Lecture 7

Today: derivation of PPT - the "easy" way

⇒ includes Coulomb effects (so prefactor in ionization probability)

SFA: $P \sim \underbrace{\quad}_{\text{prefactor}} e^{-\frac{2(2I_p)^{3/2}}{3F}} \cdot e^{-\frac{p_{\parallel}^2}{2\alpha_{\parallel}}} \cdot e^{-\frac{p_{\perp}^2}{2\alpha_{\perp}}}$

⇒ Prefactor only recovers the exponential dependence

⇒ short range potential (i.e. triangular barrier)

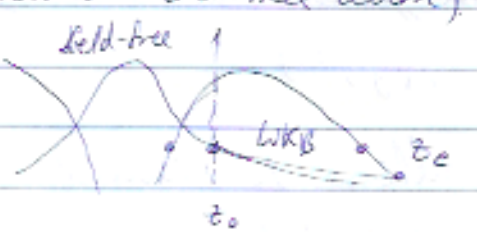
⇒ adiabatic (quasi-static limit) - means the barrier is stationary during tunneling

"tunneling regime": $\gamma \sim O(1)$ or $\gamma << 1$

"multi-photon regime": $\gamma >> 1$ ⇒ $\omega_L \sim \omega_B$

(barrier moves & interacts with the electron)

PPT ⇒ prefactor obtained by matching $\psi_0(x,y,z)$ (wavefunction of field-free atom) to the WKB solution



⇒ so the prefactor is just the amplitude of the WKB solution @ $z = z_0$

Before (in class) ⇒ $\Phi(p_x, p_y, z) = \Phi_0(p_x, p_y z_0)\sqrt{\frac{p_z(z_0)}{p_z(z)}}\, e^{-S(z)/\hbar}$

where $S(z)$ is Action: $S(z) = \int_{z_0}^{z} p_z(z)\, dz$

⇒ integrated from z_0, so $S(z_0) = 0$ ⇒ $\underbrace{\Phi(p_x p_y z_0) = \Phi_0(p_x p_y z_0)}$ matching of field-free & WKB solutions @ $z = z_0$

$\Phi(p_x, p_y, z)$ is the partial Fourier transform of $\Psi(x, y, z)$ (reminder $\vec{E} = F\cos(\omega t)\hat{z} \Rightarrow \vec{E}$ field is chosen to point in the z-direction)

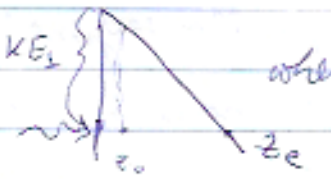
$$\Psi(x, y, z) = \frac{1}{2\pi}\int dp_x \int dp_y\, e^{ip_x x + ip_y y}\, \underbrace{\Phi(p_x, p_y, z)}_{\text{what we solve for}}$$

1-D Schrodinger eqn. for short-range potential $\Rightarrow$

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

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

short range potential $\Rightarrow$



where $KE_\perp = \frac{p_\perp^2}{2}$

Haber will need to include Coulomb effects as a perturbation to the rectangular barrier to get all z_0 to drop out of $\Phi(p_x, p_y, z)$

Reason for PFT? $\Rightarrow$ allows to reduce the full 3-D to a 1-D problem (have specific p_x, p_y, so know the "height" of the barrier)

$\Rightarrow$ can always Fourier transform back to full $\Psi(x, y, z)$

$\Rightarrow$ allows for direct calculation of probability current @ exit point: $z \to z_e$

$$\Gamma_{tm}(z) = \int dp_x\, dp_y\, p_z(z)\left|\Phi(p_x, p_y, z)\right|^2$$

(also know $p_z(z)$ if p_x, p_y are known from conservation of energy: $\frac{p_z^2 + p_\perp^2}{2m} + V(z) = -I_p$

Substitute $\boxed{\varphi(p_x, p_y, z) = \varphi_0(p_x, p_y, z_0)\sqrt{\frac{p_z(z_0)}{p_z(z)}}\, e^{-S(z)/\hbar}}$

into the 1-D schrodinger eqn, (on page 2)

+ collecting terms of order $\left(\frac{1}{\hbar}\right)^2$ (lowest order WKB)

$\Rightarrow$ Remember: WKB expands $\varphi = e^{\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n}$

where $\delta = \hbar \Rightarrow \boxed{\varphi(p_x, p_y, z) = C\, e^{S_0/\hbar + S_1}}$ (last class)

where $S_0 = -S(z)$ and $e^{S_1} = \frac{1}{\sqrt{p_z(z)}}$

C is determined by the matching: $\varphi(p_x, p_y, z_0) = \varphi_0(p_x, p_y, z_0)$

$\frac{1}{2m}\left(\frac{\partial S}{\partial z}\right)^2 - Fz = E' \Rightarrow$ Hamilton-Jacobi Eqns

$\frac{\partial S}{\partial z} = \pm\sqrt{|2(E' + Fz)|} \Rightarrow \boxed{S(z) = \int_{z_0}^{z} |2E' + 2Fz'|^{1/2}\, dz'}$

(take the + sign, since the wavefunction decays inside the barrier)

To integrate: $u = |2E' + 2Fz|$ $du = 2F\,dz \Rightarrow \int u^{1/2}\,du = \frac{2}{3}u^{3/2}$

$\Rightarrow S(z) = \frac{1}{3F}|2E' + 2Fz|^{3/2}\Big|_{z_0}^{z}$

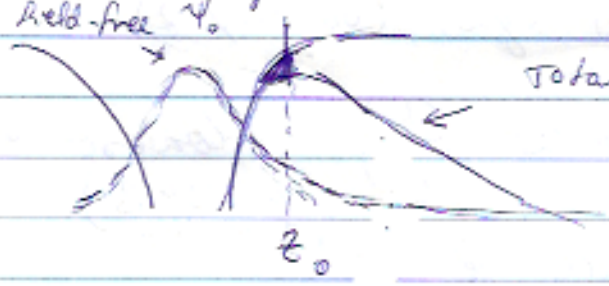
$S(z \to z_e) = \frac{1}{3F}|2E' + 2Fz_e|^{3/2} - \frac{1}{3F}|2E' + 2Fz_0|^{3/2}$

z_e is a turning point, so $2E' + 2Fz_e = 0$

Since $z_e = \frac{E'}{F}$ ($PE = E$ @ exit point)

$\boxed{S(z \to z_e) = -\frac{1}{3F}|2E' + 2Fz_0|^{3/2}}$

PPT ⇒ expand in 1st power of z_0!
(higher orders are wrong anyway!)



The shaded corner is the error @ $z = z_0$ between $\psi_0(p_x, p_y, z)$ and the "true" wavefunction: Error ~ $O(z_0^2)$

ψ_0 over-estimates the amount of decay of the wavefunction inside the barrier ⇒ under-estimates ionization probability

Expanding $S(p_x, p_y, z_e) = -\frac{1}{3F}\left[2\left(\underbrace{I_p + \frac{p_\perp^2}{2}}_{-E'} - F z_0\right)\right]^{3/2}$

assume: $I_p \gg \frac{p_\perp^2}{2}$ and $I_p \gg F z_0$

exponential suppression for $p_\perp^2 \neq 0$

is this valid?

⇒ $z_e = \frac{-E'}{F}$ ⇒ $F z_e \approx I_p \gg F z_0$

⇒ $\boxed{z_e \gg z_0}$

z_0 needs to be inside the barrier, but as small as possible (also minimizes the $O(z_0^2)$ error)

Example: Tunnel ionization of He atom

$z_{eff} = 1.34$ a.u. $\quad I_p = (z_{eff})^2 \cdot \underbrace{I_p(\text{hydrogen})}_{\frac{1}{2}\text{ a.u.}} \approx .9$ a.u.

$$E = -I_p = -\underbrace{\frac{z_{eff} \cdot e}{r}}_{\text{binding potential}} + \underbrace{eF \cdot r}_{\text{laser field (low-freq. gauge)}} + \underbrace{KE}_{0 \text{ @ turning points (i.e. entrance \& exit of barrier)}}$$

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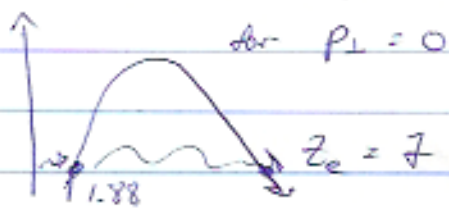
To find turning points solve Quad. eqn.: $eFr^2 - rI_p + z_{eff}e = 0$

turning points: $r = \dfrac{I_p \pm \sqrt{I_p^2 - 4(ez_{eff}\cdot F)}}{2F}$

(i.e. barrier entrance & exit)

$r \approx 1.88$; 7 for $F = .1$ a.u.



So, can pick $z_0 \approx 2$ a.u

$z_e \gg z_0$ (note z_e increases as $(p_\perp)^2 \uparrow$, while z_0 can be kept fixed)

$\Rightarrow$ more accurate approx for smaller F $\Rightarrow$ farther exit point $\Rightarrow z_e >> z_0$

Coming back to the expansion of $S(p_x, p_y, z_e)$ (page 4)

$$S(p_x, p_y, z_e) \approx +\frac{(2I_p)^{3/2}}{3F}\left[1 + \frac{p_\perp^2}{2I_p} - \frac{F z_0}{I_p}\right]^{3/2} \approx$$

$$\left[\frac{(2I_p)^{3/2}}{3F} + \frac{(2I_p)^{1/2} p_\perp^2}{2F} - (2I_p)^{1/2} z_0\right] > 0$$

- $\frac{(2I_p)^{3/2}}{3F}$: recovered before using SFA $\Rightarrow$ main exponent
- $\frac{(2I_p)^{1/2} p_\perp^2}{2F}$: perp. velocity spread with $2\sigma_\perp^2 = \frac{F}{(2I_p)^{1/2}}$
- $(2I_p)^{1/2} z_0$: to be cancelled out by the $\phi_0(p_x, p_y, z_0)$ term

$$\Rightarrow \sigma_\perp = \sqrt{\frac{\omega}{2\gamma}}$$

Remember $\phi(p_x, p_y, z_e) = \underbrace{\quad}_{\text{prefactor}} e^{-S(p_x, p_y, z_e)}$

FFT transmission amplitude

more interested in probabilities: $\phi(p_x, p_y, z_0) = \phi_0(p_x, p_y, z_0) \times \sqrt{\frac{P_t(z_0)}{P_z(z_0)}}\, e^{-S(z_0)/\hbar}$

(to include Coulomb effects)

Note: $\phi_0(p_x p_y, z) \propto e^{-(2I_p)^{1/2} z_0}$ to cancel out the arbitrary part of $S(p_x, p_y z_0)$ (decaying wavefunction example: e^{-r/a_0}))

$$\phi(p_x, p_y, z) = \frac{1}{(2\pi)^{3/2}} \int dx\, dy\, e^{-ip_x x - ip_y y} \cdot \psi(x, y, z)$$

Hydrogen asympt. wavefunction:

$$\psi_0(x, y, z) = \frac{\kappa^{3/2} e^{im\phi}}{\sqrt{2\pi}} C_{n\ell} N_{\ell m} (\kappa r)^{Q/\kappa - 1} e^{-\kappa r} P_\ell^m(\cos\theta)$$

where $\kappa = \sqrt{2I_p}$ & $C_{n\ell}$; $N_{\ell m}$ are constants

$$\psi_0(x, y, z) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \psi_m(\rho, z)$$

$$\Rightarrow \phi_0(p_x, p_y, z_0) = \frac{e^{im\phi_0}}{(2\pi)^{3/2}} (-i)^m \int_0^\infty \rho\, d\rho\, \psi_m(\rho, z_0)\, J_m(\rho p_\perp)$$

$$\propto \frac{(-i)^m e^{im\phi_0}}{(2\pi)^{1/2}} C_{n\ell} N_{\ell m} e^{-\kappa z_0} \left(\frac{p_\perp}{\kappa}\right)^m \kappa^{Q/\kappa - 1/2} z_0^{Q/\kappa}$$

$\Rightarrow$ z_0 in the exponent cancels since $\kappa = \sqrt{2I_p}$

$\Rightarrow$ also $z_0^{Q/\kappa}$ cancels. If the Coulomb (long-range) effects are included as a higher order perturbation to the

So, finally, we have $\Phi_0(p_x, p_y, z_e)$ & $e^{-S(z_e)/\hbar}$ =

$e^{-\frac{S(z_e)}{\hbar} + S_1(z_e) + S_c(z_e)}$ (Coulomb correction) calculated to 1st order in WKB

e.g. (again z_0 cancels out when we $\Phi_0 \propto e^{-S(z_e)/\hbar}$ $e^{S_c(z_e)} \propto z_0^{-Q/\kappa}$

$\Rightarrow \Phi(p_x, p_y, z_e) = \Phi_0(p_x, p_y, z_0) \cdot \sqrt{\frac{p_z(z_0)}{p_z(z_e)}}\, e^{-S_0/\hbar + S_c}$

To find current: $\Gamma_{em} = \int dp_x dp_y\, p_z(z \to z_e) \left|\Phi(p_x, p_y, z \to z_e)\right|^2$ @ $z = z_e$ (exit pt.)

$\Gamma_{lm} = \frac{\kappa^2}{2} |C_{\kappa\ell}|^2 \frac{2\ell+1}{2^m m!} \frac{(\ell+m)!}{(\ell-m)!} \left(\frac{2\kappa^3}{F}\right)^{2Q/\kappa - m - 1}$

PPT formula!

prefactor that includes Coulomb effects + depends on ℓ, m

$e^{-2\kappa^3/3F}$ Keldysh exponent since $\kappa = \sqrt{2I_p}$

"easy" derivation!

Notes on approximations (not a full solution!)

1) uses Laser-free wavefunction up to $z < z_0$

2) asymptotic solution for a triangular barrier in 0th order WKB, includes the Coulomb as a 1st order correction (using perturbation theory) ⇒ causes $z_0^{Q/\kappa}$ factor in Ψ_0

⇒ causes errors of $O(z_0^2)$ so z_0 should be as small as possible)