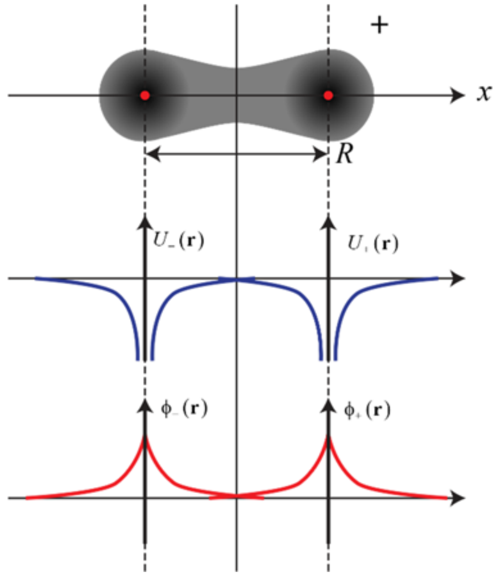
NANO 705-Notes

Hydrogen molecular ion

An appropriate basis

Molecular hydrogen is held together by covalent bonds. In fact, two hydrogen nuclei can remain bonded by a single electron in the H_2^+ molecular ion. The electron is shared by both protons, which are repelled from each other.



The electron wave function can be solved exactly using elliptical coordinates, which are quite cumbersome. We will show that a stable solution (with positive binding energy) is formed by a linear combination of the ground-state orbitals associated with each proton separately. Our goal is to establish the use of convenient basis states from which we can construct an approximate solution to a related problem of interest.

Formulation

The total energy relevant to the formation of the molecule includes the kinetic energy of the electron, the electrostatic potential energy between the electron and each proton, and the electrostatic repulsion between the protons. The hamiltonian is then

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + U_-(\mathbf{r}) + U_+(\mathbf{r}) + \frac{q^2}{4\pi\varepsilon_0 R}$$

where

$$U_\pm(\mathbf{r}) = U(|\mathbf{r} \mp \mathbf{R}/2|)$$

and

$$U(|\mathbf{r}|) = \frac{-q^2}{4\pi\varepsilon_0 r}$$

We use the H-atom ground-state orbitals as our basis functions. If the atom is centered at the origin, the wave function is

$$\phi(r) = \frac{1}{\sqrt{\pi} \cdot a_0^{3/2}} e^{-r/a_0}$$

In the molecule, we have one orbital centered around each nucleus

$$\phi_{\pm}(\mathbf{r}) = \phi(|\mathbf{r} \mp \mathbf{R}/2|)$$

The hamiltonian for each isolated atom is

$$\hat{H}_{\pm} = \frac{-\hbar^2}{2m}\nabla^2 + U(|\mathbf{r} \mp \mathbf{R}/2|)$$

Our basis consists of eigenfunctions of these separate hamiltonians

$$\hat{H}_{\pm}\phi_{\pm}(\mathbf{r}) = -E_0 \cdot \phi_{\pm}(\mathbf{r})$$

We will write the wave function for the molecule ion as

$$\psi(\mathbf{r}) = c_+\phi_+(\mathbf{r}) + c_-\phi_-(\mathbf{r})$$

This can be written in the $\phi_{\pm}$ basis as

$$\{\psi\} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

Basis functions

Let's look at the representation of a state in particular basis. We have

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle$$

Consider the expectation value

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{m,n} c_m^* c_n \langle\phi_m|\hat{H}|\phi_n\rangle}{\sum_{m,n} c_m^* c_n \langle\phi_m|\phi_n\rangle}$$

Identify the matrix elements in this basis: $[H]_{mn} = \langle\phi_m|\hat{H}|\phi_n\rangle$ and $[S]_{mn} = \langle\phi_m|\phi_n\rangle$.

$$E = \frac{\{\psi\}^\dagger [H]\{\psi\}}{\{\psi\}^\dagger [S]\{\psi\}}$$

For a given $[H]$ and $[S]$, we can find the $\{\psi\}$ satisfying $[H]\cdot\{\psi\} = E\cdot[S]\cdot\{\psi\}$. In this case, the expectation value is also the eigenvalue of $[S]^{-1}\cdot[H]$, i.e.,

$$[S]^{-1}\cdot[H]\cdot\{\psi\} = E\cdot\{\psi\}$$

These wavefunctions and their energies are not the eigenfunctions and eigenvalues of the actual hamiltonian, but provide a useful orthonormal set constructed from our selected basis functions.

Normalization

We can include a normalization constant in our wave function

$$|\,\psi\rangle = \frac{1}{Z}\sum_n c_n\,|\,\phi_n\rangle$$

If we want our wave function to be normalized, we need

$$1 = \langle\psi\,|\,\psi\rangle = \frac{1}{|Z|^2}\sum_{m,n} c_m{}^* c_n\,\langle\phi_m\,|\,\phi_n\rangle$$

so

$$|Z|^2 = \sum_{m,n} c_m{}^*\,[S]_{mn}\,c_n = \{\psi\}^\dagger[S]\{\psi\}$$

Within an arbitrary phase constant

$$Z = \sqrt{\{\psi\}^\dagger[S]\{\psi\}}$$

Solution

For the problem at hand

$$[H] = \begin{pmatrix} \langle\phi_+\,|\,\hat{H}\,|\,\phi_+\rangle & \langle\phi_+\,|\,\hat{H}\,|\,\phi_-\rangle \\ \langle\phi_-\,|\,\hat{H}\,|\,\phi_+\rangle & \langle\phi_-\,|\,\hat{H}\,|\,\phi_-\rangle \end{pmatrix}$$

and

$$[S] = \begin{pmatrix} \langle\phi_+\,|\,\phi_+\rangle & \langle\phi_+\,|\,\phi_-\rangle \\ \langle\phi_-\,|\,\phi_+\rangle & \langle\phi_-\,|\,\phi_-\rangle \end{pmatrix}$$

We can write

$$\hat{H} = \hat{H}_- + U_+(\mathbf{r}) + \frac{q^2}{4\pi\varepsilon_0 R} = \hat{H}_+ + U_-(\mathbf{r}) + \frac{q^2}{4\pi\varepsilon_0 R}$$

Let's first write the elements of $[S]$ as

$$[S] = \begin{pmatrix} 1 & s(R) \\ s(R) & 1 \end{pmatrix}$$

The diagonal elements in $[H]$ are

$$\begin{aligned}\langle\phi_-\,|\,\hat{H}\,|\,\phi_-\rangle\big(=\langle\phi_+\,|\,\hat{H}\,|\,\phi_+\rangle\big) &= \left\langle\phi_+\,|\,\hat{H}_+ + U_-(\mathbf{r}) + \frac{q^2}{4\pi\varepsilon_0 R}\,|\,\phi_+\right\rangle \\ &= \left(-E_0 + \frac{q^2}{4\pi\varepsilon_0 R}\right)\langle\phi_+\,|\,\phi_+\rangle + \langle\phi_+\,|U_-(\mathbf{r})\,|\,\phi_+\rangle \\ &= -E_0 + \frac{q^2}{4\pi\varepsilon_0 R} + a(R)\end{aligned}$$

and the off-diagonal elements are

$$\langle \phi_+ | \hat{H} | \phi_- \rangle \left(= \langle \phi_- | \hat{H} | \phi_+ \rangle \right) = \left\langle \phi_- | \hat{H}_+ + U_-(\mathbf{r}) + \frac{q^2}{4\pi\varepsilon_0 R} | \phi_+ \right\rangle$$

$$= \left(-E_0 + \frac{q^2}{4\pi\varepsilon_0 R} \right) \langle \phi_- | \phi_+ \rangle + \langle \phi_- | U_-(\mathbf{r}) | \phi_+ \rangle$$

$$= \left(-E_0 + \frac{q^2}{4\pi\varepsilon_0 R} \right) \cdot s(R) + b(R)$$

We can abbreviate

$$c = -E_0 + \frac{q^2}{4\pi\varepsilon_0 R} + a(R)$$

$$d = \left(-E_0 + \frac{q^2}{4\pi\varepsilon_0 R} \right) \cdot s(R) + b(R)$$

$$s = s(R)$$

giving

$$[H] = \begin{pmatrix} c & d \\ d & c \end{pmatrix}, \; [S] = \begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix}$$

Inverting gives

$$[S]^{-1} = \frac{1}{1-s^2} \begin{pmatrix} 1 & -s \\ -s & 1 \end{pmatrix}$$

Now

$$[S]^{-1} \cdot [H] = \frac{1}{1-s^2} \begin{pmatrix} c - sd & d - sc \\ d - sc & c - sd \end{pmatrix}$$

To solve the eigenvalue problem, we take

$$\det\left([S]^{-1} \cdot [H] - E[I] \right) = 0$$

which becomes

$$\det \begin{pmatrix} \dfrac{c-sd}{1-s^2} - E & \dfrac{d-sc}{1-s^2} \\ \dfrac{d-sc}{1-s^2} & \dfrac{c-sd}{1-s^2} - E \end{pmatrix} = 0$$

The eigenvalues are

$$E = \frac{c - sd \pm (d - sc)}{1-s^2} = \begin{cases} \dfrac{c-d}{1-s} = E_A \\ \dfrac{c+d}{1+s} = E_B \end{cases}$$

Notice

$$c+d=\left(-E_0+\frac{q^2}{4\pi\varepsilon_0 R}\right)\cdot[1+s(R)]+a(R)+b(R)$$

and

$$c-d=\left(-E_0+\frac{q^2}{4\pi\varepsilon_0 R}\right)\cdot[1-s(R)]+a(R)-b(R)$$

So our eigenvalues are

$$E_A(R)=-E_0+\frac{q^2}{4\pi\varepsilon_0 R}+\frac{a(R)-b(R)}{1-s(R)}$$

$$E_B(R)=-E_0+\frac{q^2}{4\pi\varepsilon_0 R}+\frac{a(R)+b(R)}{1+s(R)}$$

Wave functions
To find the wave functions for each eigenvalue, write

$$[S]^{-1}\cdot[H]\cdot\{\psi_{A,B}\}=E_{A,B}\cdot\{\psi_{A,B}\}$$

These give

$$\frac{1}{1-s^2}\cdot\begin{pmatrix} c-sd & d-sc \\ d-sc & c-sd \end{pmatrix}\cdot\begin{pmatrix} c_+ \\ c_- \end{pmatrix}=\frac{c\mp d}{1\mp s}\cdot\begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

These give

$$\{\psi_{A,B}\}=\frac{1}{Z_{A,B}}\cdot\begin{pmatrix} 1 \\ \mp 1 \end{pmatrix}$$

The normalization constants are

$$Z_{A,B}=\sqrt{\begin{pmatrix} 1 & \mp 1 \end{pmatrix}\begin{pmatrix} 1 & 1\mp s \\ 1\mp s & 1 \end{pmatrix}\cdot\begin{pmatrix} 1 \\ \mp 1 \end{pmatrix}}=\sqrt{2(1\mp s)}$$

The wave functions are then

$$\psi_{A,B}(\mathbf{r})=\frac{1}{\sqrt{2(1\mp s)}}\cdot[\phi_+(|\mathbf{r}-\mathbf{R}/2|)\mp\phi(|\mathbf{r}+\mathbf{R}/2|)]$$

Evaluation
We will need to perform the integrals for $a(R)$, $b(R)$, and $s(R)$ to interpret these results. First

$$a(R) = \langle \phi_- | U_+(\mathbf{r}) | \phi_- \rangle$$
$$= \int_{\mathbf{r}} d^3r \left(\frac{1}{\pi \cdot a_0{}^3}\right) \cdot \left(\frac{-q^2}{4\pi\varepsilon_0}\right) \cdot \frac{1}{|\mathbf{r} - \mathbf{R}/2|} \cdot \mathrm{e}^{-2|\mathbf{r}+\mathbf{R}/2|/a_0}$$
$$a(R) = \frac{-q^2}{4\pi^2\varepsilon_0 \cdot a_0{}^3} \cdot \int_{\mathbf{r}} d^3r \frac{1}{|\mathbf{r} - \mathbf{R}|} \cdot \mathrm{e}^{-2r/a_0}$$

We can choose to orient $\mathbf{R}$ along the z axis. Then do the ϕ integral.

$$a(R) = \frac{-q^2}{2\pi\varepsilon_0 \cdot a_0{}^3} \cdot \int_{r=0}^{\infty} dr \cdot r^2 \cdot \mathrm{e}^{-2r/a_0} \int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{1}{\sqrt{r^2 + R^2 - 2rR\cos\theta}}$$

We showed that

$$\int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{1}{\sqrt{r^2 + R^2 - 2rR\cos\theta}} = \frac{r + R - |r - R|}{rR}$$

We can break the r integral into the ranges $r \le R$ and $r > R$

$$a(R) = \frac{-q^2}{\pi\varepsilon_0 \cdot a_0{}^3} \cdot \left[\left(\frac{1}{R}\right) \cdot \int_{r=0}^{R} dr \cdot r^2 \cdot \mathrm{e}^{-2r/a_0} + \int_{r=R}^{\infty} dr \cdot r \cdot \mathrm{e}^{-2r/a_0}\right]$$

Let's define $\alpha = 2/a_0$ and $y = \alpha r$. Finally

$$a(R) = \frac{-q^2}{\pi\varepsilon_0 \cdot a_0{}^3 \cdot \alpha^3 \cdot R} \cdot \left[\int_{r=0}^{\alpha R} dy \cdot y^2 \cdot \mathrm{e}^{-y} + \alpha R \cdot \int_{r=\alpha R}^{\infty} dy \cdot y \cdot \mathrm{e}^{-y}\right]$$
$$a(R) = \frac{-q^2}{4\pi\varepsilon_0 R} \cdot \left[1 - \left(1 + \frac{R}{a_0}\right) \cdot \mathrm{e}^{-2R/a_0}\right]$$

Next we find the "exchange" integral

$$b(R) = \langle \phi_+ | U_+(\mathbf{r}) | \phi_- \rangle$$
$$= \int_{\mathbf{r}} d^3r \left(\frac{1}{\pi \cdot a_0{}^3}\right) \cdot \left(\frac{-q^2}{4\pi\varepsilon_0}\right) \cdot \frac{1}{|\mathbf{r} - \mathbf{R}/2|} \cdot \mathrm{e}^{-(|\mathbf{r}-\mathbf{R}/2|+|\mathbf{r}+\mathbf{R}/2|)/a_0}$$
$$b(R) = \frac{-q^2}{4\pi^2\varepsilon_0 \cdot a_0{}^3} \cdot \int_{\mathbf{r}} d^3r \frac{1}{|\mathbf{r} - \mathbf{R}|} \cdot \mathrm{e}^{-(r+|\mathbf{r}-\mathbf{R}|)/a_0}$$

We again choose to orient $\mathbf{R}$ along the z axis and do the ϕ integral.

$$b(R) = \frac{-q^2}{2\pi\varepsilon_0 \cdot a_0{}^3} \cdot \int_{r=0}^{\infty} dr \cdot r^2 \cdot \mathrm{e}^{-r/a_0} \int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{\mathrm{e}^{-\sqrt{r^2+R^2-2rR\cos\theta}/a_0}}{\sqrt{r^2 + R^2 - 2rR\cos\theta}}$$

The second integral gives

$$\int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{\mathrm{e}^{-\sqrt{r^2+R^2-2rR\cos\theta}/a_0}}{\sqrt{r^2 + R^2 - 2rR\cos\theta}} = -\frac{a_0{}^2}{rR}\left(\mathrm{e}^{-(r+R)/a_0} - \mathrm{e}^{-|r-R|/a_0}\right)$$

Again splitting the integral into two ranges

$$b(R)=\frac{-q^2}{\pi\varepsilon_0\cdot R\cdot a_0{}^2}\cdot\left[\int_{r=0}^{R}dr\cdot r\cdot \mathrm{e}^{-(r+R)/a_0}\cdot\sinh\left(\frac{r}{a_0}\right)+\int_{r=R}^{\infty}dr\cdot r\cdot \mathrm{e}^{-2r/a_0}\cdot\sinh\left(\frac{R}{a_0}\right)\right]$$

$$b(R)=\frac{-q^2}{4\pi\varepsilon_0\cdot a_0}\cdot\left(1+\frac{R}{a_0}\right)\cdot \mathrm{e}^{-R/a_0}$$

Lastly, we address the "overlap" integral

$$\begin{aligned} s(R)&=\langle\phi_+\mid\phi_-\rangle\\ &=\int_{\mathbf{r}}d^3r\left(\frac{1}{\pi\cdot a_0{}^3}\right)\cdot \mathrm{e}^{-(|\mathbf{r}-\mathbf{R}/2|+|\mathbf{r}+\mathbf{R}/2|)/a_0}\\ &=\frac{1}{\pi\cdot a_0{}^3}\cdot\int_{\mathbf{r}}d^3r\cdot \mathrm{e}^{-(r+|\mathbf{r}-\mathbf{R}|)/a_0}\end{aligned}$$

$$s(R)=\frac{2}{a_0{}^3}\cdot\int_{r=0}^{\infty}dr\cdot r^2\cdot \mathrm{e}^{-r/a_0}\int_{\theta=0}^{\pi}d\theta\cdot\sin\theta\cdot \mathrm{e}^{-\sqrt{r^2+R^2-2rR\cos\theta}/a_0}$$

Let's do the θ integral.

$$\int_{\theta=0}^{\pi}d\theta\cdot\sin\theta\cdot \mathrm{e}^{-\sqrt{r^2+R^2-2rR\cos\theta}/a_0}=\frac{-a_0{}^2}{rR}\cdot\left[\left(1+\frac{r+R}{a_0}\right)\cdot \mathrm{e}^{-(r+R)/a_0}-\left(1+\frac{|r-R|}{a_0}\right)\cdot \mathrm{e}^{-|r-R|/a_0}\right]$$

We can then break the r integral into three terms:

$$s_1(R)=\frac{2}{a_0{}^3}\cdot\int_{r=0}^{\infty}dr\cdot r^2\cdot \mathrm{e}^{-r/a_0}\left[\frac{-a_0{}^2}{rR}\cdot\left(1+\frac{r+R}{a_0}\right)\cdot \mathrm{e}^{-(r+R)/a_0}\right]$$

$$s_{2a}(R)=\frac{2}{a_0{}^3}\cdot\int_{r=0}^{R}dr\cdot r^2\cdot \mathrm{e}^{-r/a_0}\left[\frac{a_0{}^2}{rR}\cdot\left(1+\frac{R-r}{a_0}\right)\cdot \mathrm{e}^{-(R-r)/a_0}\right]$$

$$s_{2b}(R)=\frac{2}{a_0{}^3}\cdot\int_{r=R}^{\infty}dr\cdot r^2\cdot \mathrm{e}^{-r/a_0}\left[\frac{a_0{}^2}{rR}\cdot\left(1+\frac{r-R}{a_0}\right)\cdot \mathrm{e}^{-(r-R)/a_0}\right]$$

where $s(R)=s_1(R)+s_{2a}(R)+s_{2b}(R)$. These give

$$s_1(R)=-\left(\frac{1}{2}+\frac{a_0}{R}\right)\cdot \mathrm{e}^{-R/a_0}$$

$$s_{2a}(R)=\left(\frac{R}{a_0}+\frac{R^2}{3a_0{}^2}\right)\cdot \mathrm{e}^{-R/a_0}$$

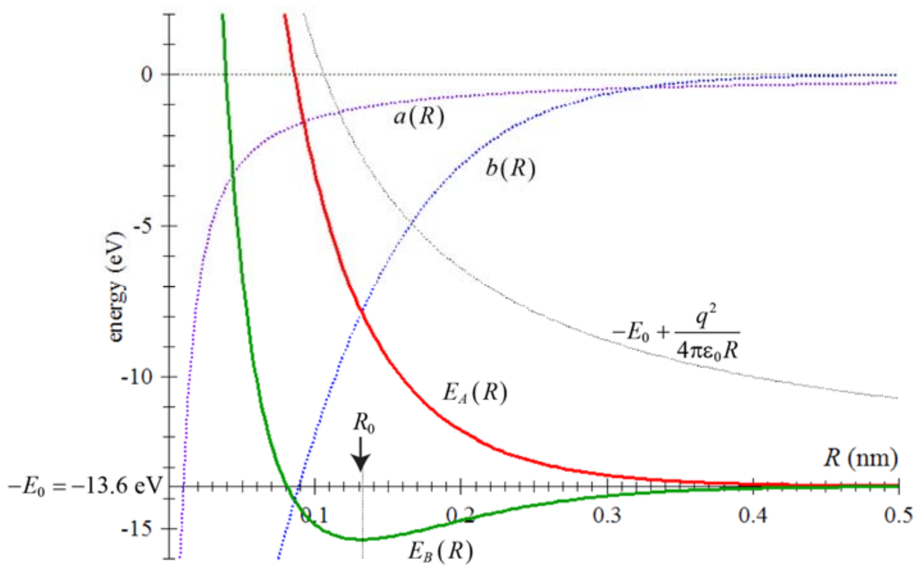
$$s_{2b}(R)=\left(\frac{3}{2}+\frac{a_0}{R}\right)\cdot \mathrm{e}^{-R/a_0}$$

The final result for the overlap integral is

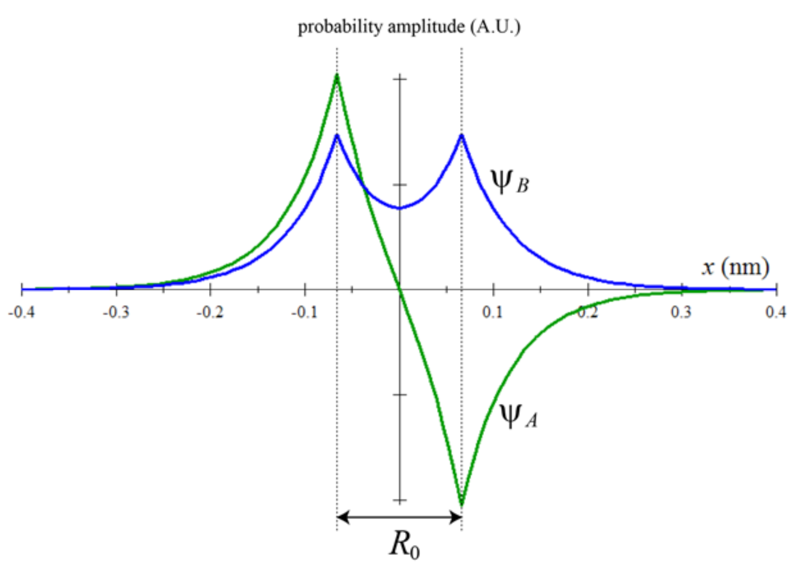
$$s(R)=\left(1+\frac{R}{a_0}+\frac{R^2}{3a_0{}^2}\right)\cdot \mathrm{e}^{-R/a_0}$$

Bound state

Now we can investigate whether a bound state ($E < -E_0$) exists for either the E_A or E_B solutions at some value of R and use the variational principle to minimize the total energy. Plotting these quantities shows that only the symmetric (E_B) solution has a minimum energy lower than that of an isolated, neutral H atom and distant proton. Using these basis functions, the optimal separation of the protons is 0.132 nm and the ground-state energy is -15.37 eV. That can be taken as an upper limit on the actual ground-state energy, which will always be lower than the expectation value found from an approximate solution.



Now we can plot the wave functions ψ_A and ψ_B, referred to as the *anti-bonding* and *bonding* orbitals, respectively, for the optimal nucleus separation R_0 (which is, in fact, applicable only to ψ_B.)



We see that ψ_A has a node at the midpoint between the nuclei, whereas ψ_B does not.

Integrals
Find

$$I_n = \int_y dy \cdot y^n \cdot \mathrm{e}^{-y}$$

where $n \in \mathbb{Z}^+$. It is easy to see that

$$I_0 = \int_y dy \cdot \mathrm{e}^{-y} = -\mathrm{e}^{-y}$$

What is I_1? We can integrate by parts: $\int u \cdot dv = u \cdot v - \int v \cdot du$, using $u = y$ and $v = -\mathrm{e}^{-y}$. Then $du = dy$ and $dv = \mathrm{e}^{-y}$. So

$$I_1 = -y \cdot \mathrm{e}^{-y} + I_0 = -(y+1) \cdot \mathrm{e}^{-y}$$

Now find I_2: Take $u = y^2$ and $v = -\mathrm{e}^{-y}$. Then $du = 2y \cdot dy$ and $dv = \mathrm{e}^{-y}$. So

$$I_2 = -y^2 \cdot \mathrm{e}^{-y} + 2I_1 = -\left(y^2 + 2y + 1\right) \cdot \mathrm{e}^{-y}$$

This process can be continued to any positive integer n, if needed.

Integral

$$I = \int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{1}{\sqrt{r^2 + R^2 - 2rR\cos\theta}}$$

Define $x = -\cos\theta$, $dx = d\theta \cdot \sin\theta$ and $A = r^2 + R^2$, $B = 2rR$.

$$\begin{aligned}
I &= \int_{x=-1}^{1} dx \cdot \frac{1}{\sqrt{A + Bx}} \\
&= \frac{2}{B} \cdot \sqrt{A + Bx}\Big|_{x=-1}^{1} \\
&= \frac{2}{B} \cdot \left(\sqrt{A+B} - \sqrt{A - Bx}\right) \\
&= \frac{1}{rR} \cdot \left(\sqrt{r^2 + R^2 + 2rR} - \sqrt{r^2 + R^2 - 2rR}\right) \\
&= \frac{r + R - |r - R|}{rR} \\
&= \frac{1}{R} + \frac{1}{r} - \left|\frac{1}{R} - \frac{1}{r}\right|
\end{aligned}$$

$$I = \begin{cases} 2/r, & r \le R \\ 2/R, & R < r \end{cases}$$

Integral
Find

$$I = \int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \mathrm{e}^{-\sqrt{r^2 + R^2 - 2rR\cos\theta}}$$

Let's use the definitions $A = \left(r^2 + R^2\right) \big/ {a_0}^2$, $B = 2rR \big/ {a_0}^2$

$$I = \int_{x=-1}^{1} dx \cdot \mathrm{e}^{-\sqrt{A+Bx}}$$

Define $z = \sqrt{A+Bx}$. Then $x = \left(z^2 - A\right) \big/ B$ and $dx = 2z \cdot dz \big/ B$. The integral becomes

$$\begin{aligned}
I &= \frac{2}{B} \int_{z}^{z} dz \cdot z \cdot \mathrm{e}^{-z} \\
&= -\frac{2}{B} \cdot (z+1) \cdot \mathrm{e}^{-z} \Big|_{z} \\
&= -\frac{2}{B} \cdot \left(\sqrt{A+Bx} + 1\right) \cdot \mathrm{e}^{-\sqrt{A+Bx}} \Big|_{x=-1}^{1} \\
I &= -\frac{{a_0}^2}{rR} \cdot \left[\left(\frac{r+R}{a_0} + 1 \right) \cdot \mathrm{e}^{-(r+R)/a_0} - \left(\frac{|r-R|}{a_0} + 1 \right) \cdot \mathrm{e}^{-|r-R|/a_0} \right]
\end{aligned}$$

Integral
Find

$$I = \int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \frac{\mathrm{e}^{-\sqrt{r^2+R^2-2rR\cos\theta}/a_0}}{\sqrt{r^2+R^2-2rR\cos\theta}} = -\frac{{a_0}^2}{rR} \left(\mathrm{e}^{-(r+R)/a_0} - \mathrm{e}^{-|r-R|/a_0} \right)$$

Again take $A = \left(r^2 + R^2\right) \big/ {a_0}^2$, $B = 2rR \big/ {a_0}^2$.

$$I = \int_{x=-1}^{1} dx \cdot \frac{\mathrm{e}^{-\sqrt{A+Bx}}}{\sqrt{A+Bx}}$$

We don't need any tricks here. The result is

$$\begin{aligned}
I &= \int_{x=-1}^{1} dx \cdot \frac{\mathrm{e}^{-\sqrt{A+Bx}}}{\sqrt{A+Bx}} \\
&= \frac{-2}{B} \mathrm{e}^{-\sqrt{A+Bx}} \Big|_{x=-1}^{1} = \frac{-2}{B} \left(\mathrm{e}^{-\sqrt{A+B}} - \mathrm{e}^{-\sqrt{A-B}} \right) \\
I &= -\frac{{a_0}^2}{rR} \left(\mathrm{e}^{-(r+R)/a_0} - \mathrm{e}^{-|r-R|/a_0} \right)
\end{aligned}$$