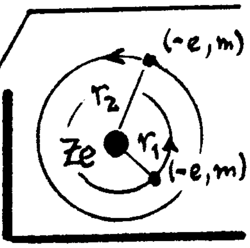
ϕ506 Problems

⑦ A 1oz. rifle bullet takes $\frac{1}{2}$ sec. to reach its target. Consider the bullet to be a mass point, and neglect effects due to air resistance, gravity, etc. Find the <u>spread</u> of successive shots at the target under optimum conditions of aiming and firing. How big is this spread if the "bullet" is a hydrogen atom?



⑧ [20 pts.]. Consider a two-electron (He-like) atom with an ∞ly heavy nucleus of charge Ze. Let the electrons be in circular orbits of radii r_1 & r_2. The problem is to estimate the lowest (i.e. ground state) energy of this system by means of the uncertainty relations.

(A) Write expressions for the <u>total</u> K.E. of the electrons in orbit, the <u>total</u> P.E. of the electrons in the presence of the nucleus, and the mutual repulsion energy between the electrons. Assume that the latter interaction keeps the electrons on opposite sides of the nucleus.

(B) Impose the uncertainty relations on the electron momenta, and find the <u>total system energy</u>: $E = \text{K.E.} + \text{P.E.} + \binom{\text{repulsion}}{\text{energy}}$ as a function of r_1 & r_2. Find the minimum in $E(r_1, r_2)$ to get the desired ground state energy.

(C) In energy units of Rydbergs ($1\,\text{Ry} = \frac{1}{2}me^4/\hbar^2 = 13.6\,\text{eV}$), calculate values of E_{min}[part (B)] and compare with experiment.

Z	1	2	3	4	5
$\lvert E_{expt.}\rvert$, Ry	1.05	5.81	14.6	27.3	44.1

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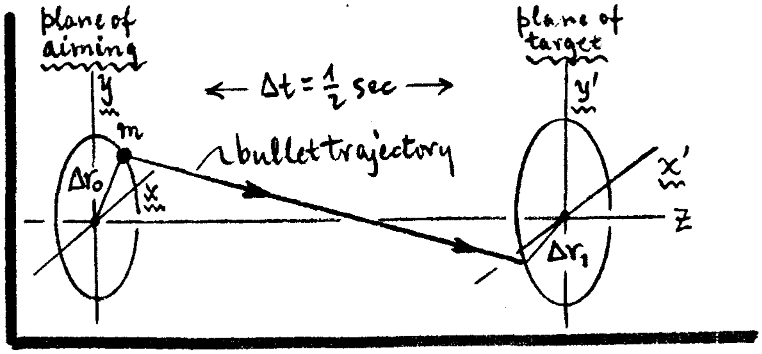
⑨ [15 pts]. At time $t=0$, the wave packet for a free particle of mass m and momentum p_0 is given by: $\phi(x,0) = A(x)\exp(ip_0x/\hbar)$. The amplitude $A(x)$ is real, and is appreciably different from zero only over $-a \leq x \leq +a$, $a = \text{cnst}$. At time $t>0$, find the interval of x-values where $\phi(x,t)$ is appreciable. I.e., if the size of $|\phi|^2$ is $\Delta x \sim a$ at $t=0$, what is its size at $t>0$?

ϕ506 Solutions

⑦ Aiming for a QM rifle bullet.



1) Assume bullet m travels ~ $\parallel$ z-axis in diagram at right. If Δx & Δy are initial aiming uncertainties, then m will strike target off-center by...

$\rightarrow \Delta r_0 = \sqrt{(\Delta x)^2 + (\Delta y)^2}$ (1), from a purely classical standpoint.

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2) BUT, localizing m to Δx & Δy $\Rightarrow$ QM momentum uncertainties $\Delta p_x \sim \frac{\hbar}{\Delta x}$ and $\Delta p_y \sim \frac{\hbar}{\Delta y}$ in the transverse direction (i.e. $\perp$ z-axis), and m moves randomly in the xy-plane @ velocity: $\Delta v = \frac{1}{m}\sqrt{(\Delta p_x)^2 + (\Delta p_y)^2}$ during its transit time Δt to the target.★ So it is off-target by an additional amount:

$$\rightarrow \Delta r_1 = \Delta v\, \Delta t \sim \left(\frac{1}{m}\sqrt{(\hbar/\Delta x)^2 + (\hbar/\Delta y)^2}\right)\Delta t = \sqrt{(\alpha/\Delta x)^2 + (\alpha/\Delta y)^2}, \qquad (2)$$

where: $\alpha = \hbar \Delta t/m$; Δr_1 is due to the QM uncertainty.

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3) Δr_0 & Δr_1 add like vectors: $\Delta \mathbf{r}_0 + \Delta \mathbf{r}_1 = \Delta \mathbf{r}$, the total spread at target. However, the directions of $\Delta \mathbf{r}_0$ & $\Delta \mathbf{r}_1$ are uncorrelated, so that...

$$\rightarrow (\Delta r)^2 = (\Delta r_0)^2 + (\Delta r_1)^2 + 2\underbrace{(\Delta \mathbf{r}_0)\cdot(\Delta \mathbf{r}_1)}_{0,\text{ on average}} \Rightarrow \Delta r = \sqrt{(\Delta r_0)^2 + (\Delta r_1)^2},$$

i.e. target spread is...

$$\rightarrow \Delta r = \sqrt{(\Delta x)^2 + (\alpha/\Delta x)^2 + (\Delta y)^2 + (\alpha/\Delta y)^2}, \quad \text{w/ } \alpha = \hbar \Delta t/m. \qquad (3)$$

$$\text{Optimization } \left(\begin{smallmatrix}\text{for } \Delta r\\ = \min\end{smallmatrix}\right) \begin{cases} \partial \Delta r/\partial \Delta x = 0 \Rightarrow (\Delta x)^2 = \alpha \\ \partial \Delta r/\partial \Delta y = 0 \Rightarrow (\Delta y)^2 = \alpha \end{cases} \Rightarrow \boxed{\Delta r_{opt} = \sqrt{4\alpha} = 2\sqrt{\frac{\hbar \Delta t}{m}}} \qquad (4)$$

In this scheme, you can never hit the target dead-center.

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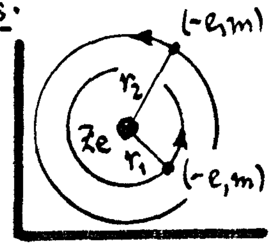
4) For $\Delta t = \frac{1}{2}$ sec & $m = 1$ oz. $= 28.4$ gm, the spread: $\Delta r_{opt} \simeq 10^{-14}$ cm, negligible. However, for an H atom, $m \simeq 1.67 \times 10^{-24}$ gm: $\Delta r_{opt} \simeq 0.036$ cm, measurable.

★ This assumes that QM is ~ over upon firing -- after initial localization to Δr_0, and the consequent QM uncertainty Δv -- m's wavepacket moves classically.

⑧ [20 pts]. Ground state of He atom via Uncertainty Relations.



(A) If the electron momenta in orbit are p_1 & p_2, then...

$$\rightarrow K = (p_1^2/2m) + (p_2^2/2m), \quad m = \text{electron mass}, \tag{1}$$

is the total electron K.E. The total electron P.E. is given by...

$$\rightarrow V = -(Ze^2/r_1) - (Ze^2/r_2), \quad \text{w/ } Ze = \text{nuclear charge}, \; -e = \text{electron charge}, \tag{2}$$

where r_1 & r_2 = electron-nuclear separations. For arbitrary electron positions $\mathbf{r}_1$ & $\mathbf{r}_2$, the e-e repulsion energy is: $U = e^2/|\mathbf{r}_1 - \mathbf{r}_2|$. But if we assume U keeps the e's on opposite sides of the nucleus, then...

$$\rightarrow U = e^2/(r_1 + r_2). \tag{3}$$

The total electron orbital energy is: E = K + V + U, or...

$$E(r_1, r_2) = \frac{1}{2m}(p_1^2 + p_2^2) - Ze^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + e^2/(r_1 + r_2). \tag{4}$$

(B) Localization of the e's to orbits of sizes r_1 & r_2 automatically generates orbital momenta at least of sizes $p_1 = \hbar/r_1$ & $p_2 = \hbar/r_2$, resp. We write equal signs here because we are looking for a minimum energy. Use this p_1 & p_2 in Eq. (4) to find the electron energy...

$$\boxed{E(r_1, r_2) = \frac{\hbar^2}{2m}\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) - Ze^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + e^2/(r_1 + r_2)}. \tag{5}$$

E will be a minimum when both $\partial E/\partial r_1 = 0$ & $\partial E/\partial r_2 = 0$, i.e. ...

$$\left.\begin{aligned} &\frac{\partial E}{\partial r_1} = \frac{e^2}{r_1^2}\left[-\left(\frac{\hbar^2}{me^2}\right)\frac{1}{r_1} + Z - \left(\frac{r_1}{r_1 + r_2}\right)^2\right] = 0, \\ \text{and}\quad &\frac{\partial E}{\partial r_2} = \frac{e^2}{r_2^2}\left[-\left(\frac{\hbar^2}{me^2}\right)\frac{1}{r_2} + Z - \left(\frac{r_2}{r_1 + r_2}\right)^2\right] = 0. \end{aligned}\right\} \tag{6}$$

These expressions are equivalent under an exchange of labelling: $r_1 \rightarrow r_2$

and $r_2 \to r_1$; i.e., r_2 plays the same role in the 2nd of Eqs.(6) as does r_1 in the first... r_1 & r_2 are equivalent. We thus set them equal, to get...

$\to r_2 = r_1$, and : $\frac{\partial E}{\partial r_1} = 0 \Rightarrow \left[-\frac{a_0}{r_1} + Z - \frac{1}{4}\right] = 0$,

i.e.// $r_2 = r_1 = a_0/(Z-\frac{1}{4})$, w/ $a_0 = \hbar^2/me^2 = 0.53\times10^{-8}$ cm {BOHR radius. (7)

This is the condition for a minimum in the energy $E(r_1, r_2)$ of Eq.(5). As we might have anticipated, the electrons behave equivalently, and get as close to the nucleus as they can. The minimum (ground state) energy is :

$\to E_{min}(Z) = E(r_1 = a_0/(Z-\frac{1}{4}), r_2 = r_1)$, in Eq.(5)

i.e.// $\boxed{E_{min}(Z) = -(Z-\frac{1}{4})^2 e^2/a_0}$ ← ground state energy. (8)

(C) In Eq.(8), we see the energy $e^2/a_0 = me^4/\hbar = 2$ Ry. So, in units of Ry★, this calculation yields the ground state energy

$|E_{min}(Z)| = 2(Z-\frac{1}{4})^2$. (9)

Comparison with known experimental values goes as follows (all in Ry):

Z	1	2	3	4	5	6
exptal, $\lvert E_{gnd}\rvert$	1.05	5.81	14.6	27.3	44.1	64.8
$\lvert E_{min}(Z)\rvert$, Eq.(9)	1.13	6.13	15.1	28.1	45.1	66.1
% error	7.6%	5.5%	3.4%	2.9%	2.3%	2.0%

(10)

The agree between expt & theory is remarkably good, considering the simplicity of our calculation. The actual QM calculation of E_{gnd} for He(Z) is quite elaborate by comparison.

★ 1 Ry (Rydberg) = $e^2/2a_0$ = 13.6 eV is the ionization energy for the H-atom.

⑨ [15 pts]. Time evolution of a free-particle wave-packet.

1. Ref CLASS NOTES p. Pack 1, Eq.(2). The spectral fcn $\varphi(k)$ is determined from the initial distribution $\phi(x,0)$ via: $\varphi(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\phi(\xi,0)\,e^{-ik\xi}\,d\xi$, so here:

$$\rightarrow \varphi(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}A(\xi)\,e^{i(k_0-k)\xi}\,d\xi\ ,\quad \text{w/}\ k_0=\frac{p_0}{\hbar}=\text{initial particle wave \#.} \tag{1}$$

$\varphi(k)$ will be appreciable only for k-values in the range: $|k_0-k|a<1$ (by definition of the range of $A(\xi)$), and in the ξ-range: $|\xi|<a$, the oscillating factor $e^{i(k_0-k)\xi}$ in (1) will not change by very much.

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2. With the above $\varphi(k)$, the free-particle wavepacket is, approximately

$$\rightarrow \phi(x,t)=\int_{k_1}^{k_2}dk\,\varphi(k)\,e^{i(kx-\omega t)}\ ,\quad \text{w/}\ \omega=\hbar k^2/2m\ \Big\}\ \text{free particle of mass } m;\ \text{NOTES, p. Pack 5, Eq(14).} \tag{2}$$

Where the limits $k_1=k_0-(1/a)$ & $k_2=k_0+(1/a)$ span the range where $\varphi(k)$ is "appreciable". Reference the integral to the central wave# k_0 by defining a new integration variable $\kappa=k_0-k$. Then Eq.(2) reads...

$$\rightarrow \phi(x,t)=\int_{-1/a}^{+1/a}d\kappa\,\varphi(k_0-\kappa)\,e^{i\left[(k_0-\kappa)x-\frac{\hbar}{2m}(k_0-\kappa)^2t\right]}$$

$$=e^{i(k_0x-\omega_0t)}\int_{-1/a}^{+1/a}d\kappa\,\varphi(k_0-\kappa)\,e^{-i\kappa\left[(x-v_0t)+\frac{\hbar\kappa}{2m}t\right]}\ , \tag{3}$$

w/ $\underline{\omega_0}=\hbar k_0^2/2m$ (central freq.) & $\underline{v_0}=\hbar k_0/m$ (propagation velocity).

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3. At $t=0$, ϕ of Eq.(3) has size δx_0 such that: $\kappa\,\delta x_0|_{\kappa=\pm 1/a}\sim 1$, i.e. $\delta x_0\sim a$, in accord with the data on $A(\xi)$. At $t>0$, the term $(\hbar\kappa/2m)t$ supplies an additional packet width: $(\hbar\kappa/2m)t|_{\kappa=\pm1/a}\sim(\hbar/2m\,\delta x_0)t$. The overall packet width (or region where ϕ is "appreciable") @ times $t>0$ is thus of order...

$$\boxed{\delta x\sim\delta x_0+(\hbar/2m\,\delta x_0)t}\ ,\quad \text{w/}\ \delta x_0=a=\text{initial width.} \tag{4}$$

Comp. w/ CLASS NOTES, p. Pack 6, Eq.(18): $\delta x=\sqrt{(\delta x_0)^2+[(\hbar/m\,\delta x_0)t]^2}$, for a free-particle Gaussian. As $t\rightarrow\infty$, δx (Gaussian) $\sim(\hbar/m\,\delta x_0)t$ is just 2x Eq.(4).