I. Degenerate Perturbation Theory

Consider a free particle in a one-dimensional periodic ring $-L/2 \leq x \leq L/2$. The energy eigenstates are $\psi_n(x) = e^{2\pi inx/L}/\sqrt{L}$ for integer n. These eigenstates are doubly-degenerate for nonzero n. Let there be a perturbing potential $V = V_0 e^{-x^2/a^2}$ with $0 < V_0 \ll 2\pi^2\hbar^2/(mL^2)$: there is a small Gaussian barrier at $x = 0$.

(a) Calculate the first-order correction to the the energy eigenvalue E_n for the degenerate situations $n \neq 0$.

Solution:
We recast the eigenstates to state kets as follows:

$$\langle x|n\rangle = \psi_n(x) = e^{2\pi inx/L}/\sqrt{L} \tag{1}$$

Note that this is doubly degenerate since the eigenstates with integer n are linearly independent to the eigenstates with integer -n . This can also be seen from the form of the system's energy given by $E_n = n^2[2\pi^2\hbar^2/(mL^2)]$ in which we see that ψ_n and ψ_{-n} lead to the same energy, assuming that the system is unperturbed. With the given pertubation, we construct the following perturbation matrix:

$$V = \begin{bmatrix} \langle n|V|n\rangle & \langle n|V|-n\rangle \\ \langle -n|V|n\rangle & \langle -n|V|-n\rangle \end{bmatrix} \tag{2}$$

We will assume that $a \ll L$ so that we can extend the interval $-L/2 \leq x \leq L/2$ to $-\infty \leq x \leq \infty$ for convenience. This is valid as the perturbation is zero outside $-a \leq x \leq a$. On that note, it is useful to have the result of a Gaussian integral as reference:

$$\int_{-\infty}^{\infty} e^{-\gamma x^2 \mathrm{d}x} = \sqrt{\frac{\pi}{\gamma}}, \tag{3}$$

We then evaluate the first element of the matrix to be

$$\begin{aligned} \langle n|V|n\rangle &= \int_{-\infty}^{\infty} (\psi_n)^* V \psi_n \, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{L}} e^{2\pi inx/L}\right)^* V_0 e^{-x^2/a^2} \frac{1}{\sqrt{L}} e^{2\pi inx/L} \, \mathrm{d}x \\ &= \frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2} \, \mathrm{d}x \\ \langle n|V|n\rangle &= \frac{V_0}{L} a\sqrt{\pi} \end{aligned} \tag{4}$$

in which we applied Eq. (3). In the same manner, we can evaluate the last element to be

$$\langle -n|V|-n\rangle = \frac{V_0}{L} a\sqrt{\pi} \tag{5}$$

As for the second element, we have

$$\begin{aligned}
\langle -n|V|n\rangle &= \int_{-\infty}^{\infty} (\psi_{-n})^* V \psi_n \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{L}} e^{-2\pi inx/L}\right)^* V_0 e^{-x^2/a^2} \frac{1}{\sqrt{L}} e^{2\pi inx/L} \,\mathrm{d}x \\
&= \frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2 + 4\pi inx/L} \,\mathrm{d}x \\
\langle -n|V|n\rangle &= \frac{V_0}{L} \int_{-\infty}^{\infty} e^{-ux^2 + vx} \,\mathrm{d}x
\end{aligned} \tag{6}$$

after replacing the following variables for easier calculation:

$$u = \frac{1}{\alpha^2}, \qquad v = \frac{4\pi inx}{L} \tag{7}$$

Then, $\langle -n|V|n\rangle$ becomes

$$\begin{aligned}
\langle -n|V|n\rangle &= \frac{V_0}{L} \int_{-\infty}^{\infty} e^{-u\left(x^2 + \frac{v}{u}x\right)} \,\mathrm{d}x \\
&= \frac{V_0}{L} \int_{-\infty}^{\infty} e^{-u\left(x^2 + \frac{v}{u}x + \left(\frac{v}{2u}\right)^2 - \left(\frac{v}{2u}\right)^2\right)} \,\mathrm{d}x \\
&= \frac{V_0}{L} e^{u\left(\frac{v}{2u}\right)^2} \int_{-\infty}^{\infty} e^{-u\left(x^2 - \frac{v}{2u}\right)^2} \,\mathrm{d}x \\
&= \frac{V_0}{L} e^{u\left(\frac{v}{2u}\right)^2} \int_{-\infty}^{\infty} e^{-uy^2} \,\mathrm{d}y \\
\langle -n|V|n\rangle &= \frac{V_0}{L} e^{u\left(\frac{v}{2u}\right)^2} \sqrt{\frac{\pi}{u}}
\end{aligned} \tag{8}$$

Substituting back u and v, we obtain

$$\langle -n|V|n\rangle = \frac{V_0}{L} a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \tag{9}$$

In the same manner, we can calculate that

$$\langle n|V|-n\rangle = \frac{V_0}{L} a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \tag{10}$$

Now, we assume that the linear combination of eigenstates that can lift the degeneracy is of the form

$$\psi = \alpha\psi_n + \beta\psi_{-n} \tag{11}$$

Then, the first order correction to the energy can be obtained from the eigenvalue problem:

$$\begin{bmatrix} \langle n|V|n\rangle & \langle n|V|-n\rangle \\ \langle -n|V|n\rangle & \langle -n|V|-n\rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E_n^{(1)} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \tag{12}$$

which can be written as

$$\begin{bmatrix} \frac{V_0}{L} a\sqrt{\pi} - E_n^{(1)} & \frac{V_0}{L} a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L} a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L} a\sqrt{\pi} - E_n^{(1)} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0 \tag{13}$$

We need to evaluate the determinant of the given matrix:

$$\begin{vmatrix} \frac{V_0}{L}a\sqrt{\pi} - E_n^{(1)} & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi} - E_n^{(1)} \end{vmatrix} = 0 \tag{14}$$

To do this, we calculate the determinant of a simpler 2×2 matrix as

$$\begin{aligned} \begin{vmatrix} A-\lambda & B \\ C & D-\lambda \end{vmatrix} &= 0 \\ (A-\lambda)(D-\lambda) - BC &= 0 \\ \lambda^2 - (A+D)\lambda + AD - BC &= 0 \end{aligned} \tag{15}$$

With the quadratic equation, the eigenvalue λ is given by

$$\begin{aligned} \lambda &= \frac{-(-(A+D)) \pm \sqrt{(A+D)^2 - 4(AD-BC)}}{2} \\ &= \frac{A+D \pm \sqrt{A^2+D^2+2AD-4(AD-BC)}}{2} \\ &= \frac{1}{2}\left[A+D \pm \sqrt{A^2+D^2+2AD-4(AD-BC)}\right] \\ \lambda &= \frac{1}{2}\left[A+D \pm \sqrt{(A-D)^2+4BC}\right] \end{aligned} \tag{16}$$

If we apply this to our problem, we know that $A = D$ and $B = C$. Thus,

$$\lambda = \frac{1}{2}\left[2A \pm \sqrt{4B^2}\right] = \frac{1}{2}\left[2A \pm 2B\right] = A \pm B \tag{17}$$

Therefore, the first-order correction to the eigenvalue energy is calculated to be

$$E_n^{(1),\pm} = \frac{V_0}{L}a\sqrt{\pi} \pm \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} = \frac{V_0}{L}a\sqrt{\pi}\left(1 \pm e^{-\left(\frac{2\pi na}{L}\right)^2}\right) \tag{18}$$

(b) Obtain the linear combination of ψ_n and ψ_{-n} that diagonalize the perturbation matrix.

Solution:
Substituting $E_n^{(1),+}$ to Eq. (13), we have

$$\begin{aligned} \begin{bmatrix} \frac{V_0}{L}a\sqrt{\pi} - \frac{V_0}{L}a\sqrt{\pi}\left(1 + e^{-\left(\frac{2\pi na}{L}\right)^2}\right) & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi} - \frac{V_0}{L}a\sqrt{\pi}\left(1 + e^{-\left(\frac{2\pi na}{L}\right)^2}\right) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} &= 0 \\ \begin{bmatrix} -\frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & -\frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} &= 0 \end{aligned} \tag{19}$$

By solving this linear system of equations, we find that $\beta = \alpha$. As for $E_n^{(1),-}$, we get

$$\begin{aligned} \begin{bmatrix} \frac{V_0}{L}a\sqrt{\pi} - \frac{V_0}{L}a\sqrt{\pi}\left(1 - e^{-\left(\frac{2\pi na}{L}\right)^2}\right) & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi} - \frac{V_0}{L}a\sqrt{\pi}\left(1 - e^{-\left(\frac{2\pi na}{L}\right)^2}\right) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} &= 0 \\ \begin{bmatrix} \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \\ \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} & \frac{V_0}{L}a\sqrt{\pi}\, e^{-\left(\frac{2\pi na}{L}\right)^2} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} &= 0 \end{aligned} \tag{20}$$

In the same manner, we find that $\beta = -\alpha$. Now, we need to normalize the obtained eigenvectors. To do this, we let α be real for simplicity. Then, with the normalization condition, we have

$$\begin{aligned} |\alpha|^2 + |\beta|^2 &= 1 \\ |\alpha|^2 + |\pm\alpha|^2 &= 1 \\ 2\alpha^2 &= 1 \quad \longrightarrow \quad \alpha = \frac{1}{\sqrt{2}} \end{aligned} \tag{21}$$

Recall that the linear combination of the degenerate eigenstates is of the form in Eq. (11). Thus, we get

$$\begin{aligned} \psi_+ &= \frac{1}{\sqrt{2}}\psi_n + \frac{1}{\sqrt{2}}\psi_{-n} \\ &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}e^{2\pi inx/L} + \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}e^{-2\pi inx/L} \\ &= \frac{1}{\sqrt{2L}}\left(e^{2\pi inx/L} + e^{-2\pi inx/L}\right) \\ \psi_+ &= \sqrt{\frac{2}{L}}\cos\frac{2\pi nx}{L} \end{aligned} \tag{22}$$

as the eigenstate associated to $E_n^{(1),+}$ while we have

$$\begin{aligned} \psi_- &= \frac{1}{\sqrt{2}}\psi_n - \frac{1}{\sqrt{2}}\psi_{-n} \\ &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}e^{2\pi inx/L} - \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}e^{-2\pi inx/L} \\ &= \frac{1}{\sqrt{2L}}\left(e^{2\pi inx/L} - e^{-2\pi inx/L}\right) \\ &= \frac{1}{\sqrt{2L}}2i\sin\frac{2\pi nx}{L} \\ \psi_+ &= i\sqrt{\frac{2}{L}}\sin\frac{2\pi nx}{L} \end{aligned} \tag{23}$$

as the eigenstate associated to $E_n^{(1),-}$.

II. Variational Method

Use a Gaussian trial wavefunction to estimate the ground state energy of a bound electron in a hydrogen atom.

(a) Compare your result with the exact ground state energy -1 Ry (as a dimensionless ratio).

Solution:

A Gaussian wavefunction is usually of the form

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} \tag{24}$$

To mimic this, we let our trial wavefunction to be of the form

$$\langle r|\alpha\rangle = \psi(r) = Ne^{-r^2/\beta^2} \tag{25}$$

in which it is recasted as a state ket. Note that N is a normalization constant. Also, it is useful have the following variations of the Gaussian integral as reference for later calculations:

$$\int_0^\infty e^{-ar^2}\mathrm{d}r = \frac{1}{2}\sqrt{\frac{\pi}{a}}, \quad \int_0^\infty r^2 e^{-ar^2}\mathrm{d}r = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}, \quad \int_0^\infty r^4 e^{-ar^2}\mathrm{d}r = \frac{3}{8}\sqrt{\frac{\pi}{a^5}} \tag{26}$$

$$\int_0^\infty r e^{-ar^2}\mathrm{d}r = \frac{1}{2a} \tag{27}$$

Now, we want to calculate N. Using the normalization condition, we have

$$\begin{aligned} \int (\psi)^* \psi \, \mathrm{d}\mathcal{V} &= 1 \\ \left(\int_0^{2\pi} \mathrm{d}\phi\right)\left(\int_0^{\pi} \sin\theta \, \mathrm{d}\theta\right)\left(\int_0^\infty \left(Ne^{-r^2/\beta^2}\right)^* Ne^{-r^2/\beta^2} r^2 \, \mathrm{d}r\right) &= 1 \\ 4\pi N^2 \int_0^\infty r^2 e^{-2r^2/\beta^2} \, \mathrm{d}r &= 1 \\ 4\pi N^2 \cdot \frac{1}{4}\sqrt{\pi\left(\frac{\beta^2}{2}\right)^3} &= 1 \end{aligned} \tag{28}$$

in which we applied Eq. (26). Thus, we get

$$N = \sqrt[4]{\left(\frac{2}{\pi\beta^2}\right)^3} \tag{29}$$

Note that the Hamiltonian of this system is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 - k\frac{e^2}{r} \tag{30}$$

where $k = 1/(4\pi\epsilon_0)$. In spherical coordinates, ∇^2 is of the form

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{31}$$

To obtain the energy associated with the trial wavefunction, we calculate for the expectation value of the Hamiltonian

$$E = \langle\alpha|H|\alpha\rangle = \langle\alpha|T|\alpha\rangle + \langle\alpha|V|\alpha\rangle \tag{32}$$

The kinetic energy term leads to

$$
\begin{aligned}
\langle\alpha|T|\alpha\rangle &= \int (\psi)^* T\psi \, \mathrm{d}\mathcal{V} \\
&= \left(\int_0^{2\pi} \mathrm{d}\phi\right)\left(\int_0^{\pi} \sin\theta \, \mathrm{d}\theta\right)\left(\int_0^{\infty} \left(Ne^{-r^2/\beta^2}\right)^* \left(-\frac{\hbar^2}{2m}\nabla^2 Ne^{-r^2/\beta^2}\right) r^2 \, \mathrm{d}r\right) \\
&= -\frac{\hbar^2}{2m}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot 4\pi \int_0^{\infty} e^{-r^2/\beta^2} \left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} e^{-r^2/\beta^2}\right)\right) r^2 \, \mathrm{d}r \\
&= -\frac{\hbar^2}{2m}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot 4\pi \left[-\frac{2}{\beta^2}\int_0^{\infty} e^{-r^2/\beta^2}\left(\frac{\partial}{\partial r} r^3 e^{-r^2/\beta^2}\right) \mathrm{d}r\right] \\
&= \frac{\hbar^2}{2m}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot \frac{8\pi}{\beta^2}\left[-\frac{2}{\beta^2}\int_0^{\infty} r^4 e^{-2r^2/\beta^2} \, \mathrm{d}r + 3\int_0^{\infty} r^2 e^{-2r^2/\beta^2} \, \mathrm{d}r\right] \\
&= \frac{\hbar^2}{2m}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot \frac{8\pi}{\beta^2}\left[-\frac{2}{\beta^2}\left(\frac{3}{8}\sqrt{\pi\left(\frac{\beta^2}{2}\right)^5}\right) + 3\left(\frac{1}{4}\sqrt{\pi\left(\frac{\beta^2}{2}\right)^3}\right)\right] \\
&= \frac{\hbar^2}{2m}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot \frac{8\pi}{\beta^2}\left[-\frac{3}{8} + \frac{3}{4}\right]\sqrt{\pi\left(\frac{\beta^2}{2}\right)^3} \\
\langle\alpha|T|\alpha\rangle &= \frac{3\hbar^2}{2m\beta^2}
\end{aligned}
\tag{33}
$$

in which we applied the integrals in Eq. (26). Note that ∇^2 reduces to its first term in Eq. (31) since the wavefunction is only dependent on r. As for the potential energy term, we have

$$
\begin{aligned}
\langle\alpha|V|\alpha\rangle &= \int (\psi)^* V\psi \, \mathrm{d}\mathcal{V} \\
&= \left(\int_0^{2\pi} \mathrm{d}\phi\right)\left(\int_0^{\pi} \sin\theta \, \mathrm{d}\theta\right)\left(\int_0^{\infty} \left(Ne^{-r^2/\beta^2}\right)^* \left(-k\frac{e^2}{r} Ne^{-r^2/\beta^2}\right) r^2 \, \mathrm{d}r\right) \\
&= -k\frac{e^2}{r}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot 4\pi \int_0^{\infty} r \, e^{-2r^2/\beta^2} \, \mathrm{d}r \\
&= -k\frac{e^2}{r}\sqrt{\left(\frac{2}{\pi\beta^2}\right)^3} \cdot 4\pi \left(\frac{1}{2}\frac{\beta^2}{2}\right) \\
\langle\alpha|V|\alpha\rangle &= -k\frac{2e^2}{\beta}\sqrt{\frac{2}{\pi}}
\end{aligned}
\tag{34}
$$

in which we applied an integral in Eq. (27). Substituting in Eqs. (33) and (34) to Eq. (32), we have

$$
E = \frac{3\hbar^2}{2m\beta^2} - k\frac{2e^2}{\beta}\sqrt{\frac{2}{\pi}} \tag{35}
$$

We need to minimize this with respect to β as follows:

$$
\frac{\partial E}{\partial \beta} = -2\frac{3\hbar^2}{2m\beta^3} - (-1)k\frac{2e^2}{\beta^2}\sqrt{\frac{2}{\pi}} = 0 \tag{36}
$$

in which we obtain β as

$$\beta = \frac{1}{k}\frac{3\hbar^2}{2e^2 m}\sqrt{\frac{\pi}{2}} \tag{37}$$

Substituting β to Eq. (35), we have

$$\begin{aligned} E_{\text{min}} &= \frac{3\hbar^2}{2m}\left(k\frac{2e^2 m}{3\hbar^2}\sqrt{\frac{2}{\pi}}\right)^2 - 2ke^2\sqrt{\frac{2}{\pi}}\left(k\frac{2e^2 m}{3\hbar^2}\sqrt{\frac{2}{\pi}}\right) \\ &= k^2 e^4 \frac{2m}{3\hbar^2}\frac{2}{\pi} - 2k^2 e^4 \frac{2m}{3\hbar^2}\frac{2}{\pi} \\ E_{\text{min}} &= -\frac{4}{3\pi}\frac{k^2 m e^4}{\hbar^2} \end{aligned} \tag{38}$$

Note that the energy of this system is given by

$$E_n = -\frac{hcR_H}{n} \tag{39}$$

where the Ryberg constant is

$$R_H = \frac{me^4}{8\epsilon_0^2 h^3 c} \tag{40}$$

Thus, the exact ground state is of the form

$$E_{\text{gs}} = -hcR_H = -hc\frac{me^4}{8\epsilon_0^2 h^3 c} = -\frac{me^4}{8\epsilon_0^2 h^2} = -\frac{me^4}{2\cdot 2^2\epsilon_0^2(2\pi\hbar)^2} = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2} = -\frac{1}{2}\frac{k^2 m e^4}{\hbar^2} \tag{41}$$

Comparing this to our obtained E_{min}, we have

$$E_{\text{min}} = \frac{4}{3\pi}\cdot 2E_{\text{gs}} \approx 0.85 E_{\text{gs}} \tag{42}$$

We know that $E_{\text{gs}} = -1\,\text{Ry}$. Then, we get

$$E_{\text{min}} \approx -0.85\,\text{Ry} \tag{43}$$

which is higher than the exact ground energy. This is expected as it is proven that, depending on the used trial wavefunction, the expectation value of the Hamiltonian will result to the ground state energy or be an overestimate of this energy. In this sense, this also shows that a Gaussian wavefunction is not the form of the actual ground state for the given system.

(b) Compare the standard deviation of this Gaussian with the Bohr radius a_0 (as a dimensionless ratio).

Solution:
Recall the form of the Gaussian wavefunction in Eq. (24). We can calculate for the standard deviation σ by either comparing its normalization constant or the exponent of exponetial function with the trial wavefunction. We choose the latter for easier calculation as follows:

$$-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2} = -\frac{r^2}{\beta^2} \quad \longrightarrow \quad \sigma^2 = \frac{1}{2}\beta^2 \tag{44}$$

Now, note that the Bohr radius is given by

$$a_0 = \frac{1}{k}\frac{\hbar^2}{me^2} \tag{45}$$

Substituting β from Eq. (37) and using Eq. (45), we get

$$\sigma^2 = \frac{1}{2}\left(\frac{1}{k}\frac{3\hbar^2}{2e^2m}\sqrt{\frac{\pi}{2}}\right)^2 = \frac{1}{2}\left(\frac{3}{2}a_0\right)^2\frac{\pi}{2} \tag{46}$$

which results to

$$\sigma = \frac{3\sqrt{\pi}}{4}a_0 \approx 1.33\,a_0 \tag{47}$$

This shows that using a Gaussian wavefunction leads to a higher standard deviation than that of the expected value.