Lecture 8

Recap: Derived PPT formula using the method of partial Fourier Transform (PFT)

PFT: $\phi(p_x, p_y, z) = \iint dp_x\, dp_y\, e^{-ip_x x - ip_y y}\, \psi(x, y, z)$

($\vec{E}$ field points along $\hat{z}$)

PFT + $\underbrace{\text{short-range}}_{V = -Fz}$ Coulomb potential $\Rightarrow$ 3-D Schrodinger Eqn. is reduced to 1-D

$\Rightarrow \vec{E} = -F\hat{z}$

(Note short-range potential = triangular barrier)

Full wavefunction $\psi(x, y, z) = \iint dp_x\, dy\, \underbrace{e^{ip_x x + ip_y y} \times \phi(p_x, p_y, z)}$

substitute that into the full 3-D Schrodinger Eqn!

3-D $\Rightarrow$ $\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\phi(p_x, p_y, z)\, e^{ip_x x + ip_y y}$

linear PDE

$= \underbrace{(E - V)}_{(-I_p + Fz)}\ \phi(p_x, p_y, z)\, e^{ip_x x + ip_y y}$

1-D

linear ODE $\Rightarrow$

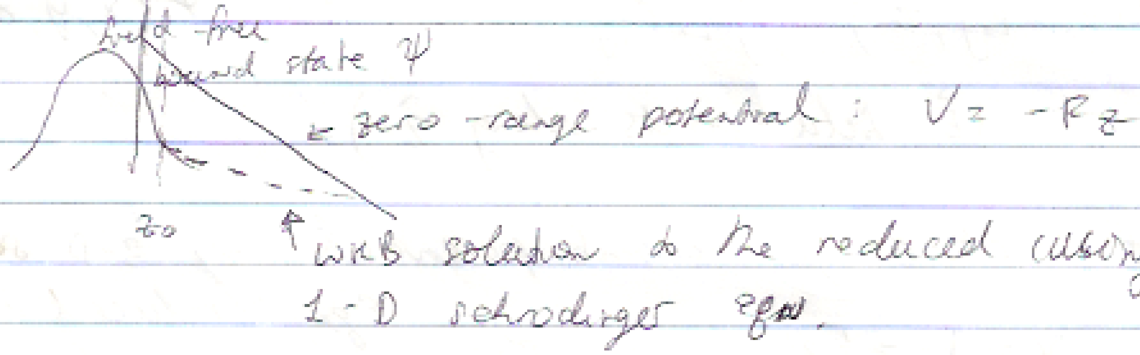
(in a.u.)

$$-\frac{1}{2}\frac{\partial^2 \phi(p_x, p_y, z)}{\partial z^2} = \Big[\overbrace{-I_p - \underbrace{\left(\frac{p_x^2}{2} + \frac{p_y^2}{2}\right)}_{\frac{p_\perp^2}{2}}}^{E'} + F \cdot z\Big]\phi(p_x, p_y, z)$$

3-D Problem reduced to 1-D tunneling problem by assuming short-range pot. & using PFT!

(2)

To obtain PPT: match field free wavefunction to the ____ of a 1-D schrodinger Eqn. @ some point $z = z_0$ inside the barrier



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another way to reduce the full 3D schrodinger Eqn. (atomic potential + laser field) to 1D without assuming short range potential (exact for a Hydrogen atom)

$\Rightarrow$ Parabolic coordinates (Landau & Lifshitz)

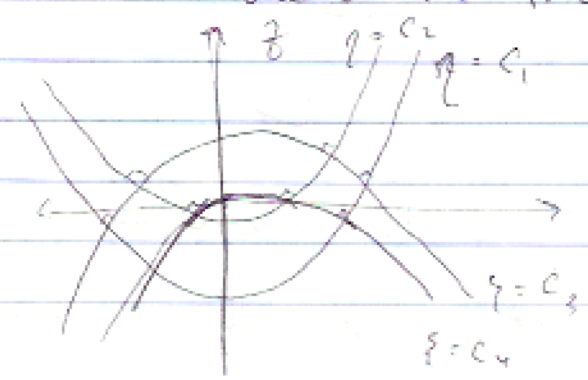
$\xi, \eta, \phi \Rightarrow \quad x = \sqrt{\xi\eta}\cos\phi \; ; \quad y = \sqrt{\xi\eta}\sin\phi \; ; \quad z = \frac{1}{2}(\xi - \eta)$

ϕ : azim

$$r = \sqrt{x^2 + y^2 + z^2} = \frac{1}{2}(\xi + \eta) \; ; \quad \xi, \eta > 0 \quad \text{since } r \geq z$$

$$\Rightarrow \xi = r + z \; , \quad \eta = r - z \; , \quad \phi = \tan^{-1}(y/x)$$

surfaces $\xi = \text{const}$; $\eta = \text{const}$ are paraboloids of revolution about the z-axis (focus @ the origin)



$\hat{\eta} \perp \hat{\xi}$ (orthogonal)

Laplacian: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{4}{\xi+\eta}\left[\frac{\partial}{\partial \xi}\left(\xi\frac{\partial}{\partial \xi}\right) + \frac{\partial}{\partial \eta}\left(\eta\frac{\partial}{\partial \eta}\right)\right]$

$+ \frac{1}{\xi\eta}\frac{\partial^2}{\partial \phi^2}$

$-\frac{1}{2}\nabla^2\Psi = (E-V)\Psi$ where $V = \underbrace{-\frac{1}{r}}_{\text{coulomb}} \underbrace{- eFz}_{\text{laser}} = \underbrace{\frac{-2}{\xi+\eta}}_{\text{coulomb}} + \underbrace{\frac{F}{2}(\xi-\eta)}_{\text{laser}}$

$\nabla^2\Psi + 2(E-V)\Psi = 0$

$\Downarrow$

$$\frac{4}{\xi+\eta}\left[\frac{\partial}{\partial \xi}\left(\xi\frac{\partial\Psi}{\partial \xi}\right) + \frac{\partial}{\partial \eta}\left(\eta\frac{\partial\Psi}{\partial \eta}\right)\right] + \frac{1}{\xi\eta}\frac{\partial^2\Psi}{\partial\phi^2} + 2\Psi\left(E + \frac{2}{\xi+\eta} - \frac{F}{2}(\xi-\eta)\right) = 0$$

assume solution of the form: $f_1(\xi) f_2(\eta) e^{im\phi} = \Psi(\xi,\eta,\phi)$

(like in spherical coords: $f(r)\cdot P(\theta)\, e^{im\phi}$)

substituting $\Psi = f_1(\xi) f_2(\eta) e^{im\phi}$ and multiplying by

$\frac{1}{4}(\xi+\eta)\cdot\frac{1}{\Psi(\xi,\eta,\phi)}$

$$\Rightarrow \left[\frac{1}{\partial\xi}\left(\xi\frac{\partial f_1}{\partial \xi}\right)\times \underbrace{f_2(\eta)\cdot e^{im\phi}} + \frac{\partial}{\partial\eta}\left(\eta\frac{\partial f_2(\eta)}{\partial \eta}\right)\cdot f_1(\xi)\, e^{im\phi}\right]$$

$$\times \frac{1}{f_1(\xi) f_2(\eta) e^{im\phi}} + -\frac{1}{4}\underbrace{\left(\frac{\xi+\eta}{\xi\eta}\right)}_{\frac{1}{\eta}+\frac{1}{\xi}}\cdot m^2 + \frac{1}{2}\Big(E(\xi+\eta) + 2$$

$$-\frac{F}{2}(\xi^2-\eta^2)\Big) = 0$$

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$$\Rightarrow \underbrace{\frac{1}{f_1(\xi)}\frac{1}{\partial\xi}\left(\xi\frac{\partial f_1}{\partial\xi}\right)-\frac{1}{4}\frac{m^2}{\xi}+\frac{1}{2}E\xi-\frac{F}{4}\xi^2}_{\text{terms only dep. on } \xi} = -\beta_1$$

$$+\underbrace{\frac{1}{f_2(\eta)}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial f_2(\eta)}{\partial\eta}\right)-\frac{1}{4}\frac{m^2}{\eta}+\frac{1}{2}E\eta+\frac{F}{4}\eta^2}_{\text{terms only dep. on } \eta} = -\beta_2 \qquad = -1$$

$\Rightarrow$ since the variables are separated, each expression has to equal to a constant (same is done when finding $\Psi(r,\theta,\phi)$ for a hydrogen atom $\Rightarrow$ get constants n, l, m)

where $-\beta_1 + -\beta_2 = -1 \Rightarrow \boxed{\beta_1+\beta_2=1}$

we finally get 2 1-D ODE!

$\Rightarrow \left\{ \begin{array}{l} \Rightarrow \text{took the full 3-D problem, Coulomb field + laser \&} \\ \text{reduced it to 2 uncoupled ODE's by transforming to} \end{array}\right.$

parabolic coords:

$$\Rightarrow \frac{d}{d\xi}\left(\xi\frac{df_1}{d\xi}\right)+\left(\frac{1}{2}E\xi-\frac{1}{4}\frac{m^2}{\xi}-\frac{F}{4}\xi^2\right)f_1=-\beta_1 f_1$$

$$\Rightarrow \frac{d}{d\eta}\left(\eta\frac{df_2}{d\eta}\right)+\left(\frac{1}{2}E\eta-\frac{1}{4}\frac{m^2}{\eta}+\frac{F}{4}\eta^2\right)f_2=-\beta_2 f_2$$

substitute $f_1 = \chi_1/\sqrt{\xi}$ $\quad f_2 = \chi_2/\sqrt{\eta}$

Now this looks like a schrodinger eqn! (in a.u.)

$$\Rightarrow \frac{d^2\chi_1}{d\xi^2} + \underbrace{\left(\frac{1}{2}E + \frac{\beta_1}{\xi} - \frac{m^2-1}{4\xi^2} - \frac{1}{4}F\xi\right)}_{2(E_1 - U_1(\xi))}\chi_1 = 0$$

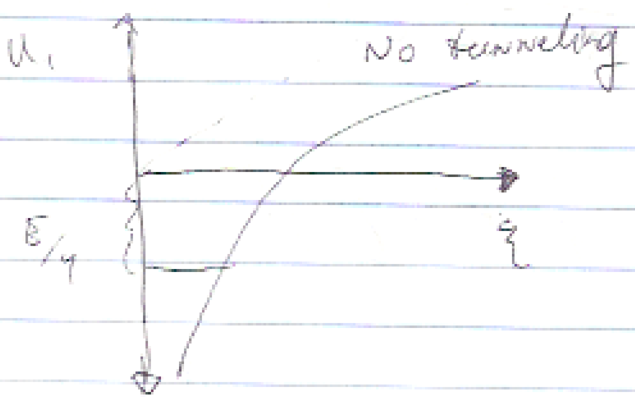
$$\Rightarrow \frac{d^2\chi_2}{d\eta^2} + \underbrace{\left(\frac{1}{2}E + \frac{\beta_2}{\eta} - \frac{m^2-1}{4\eta^2} + \frac{1}{4}F\eta\right)}_{2(E_2 - U_2(\xi))}\chi_2 = 0$$

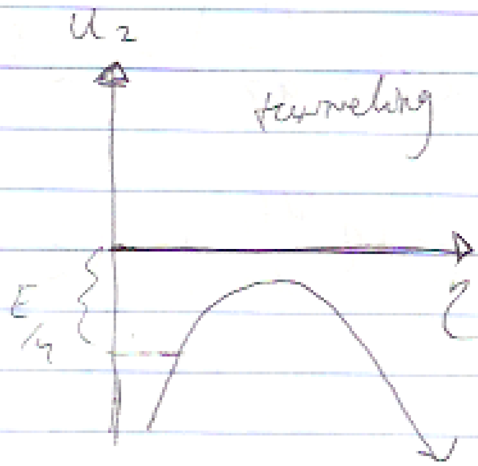
where $E_1 = E_2 = \frac{E}{4} = \frac{-I_p}{4}$

$$U_1(\xi) = \frac{-\beta_1}{2\xi} + \frac{m^2-1}{8\xi^2} + \frac{1}{8}F\xi$$

$$U_2(\eta) = \frac{-\beta_2}{2\eta} + \frac{m^2-1}{8\eta^2} - \frac{1}{8}F\eta$$

take $m = \pm 1$





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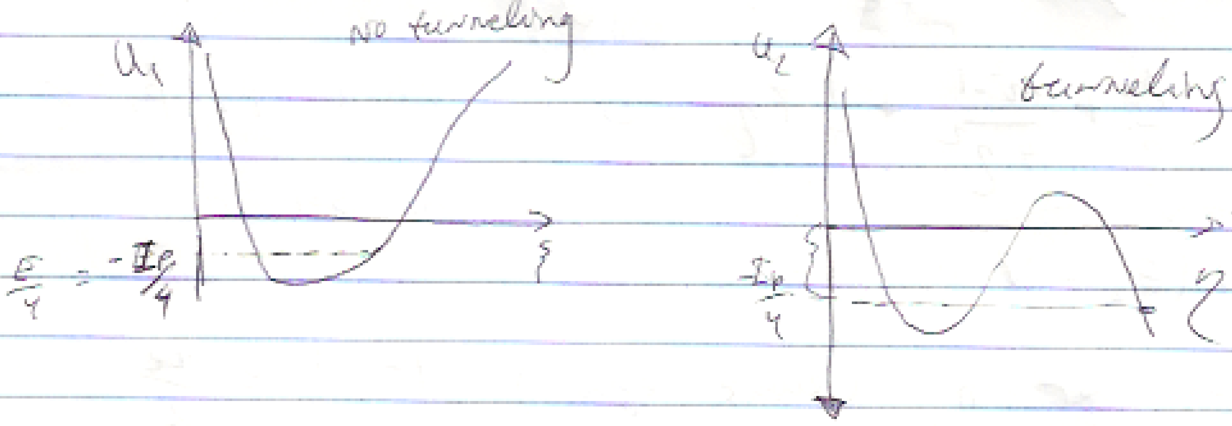
for $|m| > 1$

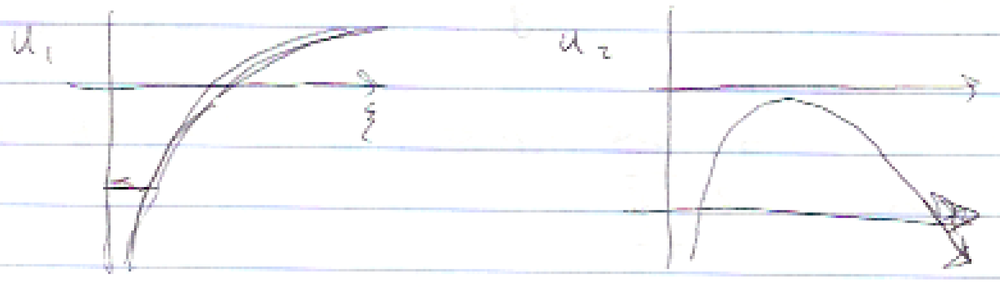


tunneling along η only!

after tunneling: $\eta \gg \xi$ $\quad r - z \gg r + z$

$-2z \gg 0 \Rightarrow$ tunneling opposite to the direction of the E-field (neg. charge on electrons)

Example: He in ground $s=1$ state $\Rightarrow m = 0$



$\xi_e \approx 0 = r_e + z_e \qquad \eta_e = r_e - z_e$

$r_e \approx -z_e$

(all the displacement is essentially along z! @ exit point) $\qquad \eta_e \approx -2z_e$

$\Rightarrow$ Exit point from the tunnel given by $z_e \approx -\frac{\eta_e}{2}$

where we get η_e by solving:

$$\underbrace{\frac{1}{2}E + \frac{\beta_2}{\eta} + \frac{1}{4\eta^2} + \frac{1}{4}F\eta}_{2(E_2 - V_2(\eta_e))} = 0$$ where $\beta_2 = \beta_1 = \frac{1}{2}$ for $S=1$ He

Solving for η_e (cubic eqn.) $|z_e| \approx \frac{\eta_e}{2}$

Compare to cartesian coords:

$$(E - V) = -I_p + \frac{1}{r} + F \cdot z \Rightarrow \frac{1}{r} \approx \frac{+1}{|z|} @ z_e$$

$$\Rightarrow I_p \approx F \cdot z + \frac{1}{z}$$

$\Rightarrow$ quadratic eqns. $\Rightarrow F \cdot z^2 - I_p z + 1 = 0$

$$\Rightarrow z_e = \underbrace{\frac{I_p + \sqrt{I_p^2 - 4F}}{2F}}_{7.7\text{ au}} < \underbrace{\frac{I_p}{F}}_{\approx 9\text{ au}} \text{ (triangular approx)}$$

For $F \approx .1$ au

In cartesian coords over-barrier ionization (OBI) happens for $F > \frac{I_p^2}{4}$

$$\Rightarrow \text{Cubic Eqn.} \quad F\eta^3 + 2\underset{-I_p}{E}\eta^2 - 2\eta + 1 = 0$$

$$|z_e| \approx \frac{\eta_e}{2} \approx \frac{16.8}{2} \approx 8.4 \text{ a.u}$$

$\Rightarrow$ Ironically, triangular approx. might be more accurate @ certain intensities than solving laser + atomic pot. in Cartesian coord.

$$\underbrace{7.7_{au}}_{\text{cartesian}} < \underbrace{8.4_{au}}_{\text{parabolic}} < \underbrace{9_{au}}_{\text{triangular approx.}}$$

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Note: * the inaccuracies came not from using cartesian coords, but from the need to make 1-D assumption when using them

* In parabolic coord. the schrodinger eqn. naturally seperates into 2 1-D independent eqns, where tunnelling can only happen along the coord., η

* OBI occurs @ higher intensities than we'd think based on 1-D Cartesian picture $\Rightarrow$ extended tunneling regime!

(in above example $F \approx 0.34$ for OBI, not 0.2 as we'd get from $F = \frac{I_p^2}{4}$