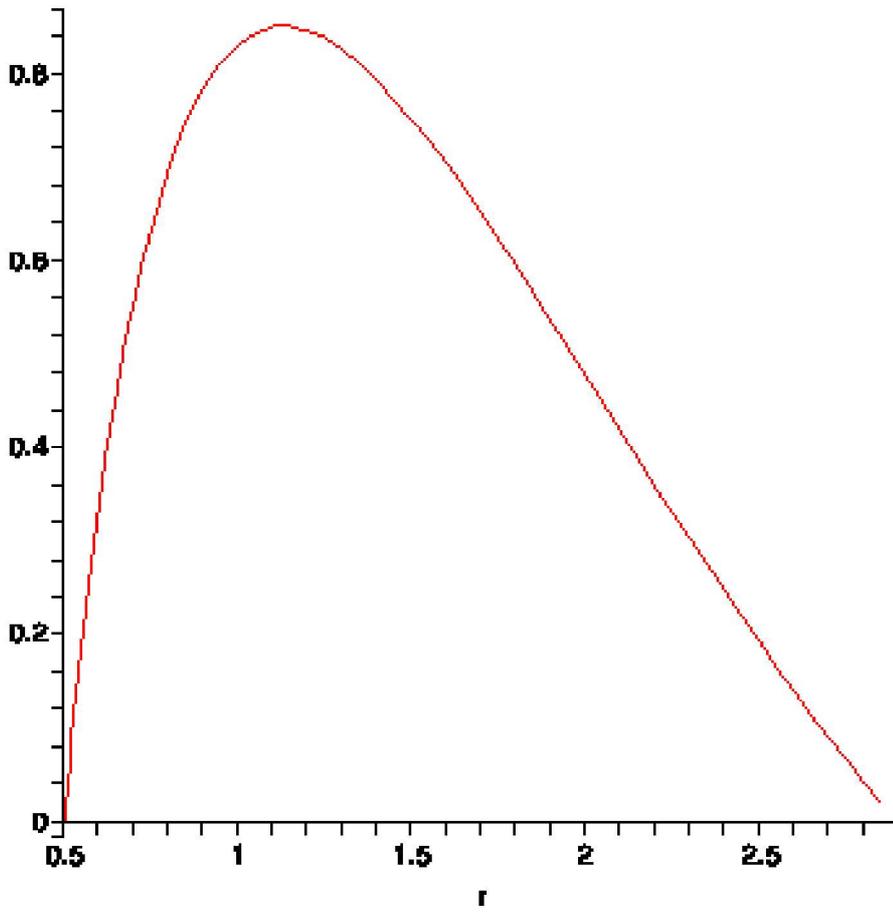


Figure 3: the ground state wavefunction for $R_1 = 0.5$ and $R_2 = 13$



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