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Lecture 6

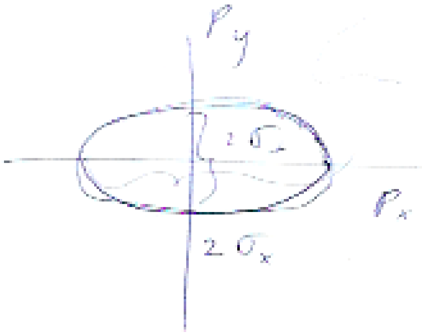
Outline: → Review from last ~~class~~ lecture

Last class: SFA ⇒ $\langle V | \Psi(t) \rangle$ = an (time reversed S-matrix)

$$P(V, t=0) = P(V, @\text{ detector}) = |\langle V | \Psi(0) \rangle|^2$$

(for linear light)

$$P \sim \underbrace{e^{-\frac{2(2I_p)^{3/2}}{3F}}}_{P_0} \cdot e^{-\frac{V_\perp^2}{2\sigma_\perp^2}} \, e^{-\frac{V_x^2}{2\sigma_x^2}}$$

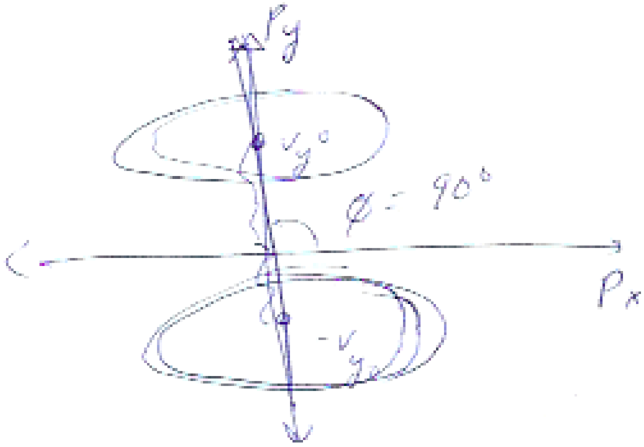


For elliptical polarization:

$$\vec{E} = F\left(\frac{1}{(1+\varepsilon^2)^{1/2}} \cos(\omega t)\, \hat{x} + \frac{\varepsilon}{(1+\varepsilon^2)^{1/2}} \sin(\omega t)\, \hat{y} \right)$$

$\sigma_\perp$, σ_x same but V_y is no longer centered @

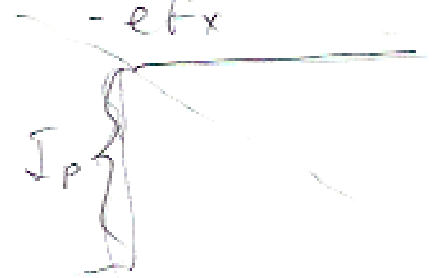
zero: $P = P_0 \, e^{-\frac{V_x^2}{2\sigma_x^2}} \, e^{-\frac{V_z^2}{2\sigma_z^2}} \cdot e^{-(V_y \pm V_y^0)^2}$



<u>Neglects coulomb effects!</u>

Coulomb correction $+\Delta\phi$ for counter; $-\Delta\phi$ for clockwise light

Neglecting Coulomb forces ⇒ tunneling through a rect. barrier of height I_p



$V(x) = \text{const}$

$\frac{\partial V}{\partial x} = 0$

(quasi-static approximation)

Today: 1) Fully solve the tunneling through the triangular barrier (have to assume an incident e^{ikx})

ADK PPT
2) obtain the same solution using WKB approx.
3) match the WKB solution to the wavefunction of an atom, thus taking account (in part) of Coulomb effects

PPT – Perelomov, Popov & Terent'ev '60s
ADK – Ammosov, Delone, Krainov '80s
→ most widely used in tunneling theory of atoms.

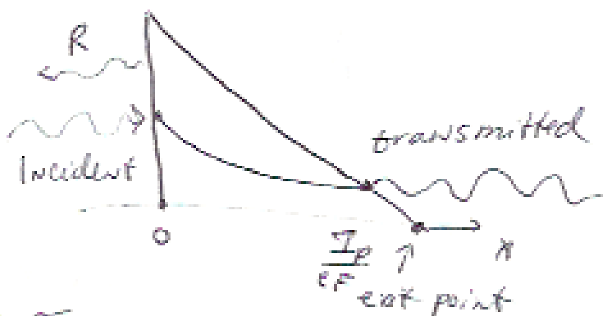
⇒ simplified derivation using partial Fourier transform: Murray et. al PRA '10 (online reference)

tunneling through a rectangular barrier:

⇒ neglects Coulomb forces ⇒ same result as from the SFA: $P \sim e^{-\frac{2(2I_p)^{3/2}}{3F}}$

barrier height: I_p

" slope: $-eF\cdot x$



Neglecting Coulomb } $V(x)-E = I_p - eF\cdot x$ for $x>0$

Schrodinger Eqn.: $\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \underbrace{(I_p - Fx)}_{V(x)-E} = 0$ for $x>0$

⇒ $\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E-V(x))\psi$

(no time-dependence if E is constant ⇒ adiabatic process.)

E – energy of the incident electron

divide by F and change variables to: $\boxed{y = \left(\frac{I_p}{F}-x\right)\cdot\left(\frac{2m}{\hbar^2}\cdot F\right)^{1/3}}$

$$\frac{\partial\psi}{\partial y} = \frac{\partial\psi}{\partial x}\cdot\frac{\partial x}{\partial y} = \frac{\partial\psi}{\partial x}\cdot(-1)\cdot\left(\frac{2m}{\hbar^2}\cdot F\right)^{-1/3}$$

$$\frac{\partial^2\psi}{\partial y^2} = \frac{\partial^2\psi}{\partial x^2}\frac{\partial x}{\partial y}\cdot(-1)\left(\frac{2m}{\hbar^2}\cdot F\right)^{-1/3} = \frac{\partial^2\psi}{\partial x^2}\left(\frac{2m}{\hbar^2}\cdot F\right)^{-2/3}$$

$$= \underbrace{\left(\frac{2m}{\hbar}\cdot F\right)^{1/3}\cdot\left(\frac{I_p}{F}-x\right)}_{y}\psi \Rightarrow \boxed{\frac{\partial^2\psi}{\partial y^2} - y\psi = 0}$$

airy function solutions!

$$Ai(y) = \frac{1}{\pi}\int_0^\infty \cos\left(\tfrac{1}{3}t^3 + yt\right)dt$$

$$Bi(y) = \frac{1}{\pi}\int_0^\infty \left(e^{-\frac{1}{3}t^3 + yt} + \sin\left(\tfrac{1}{3}t^3 + yt\right)\right)dt$$

airy functions in asymptotic limit:

for y large (high barrier)

$\boxed{Ai(y) \sim \frac{e^{-\frac{2}{3}y^{3/2}}}{2\sqrt{\pi}\,y^{1/4}}}$ ⇐ decaying solution

$Bi(y) \sim \frac{e^{+\frac{2}{3}y^{3/2}}}{\sqrt{\pi}\,y^{1/4}}$

Fowler - Nordheim tunneling ⇒ tunneling of the electron through a triangular barrier (used for tunneling in metals in static electric field, or metal - semiconductor junctions)

⇒ same tunneling exponent as using SFA for tunnel ionization.

⇒ need to take account of Coulomb effects ⇒ } PPT
⇒ recover a pre-exponent.

1) wavefunction inside the atom 2) match inside the barrier at $z = z_0$

3) solve for the triangular barrier using WKB

⇒ recover the same tunneling exponent as Fowler - Nordheim & SFA: $P \sim e^{-\frac{2(2I_p)^{3/2}}{3F}}$

but now has a <u>pre-exponent</u> due to the wavefunction inside the atom ⇒

Perelomov Popov & Terent-ev

<u>PPT</u> (most widely used tunneling theory of atoms)

⇒ matches the field - free bound wave-function to WKB approximation solution for free electron in a static field

<u>ADK</u> - similar results (equal under certain conditions)

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$$W_{ADK,PPT} = |C_{n^*l^*}|^2 f_{lm} E_i \sqrt{\frac{6}{\pi}} \left(2\frac{(2I_p)^{3/2}}{F} \right)^{2n^* - m - 3/2} \times \exp\left[-\frac{2(2I_p)^{3/2}}{3F} \right)$$

$n, l, m \Rightarrow$ quantum #s

n^* - effective principal quantum # (Slater's Rules)

$Z_{eff} = Z - s$, where Z - nuclear charge;

s - screening from other electrons

n	1	2	3	4	5	6
n^*	1	2	3	3.7	4	4.2

(takes account of screening from different electron orbitals)

approximation for single electron wavefunction:

$$\Psi_{n^*s}(r) = r^{n^*-1} \exp\left[-\frac{\overbrace{(Z-s)}^{Z_{eff}} \cdot r}{n^*} \right]$$

(matched from experimental data)

compare to hydrogen-like atoms:

$$R_{nl}(r) \sim r^l \exp\left(-\frac{Zr}{n} \right)$$

$$|C_{n^*l^*}|^2 = \frac{2^{2n^*}}{n^* \Gamma(n^*+l^*+1)\, \Gamma(n^*-l^*)}$$

$$f_{lm} = \frac{(2l+1)(l+|m|)!}{2^{|m|} |m|! (l-|m|)!}$$

Derivation of PPT using Fourier Transform

Linear light, field points along $\hat{z}$

$$\Psi(x,y,z) = \frac{1}{2\pi}\underbrace{\int dp_x \int dp_y \, e^{ip_x x + ip_y y}}_{\text{Fourier transform in 2-D}} \phi(p_x, p_y, z)$$

$$\Rightarrow \phi(p_x, p_y, z) = \frac{1}{2\pi}\int dx \int dy \, e^{-ixp_x - iyp_y} \Psi(x,y,z)$$

Schrodinger eqn. : $-\frac{\hbar^2}{2m}\nabla^2\Psi = (E-V)\Psi$

short-range potential (length-gauge) : $V = \underbrace{0}_{1/r \to 0} - Fz = -Fz$

matching different Fourier components:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \phi(p_x, p_y, z)}{\partial z^2} = (E' + Fz)\,\phi(p_x, p_y, z)$$

where $E' = -\left(I_p + \frac{p_x^2}{2} + \frac{p_y^2}{2}\right)$

1-D problem from fully 3-D Schrodinger Eqn.!

(note: works for short-range potentials (i.e. triangular barrier)

<u>WKB solution</u> : $\phi(p_x, p_y, z) = \frac{C}{\sqrt{p_z(z)}} e^{-S(p_x, p_y, z)/\hbar}$

where $p_z(z) = \left|\partial S/\partial z\right| \Rightarrow$ momentum

$-iS(p_x, p_y, p_z) \Rightarrow$ classical action : $\int_{z_0}^{z} p_z \, dz$

(imaginary because the tunneling is under the barrier)

(remember Feynman's integrals: $\Psi \sim e^{iS}$

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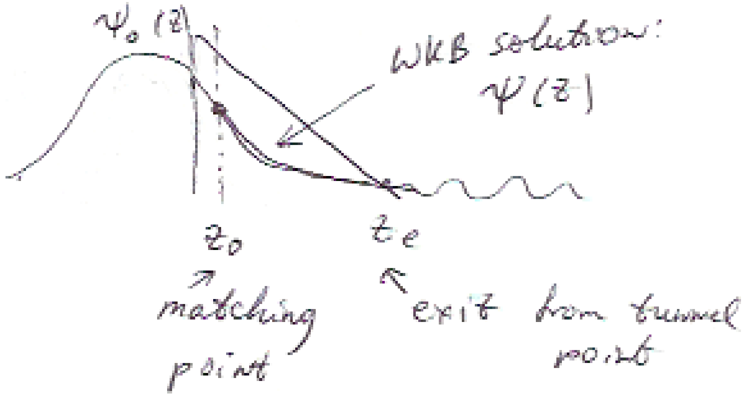
matching to the initial wavefunction of field-free atom: $\Psi_0(z)$



$$\underbrace{\Psi(z_0)}_{\text{WKB solution inside the barrier}} = \Psi_0(z_0)$$

picking C to match at $z = z_0$ so that: $\Psi(z_0) = \Psi_0(z_0)$,

we get:
$$\boxed{\Phi(p_x, p_y, z) = \underbrace{\phi_0(p_x, p_y, z_0)}_{\text{p. Fourier transform of } \Psi_0(z) = \Psi_0(x,y,z) \text{ evaluated @ } z = z_0} \sqrt{\frac{p_z(z_0)}{p_z(z)}} \times \exp\left[-\frac{S(z)}{\hbar}\right]}$$

where
$$S(z) = \int_{z_0}^{z} \Big(\underbrace{-2m\cdot[E' + Fz']}_{|p_z|}\Big)^{1/2} dz$$
since $E' + Fz' < 0$ inside a barrier

z_e - exit point $\Rightarrow$ $z_e = -\dfrac{E'}{F} = \dfrac{I_p + \frac{p_x^2}{2} + \frac{p_y^2}{2}}{F}$

Review of WKB:
$$\underbrace{\hbar^2}_{\epsilon^2 \ll 1} \phi'' + \underbrace{g(z)}_{2m(E' + F\cdot z) = p_z^2} \phi = 0$$

$$\phi = e^{\frac{1}{\delta}\sum_{n=0}^{\infty} \delta^n S_n}$$
where $\delta \ll 1$ (WKB solution)

taking first 2 terms of the expansion: $\phi \simeq e^{\frac{S_0}{\delta} + S_1}$

$$\phi' = \left(\frac{S_0'}{\delta} + S_1'\right)\phi \qquad \phi'' = \left[\left(\frac{S_0'}{\delta} + S_1'\right)^2 + \left(\frac{S_0''}{\delta} + S_1''\right)\right]\phi$$

to 0th order (powers of $\frac{1}{\delta^2}$)

$$\Rightarrow \hbar^2 \left(\frac{S_0'}{\delta}\right)^2 = -g(z) \quad \Rightarrow \delta = \hbar$$

$$\Rightarrow S_0' = \pm\sqrt{2m\,|g(z)|} \quad \Rightarrow S_0 = \pm \underbrace{\int_{z_0}^{z} \sqrt{2m\cdot|E' + Fz'|}\, dz}_{\int_{z_0}^{z} p_z\, dz \;\Rightarrow\; \text{action inside the barrier}}$$

to 1st order: power of $\frac{1}{\delta} = \frac{1}{\hbar}$

$$\Rightarrow \frac{2 S_0' S_1'}{\hbar} + \frac{S_0''}{\hbar} = 0 \quad \Rightarrow -\frac{1}{2}\frac{S_0''}{S_0'} = S_1'$$

$$\Rightarrow S_1 = -\ln\left(\sqrt{S_0'}\right) + K$$

$\Rightarrow$ taking only a decaying solution (inside the barrier)

$$\phi \approx \frac{C}{\sqrt{p_z}}\, e^{-\int_{z_0}^{z} p_z(z)\, dz/\hbar}$$

where $S_0 = -S(p_x, p_y, z) = -\int_{z_0}^{z} p_z(z)\, dz =$

$$-\int_{z_0}^{z} (2m\,|E' + Fz|)^{1/2}\, dz$$