Rutgers - Physics Graduate Qualifying Exam
Quantum Mechanics: January 12, 2007

QA

Consider the wave function in one dimension

$$\psi(x) = C \exp -a|x| \tag{1}$$

where a is a positive real number. Normalize it, and then calculate $p^2\psi(x)$. Does your answer give the correct sign for $< p^2 >$?

Solution: QA

To make

$$\int_{-\infty}^{\infty} dx|\psi(x)|^2 = 1 \tag{2}$$

$c = \sqrt{a}$.

$$p^2\psi(x) = -\hbar^2 \frac{d^2\psi(x)}{dx^2}. \tag{3}$$

Now the first derivative of $\exp -a|x|$ is discontinuous at $x = 0$. Therefore,

$$\frac{d^2\psi(x)}{dx^2} = a^2 \exp^{-a|x|} - 2a\delta(x). \tag{4}$$

Thus

$$p^2\psi(x) = -\hbar^2 a^2 + 2\hbar^2 a^{3/2}\delta(x). \tag{5}$$

If one leaves out the δ-function, one gets

$$< p^2 >= -\hbar^2 a^2 < 0. \tag{6}$$

This is clearly wrong. Since p is hermitian,

$$< p^2 >= |p|\psi > |^2 \geq 0 \tag{7}$$

for any $|\psi >$. Including the δ-function gives, however,

$$< p^2 >= -\hbar^2 a^2 + 2\hbar^2 a^2 = +\hbar^2 a^2 > 0. \tag{8}$$

QB

A particle of mass, m, is confined by the potential

$$\begin{aligned} V(x) &= \infty, \qquad & x < 0 \\ V(x) &= x^2, \qquad & x > 0. \end{aligned}$$

Find its energy eigenvalues.

Solution: QB

If $V(x)$ were x^2 everywhere, the answer is well known:

$$E_n = \hbar\omega(n + \frac{1}{2}), \tag{9}$$

where $\omega = \sqrt{k/m} = \sqrt{2/m}$ and $n = 0, 1, 2, 3...$ Now the Schrödinger equation is local, so these wave functions, $\psi_n(x)$ will work for $x > 0$. However, we must impose the boundary condition $\psi_n(x) = 0$ since $V = \infty$ for $x < 0$, just as for an infinite well. So only odd wave functions, $\psi_n(-x) = -\psi_n(x)$ will work at $x = 0$. An odd wave function will have an odd number, n, of nodes, so the answer is $\hbar\omega(n + 1/2)$ with n odd, i.e.

$$E_n = \hbar\sqrt{\frac{2}{m}}(2n' + \frac{3}{2}), \tag{10}$$

with $n' = 0, 1, 2, 3....$

QC1

Consider free particles

$$H_0 = \frac{p^2}{2m}$$

moving on a 1-dimensional ring of length L.

(a) Write down the energy levels and show each level ($exceptE = 0$) is doubly degenerate.

(b) Given a hamiltonian H_0 and an energy level E that is n times degenerate, $n > 1$. Adding to H_0 a small perturbation H_I, describe how to carry out perturbation theory for the level E.

(c) Add a perturbation

$$H_1 = -V_o e^{-x^2/a^2} \qquad a \ll L$$

Calculate the perturbed energy spectrum to first order and plot your results.

(d) Under what conditions is first order perturbation theory valid?

Solution – N. ANDREI

(3A)

1. Free electrons

$$E = \frac{p^2}{2m}$$

periodic BC: $p = \frac{2\pi}{L} n$

so

$n \neq 0$ $\quad E_n = \left(\frac{2\pi}{L}\right)^2 n^2 = E_{-n}$ $\quad$ doubly degenerate

$n = 0$ $\quad E_0 = 0$ $\quad$ not degenerate

2. perturbing a degenerate – need to choose to correct combination in the degenerate subspace.

$\psi^{(0)} = c_1 \psi_1^{(0)} + c_2 \psi_2^{(0)}$ so that for a perturbation H_I

$$\begin{cases} \left((H_I)_{11} - E^{(1)}\right) c_1 + (H_I)_{12}\, c_2 = 0 \\ (H_I)_{21}\, c_1 + \left((H_I)_{22} - E^{(1)}\right) c_2 = 0 \end{cases}$$

$\Rightarrow$

$$E^{(1)} = \frac{1}{2}\left\{ (H_I)_{11} + (H_I)_{22} \pm \sqrt{\left((H_I)_{11} - (H_I)_{22}\right)^2 + 4\,(H_I)_{12}^2} \right\}$$

3. Perturbing with $\quad H_I = -V_0\, e^{-x^2/a^2} \quad a \ll L$

the correct linear combinations are

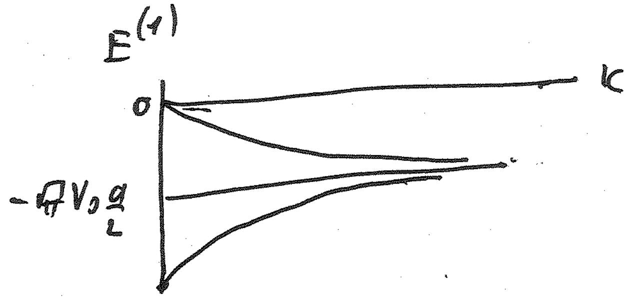
$$\psi_1^{(0)} = \left(\frac{2}{L}\right)^{1/2} \cos kx$$

$$\psi_2^{(0)} = \left(\frac{2}{L}\right)^{1/2} \sin kx \qquad k = \frac{2\pi}{L} n \qquad n = 1, 2, 3 \ldots \quad \text{only positive}$$

so

$$E_k^{(1)} = -\frac{V_0}{L} \int_{-\infty}^{\infty} (1 \pm \cos 2kx)\, e^{-x^2/a^2}\, dx \qquad a \ll L.$$

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



4. 1^{st} order applicable only if $E^{(1)} \ll E^{(0)}$

i.e. $$k^2 a^2 \gg \frac{a}{L} \frac{V_0}{\hbar^2/2ma^2}$$

i.e.

$$n \gg \frac{1}{2\pi} \left(\frac{L}{a}\right)^{1/2}.$$

limit applies only to symmetric states (perturbation vanishes

QC2

(a) Show that for the one-dimensional harmonic oscillator

$$\langle 0|e^{ikx}|0\rangle = e^{-k^2\langle 0|x^2|0\rangle/2}$$

(b) Calculate $\langle 0|\delta(x-a)|0\rangle$.

(c) What is the physical meaning of the quantity you calaculated. Discuss the cases $a = 0$ and $a = \infty$.

3B).

1. show that for a 1-d Harmonic oscillator

$$f(k) = \langle 0 | e^{ik\hat{x}} | 0 \rangle = e^{-\frac{1}{2}k^2 \langle 0 | \hat{x}^2 | 0 \rangle}$$

Recall

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} K_0 \hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_0^2 \hat{x}^2$$

defining

$$\hat{a} = \left(\frac{m\omega_0}{2\hbar}\right)^{1/2} \left(\hat{x} + \frac{i}{m\omega_0}\hat{p}\right)$$

$$\hat{a}^+ = \left(\frac{m\omega_0}{2\hbar}\right)^{1/2} \left(\hat{x} - \frac{i}{m\omega_0}\hat{p}\right)$$

we have:

$$[\hat{a}, \hat{a}^+] = 1$$

$$H = \hbar\omega_0 (\hat{a}^+ \hat{a} + \tfrac{1}{2}).$$

then i) $|0\rangle$ is defined by $\hat{a}|0\rangle = 0$

ii) $\hat{x} = \frac{1}{2}(\hat{a} + \hat{a}^+) \left(\frac{m\omega_0}{2\hbar}\right)^{-1/2}$

Now conside $f(k)$. Expand in powers of k

$f(0) = 1$

$f'(0) = 0$

same expansion for both.

$f''(\ldots) \ldots \langle 0 | \hat{x}^2 | 0 \rangle = \ldots (m\omega_0)^{-1} \ldots (\hat{a} + \hat{a}^+) \ldots (m\omega_0)^{-1} (\ldots) = \frac{\hbar}{\ldots}$

2. $g(a) = \langle 0 | \delta(\hat{x} - a) | 0 \rangle$ gives the probability to find the particle at $x = a$ (in the ground state)

But

$$g(a) = \int \frac{dk}{2\pi} e^{-ika} \langle 0 | e^{ik\hat{x}} | 0 \rangle$$

$$= \int \frac{dk}{2\pi} e^{-ika} e^{-\frac{1}{2}k^2 \frac{\hbar}{2m\omega_0}}$$

~~$= \sqrt{\frac{2\pi}{(\hbar/2m\omega_0)}} e^{-k^2/(\hbar/2m\omega_0)}$~~

$$= \sqrt{\frac{2\pi}{\hbar/2m\omega_0}} \; e^{-\frac{1}{2}k^2 \frac{1}{(\hbar/2m\omega_0)}}$$

QD1

Consider the one dimensional particle of mass m in the potential $U(x)$ such that $U(x) \to 0$ as $|x| \to \infty$.

- (a) Write down the stationary Schroödinger equation in momentum representation.
- (b) Specialize the above mentioned equation for

$$U(x) = -\alpha \left(\delta(x-L) + \delta(x+L)\right) . \tag{11}$$

  Here $\delta(x)$ is the Dirac δ-function and α and L are some dimensionful positive constants.

- (c) Using the Schroödinger equation in momentum representation find the energy spectrum of bound states for (11) and the corresponding normalized wavefunctions.
- (d) The model (11) can be thought as a toy, one dimensional, model for the ion H_2^+, where the particle m plays a role of electron interacting with heavy "protons" located at $x = \pm L$. The interaction (11) induces an effective force acting between the "protons". Calculate this force in the limit of large inter-proton separation.

Useful integrals ($x \geq 0$)

$$\begin{aligned}
\int_{-\infty}^{\infty} \mathrm{d}t \, \frac{\cos(tx)}{1+t^2} &= \pi \, \mathrm{e}^{-x} \\
\int_{-\infty}^{\infty} \mathrm{d}t \, \frac{\cos^2(tx)}{(1+t^2)^2} &= \frac{\pi}{4} \left(1 + (1+2x)\,\mathrm{e}^{-2x}\right) \\
\int_{-\infty}^{\infty} \mathrm{d}t \, \frac{\sin^2(tx)}{(1+t^2)^2} &= \frac{\pi}{4} \left(1 - (1+2x)\,\mathrm{e}^{-2x}\right)
\end{aligned} \tag{12}$$

Solution: QD1

(a) In the momentum representation the kinetic energy $\hat{T} = \hat{p}^2/(2m)$ is an operator of multiplication

$$\hat{T}\,\Psi(p) \equiv \frac{p^2}{2m}\,\Psi(p) ,$$

while the potential energy $\hat{U}$ is an integral operator

$$\hat{U}\,\Psi(p) \equiv \int_{-\infty}^{\infty} \mathrm{d}p' \, U(p,p')\,\Psi(p') .$$

Here the kernel is given by

$$U(p,p') = \tilde{U}(p-p') , \qquad \tilde{U}(p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \mathrm{d}x \, U(x)\, \mathrm{e}^{-\frac{ipx}{\hbar}} .$$

The stationary Schroödinger equation ($\hat{H}\,\Psi = E\,\Psi$) in momentum representation has a form of integral equation

$$\frac{p^2}{2m}\,\Psi(p) + \int_{-\infty}^{\infty} \mathrm{d}p \, \tilde{U}(p-p')\,\Psi(p') = E\,\Psi(p) . \tag{13}$$

(b) For the potential (11) the kernel $\tilde{U}$ reads explicitly as follows

$$\tilde{U}(p) = -\frac{\alpha}{2\pi\hbar}\int_{-\infty}^{\infty} dx\,\left(\delta(x+L)+\delta(x-L)\right)\,e^{-\frac{ipx}{\hbar}} = -\frac{\alpha}{2\pi\hbar}\left(e^{\frac{ipL}{\hbar}}+e^{-\frac{ipL}{\hbar}}\right),$$

and Eq.(13) takes the form

$$\frac{p^2}{2m}\,\Psi(p) - \frac{\alpha}{2\pi\hbar}\left(C_+\,e^{\frac{ipL}{\hbar}} + C_-\,e^{\frac{ipL}{\hbar}}\right) = E\,\Psi(p)\,, \tag{14}$$

where

$$C_\pm = \int_{-\infty}^{\infty} dp\; e^{\mp\frac{ipL}{\hbar}}\Psi(p)\,. \tag{15}$$

(c) Introduce the dimensionless quantities

$$\kappa^2 = -\frac{2mL^2}{\hbar^2}\,E\,,\quad g = \frac{m\alpha L}{\hbar^2}\,.$$

As follows from Eq.(14)

$$\Psi(p) = \frac{g}{\pi}\left(C_+e^{\frac{ipL}{\hbar}} + C_-e^{-\frac{ipL}{\hbar}}\right)\frac{1}{(\frac{pL}{\hbar})^2+\kappa^2}\,\frac{L}{\hbar}\,. \tag{16}$$

Substituting (16) in (15), and using the integrals (see (12))

$$\frac{L}{\hbar}\int_{-\infty}^{\infty}\frac{dp}{(\frac{pL}{\hbar})^2+\kappa^2} = \frac{\pi}{\kappa}\,,\qquad \frac{L}{\hbar}\int_{-\infty}^{\infty}dp\,\frac{e^{\pm\frac{2ipL}{\hbar}}}{(\frac{pL}{\hbar})^2+\kappa^2} = \frac{\pi}{\kappa}\,e^{-2\kappa}\qquad(\kappa>0)\,,$$

one finds

$$C_+ = \frac{g}{\kappa}\left(C_+ + e^{-2\kappa}\,C_-\right),\qquad C_- = \frac{g}{\kappa}\left(e^{-2\kappa}\,C_+ + C_-\right). \tag{17}$$

Homogeneous linear system (17) has a non-trivial solution if

$$\det\begin{pmatrix}\frac{g}{\kappa}-1 & \frac{g}{\kappa}\,e^{-2\kappa}\\ \frac{g}{\kappa}\,e^{-2\kappa} & \frac{g}{\kappa}-1\end{pmatrix} = \left[1-\frac{g}{\kappa}\left(1+e^{-2\kappa}\right)\right]\left[1-\frac{g}{\kappa}\left(1-e^{-2\kappa}\right)\right] = 0\,,$$

or

$$1+e^{-2\kappa} = \frac{\kappa}{g}\,,\qquad 1-e^{-2\kappa} = \frac{\kappa}{g}\,. \tag{18}$$

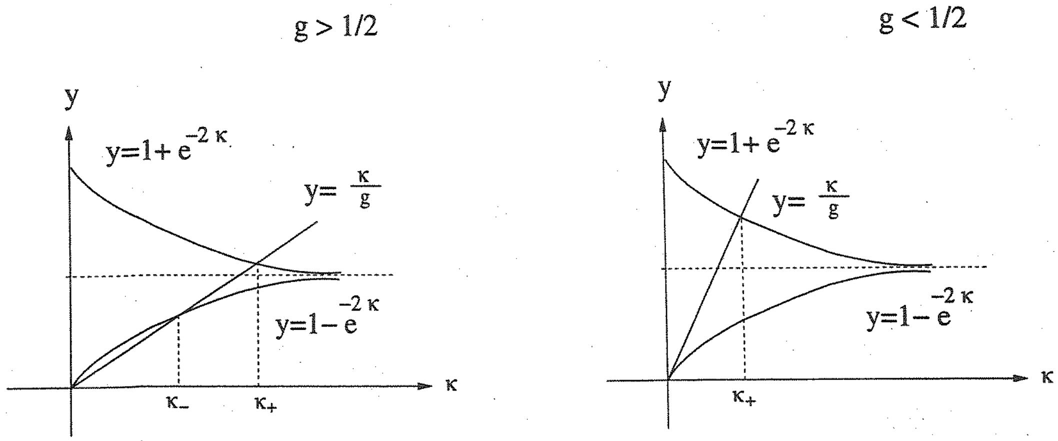
Equations (18) define the bound states energy spectrum. The first one has a real root $\kappa_+ = \kappa_+(g)$ for any $g>0$ (see Fig.). It corresponds to the ground state energy:

$$E_+ = -\frac{\hbar^2}{2mL^2}\,\kappa_+^2(g) < 0\,.$$

In this case $C_+ = C_-$ (see Eqs. (17)) and the wavefunction is an even function of p:

$$\Psi_+(p) = A_+\sqrt{\frac{L}{\hbar}}\,\frac{\cos(\frac{ipL}{\hbar})}{(\frac{pL}{\hbar})^2+\kappa_+^2}\,, \tag{19}$$

where A_+ is a (dimensionless) normalization constant.



For $g > \frac{1}{2}$ the second equation in (18) possesses the root $\kappa_- = \kappa_-(g)$ (see Fig.). It corresponds to an exited states with the energy

$$0 > E_- = -\frac{\hbar^2}{2mL^2}\ \kappa_-^2(g) > E_+ \ .$$

In this case $C_+ = -C_-$ and the wavefunction is an odd function of p.

$$\Psi_-(p) = A_-\ \sqrt{\frac{L}{\hbar}}\ \frac{\sin(\frac{ipL}{\hbar})}{(\frac{pL}{\hbar})^2 + \kappa_-^2}\ . \tag{20}$$

The constants $A_\pm$ in (19), (20) are determined by the normalization conditions

$$\int_{-\infty}^{\infty} \mathrm{d}p\ |\Psi_\pm(p)|^2 = 1\ . \tag{21}$$

Using (12), one finds

$$A_\pm = \frac{2\,\kappa_+^{\frac{3}{2}}}{\pi^{\frac{1}{2}}\sqrt{1 \pm (1 + 2\kappa_\pm)\,\mathrm{e}^{-2\kappa_\pm}}}\ .$$

(d) Eqs.(18) can be solved iteratively for $g \gg 1$. In particular

$$\kappa_\pm = g\ \big(1 \pm \mathrm{e}^{-2g}\big) + O(g^2\mathrm{e}^{-4g})\ .$$

An effective potential energy $U_\pm^{(\mathrm{eff})}(r)$ of the inter-proton interaction coincides with $E_\pm$, therefore

$$U_\pm^{(\mathrm{eff})}(r) \approx -\frac{m\alpha^2}{2\hbar^2}\ \big(1 \pm 2\,\mathrm{e}^{-\frac{m\alpha r}{\hbar^2}}\big) \quad \text{with} \quad r \equiv 2L \gg \frac{\hbar^2}{m\alpha}\ .$$

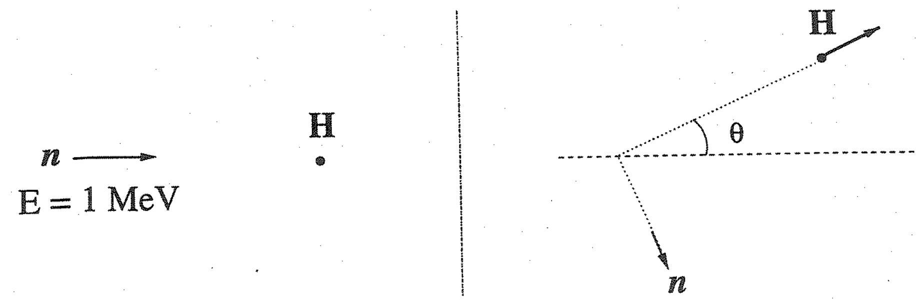
It leads to an (exponentially) small force acting between the "protons":

$$F_\pm = -\frac{\mathrm{d}U_\pm^{(\mathrm{eff})}}{\mathrm{d}r} \approx \mp\frac{m^2\alpha^3}{\hbar^4}\ \mathrm{e}^{-\frac{m\alpha r}{\hbar^2}}$$

The force F_+ corresponding to the ground state, is an attractive force. The force F_- corresponding to the exited bound state, is a repulsive force.

QD2

A fast neutron at energy 1 MeV collides with an unexited Hydrogen atom. The atom was initially at rest. After the collision, the atom has been detected as moving at angle θ to the impact direction (see Fig.). Find a probability that the atom remained in the ground state.



Solution: QD2

Let a_B and R be the Bohr radius and the proton radius respectively. Also, $\vec{v}_n$ ($v_n = \sqrt{2m_nE}$) be the incident velocity of the neutron.
Since $R/a_B \sim 10^{-4}$, the collision time $\tau \sim R/v_n$ is much less then the electron period $\tau_e \sim 137\, a_B/c$. Indeed,

$$\frac{\tau}{\tau_e} \sim \frac{1}{137}\frac{R}{a_B}\frac{c}{v_n} \sim 10^{-6}\,\frac{c}{v_n} \sim 10^{-6}\sqrt{\frac{m_nc^2}{E}} \sim 10^{-6}\,\sqrt{1000} \sim 10^{-4} \ll 1\,.$$

Therefore we can assume that the electron wavefunction remains unchanged during the collision process. In the inertial reference frame where the atom is at rest after the collision, the initial electron wavefunction reads as follows:

$$\Psi_{in}(\vec{r}) = \mathrm{e}^{\mathrm{i}\frac{m_e\vec{v}_a}{\hbar}\cdot\vec{r}}\,\Psi_0(\vec{r})\,, \tag{22}$$

where

$$\Psi_0(\vec{r}) \sim \mathrm{e}^{-\frac{r}{a}}\,,$$

and $\vec{v}_a$ is the outgoing velocity of atom. In writing of Eq.(22) we use the transformation law, $\Psi(\vec{r}) = \mathrm{e}^{\mathrm{i}\frac{m_e}{\hbar}\,\vec{v}\cdot\vec{r}'}\,\Psi'(\vec{r}')$, for the wavefunction under the Galilean boost $\vec{r} = \vec{r}' + \vec{v}t$.[1] A probability to find the atom at the ground state after the collision is given by

$$\begin{aligned} P &= \frac{\int d^3\vec{r}\,\mathrm{e}^{\mathrm{i}\frac{m_e}{\hbar}\,\vec{v}_a\cdot\vec{r}}\,\mathrm{e}^{-\frac{2r}{a_B}}}{\int d^3\vec{r}\,\mathrm{e}^{-\frac{2r}{a_B}}} = \frac{\int_0^\infty drr^2\,\mathrm{e}^{-\frac{2r}{a_B}}\,\int_0^\pi d(-\cos\theta)\,\mathrm{e}^{\mathrm{i}\frac{m_ev_ar}{\hbar}\cos\theta}}{\int_0^\infty drr^2\,\mathrm{e}^{-\frac{2r}{a_B}}\,\int_0^\pi\, d(-\cos\theta)} = \\ &= \frac{a}{4\mathrm{i}\nu}\,\frac{\int_0^\infty drr\,\left(\mathrm{e}^{-\frac{2r}{a}(1-\mathrm{i}\nu)} - \mathrm{e}^{-\frac{2r}{a}(1+\mathrm{i}\nu)}\right)}{\int_0^\infty drr^2\,\mathrm{e}^{-\frac{2r}{a}}} \\ &= \frac{1}{2\mathrm{i}\nu}\left[\frac{1}{(1-\mathrm{i}\nu)^2} - \frac{1}{(1+\mathrm{i}\nu)^2}\right] \times \frac{\int_0^\infty dx\;x\;\mathrm{e}^{-x}}{\int_0^\infty dx\;x^2\;\mathrm{e}^{-x}} \\ &= \frac{2}{(1+\nu^2)^2} \times \frac{1}{2}\,, \qquad \text{where} \quad \nu = \frac{m_ea_Bv_a}{2\hbar}\,. \end{aligned}$$

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[1] This transformation law can be obtained by decomposing the wavefunction $\Psi'(\vec{r}')$ into plan waves $\mathrm{e}^{\mathrm{i}\frac{\vec{p}'\cdot\vec{r}'}{\hbar}}$. The transformation laws for the plane wave follows from the relation $\vec{p} = \vec{p}' + m_e\vec{v}$.

The outgoing velocity $\vec{v}_a$ can be found using the energy-momentum conservation law. For pure ellastic collision one has [2]:

$$2m_n E = v_n^2 = v_a^2 + (v_n')^2 \,, \quad v_n = v_a \cos\theta + v_n' \cos(\theta') \,, \quad v_a \sin\theta = v_n' \sin(\theta') \,.$$

Then $v_a = \sqrt{2m_n E}\ \cos\theta$ and, finally,

$$P = \frac{1}{(1 + \frac{m_e}{4m_n}\frac{E}{E_0}\ \cos^2\theta)^2} = \frac{1}{(1 + 10. \times \cos^2\theta)^2} \,,$$

with

$$E = \frac{m_n v_n^2}{2} = 10^6\ \text{eV} \,, \quad E_0 = \frac{\hbar^2}{2m_e a_B^2} = 13.6\ \text{eV} \,, \quad \frac{m_e}{m_n} \approx 0.54 \times 10^{-3} \,.$$

[2]We neglect here the mass difference between H and n.