Lecture 8 11.11.13

Next Lecture: NON-adiabatic effects

Today: exact solution for strong field ionization in the adiabatic, $\gamma \ll 1$ limit

$\Rightarrow$ Corresponds to tunneling in a static electric field

$\Rightarrow$ Can take account of the Coulomb field inside the barrier

$\Rightarrow$ NO need for short-range potential approx., whereby $V_c \propto -\frac{1}{r} \approx 0$ inside the barrier, resulting in a triangular barrier

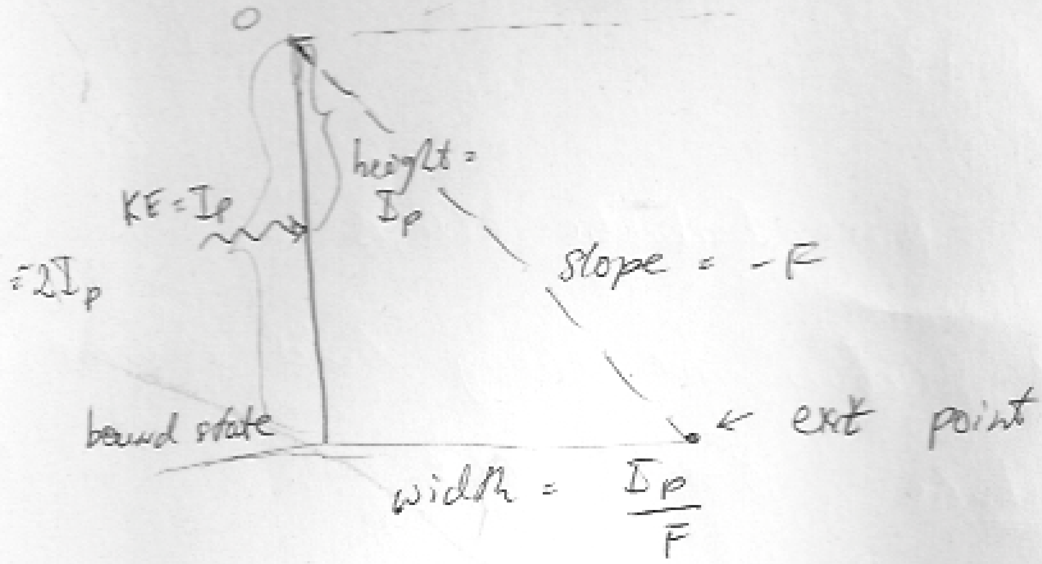
From virial theorem: $\langle KE \rangle = -\frac{1}{2} \langle PE \rangle$

$$\langle KE \rangle + \langle PE \rangle = E_{TOT} = -I_p$$

$$-\frac{1}{2}\langle PE \rangle + \langle PE \rangle = \frac{\langle PE \rangle}{2} = -I_p \Rightarrow \langle PE \rangle = -2I_p$$

$$\langle KE \rangle = I_p$$

$\Rightarrow$ Hence short-range pot. approx. results in tunneling through a triangular barrier of height I_p & width $\frac{I_p}{F}$



⇒ Can be solved exactly

⇒ results in tunneling probability given by: $|\Psi|^2 \propto e^{-\frac{2(2I_p)^{3/2}}{3F}}$

⇒ same as " " through a static triangular barrier

⇒ also comes out of SFA in the adiabatic $\gamma \ll 1$ limit

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An exact solution for a Hydrogen-like atom in a static field also exists!

⇒ change to Parabolic coordinates (Landau & Lifshitz)

ξ, η, ϕ ⇒ $x = \sqrt{\xi\eta}\cos\phi$; $y = \sqrt{\xi\eta}\sin\phi$; $z = \frac{1}{2}(\xi - \eta)$

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

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

surfaces ξ = const; η = const. are paraboloids of revolution about the z-axis (focus @ the origin)

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

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③

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

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

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

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

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

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

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

$\Rightarrow$ since the variables are separated, each expression has to equal to a constant (same is done when solving $\Psi(r,\theta,\varphi)$ 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!

$\Rightarrow$ { $\Rightarrow$ turn the full 3-D problem, Coulomb field + linear ε reduced it to 2 uncoupled ODE's by transforming to 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 we can use a schrödinger eqn! (m=0 a)

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

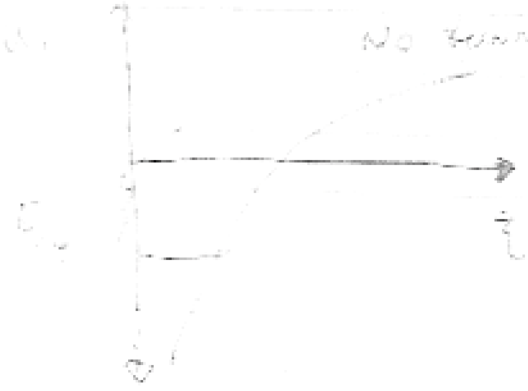
$$\Rightarrow \frac{d^2 \chi_2}{d\eta^2} + \underbrace{\left(\frac{1}{2} E - \frac{\beta_2}{\eta} - \frac{m^2-1}{4\eta^2} + \frac{1}{4} F \eta \right)}_{2(E_2 - U_2(\xi))} \chi_2 = 0$$

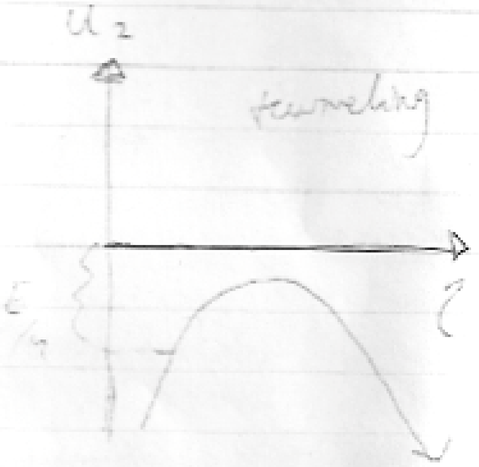
where $E_1 = E_2 = \frac{E}{4} = -\frac{I_p}{4}$

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

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

take $m = \pm 1$





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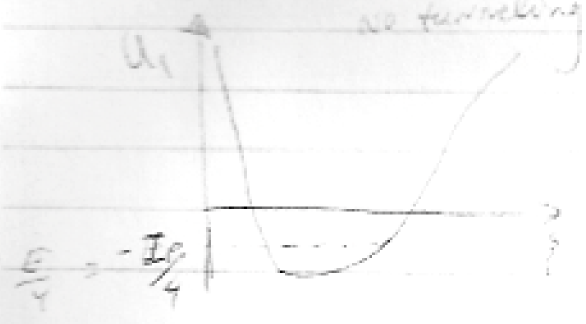
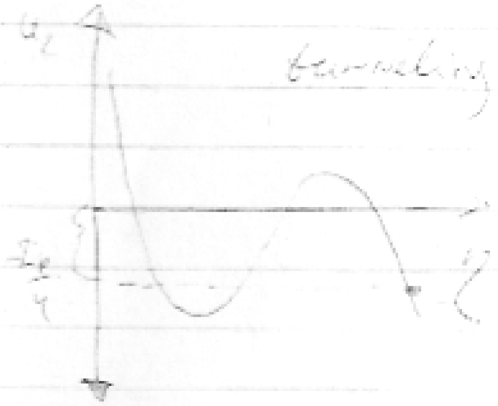
for $|m| > 1$



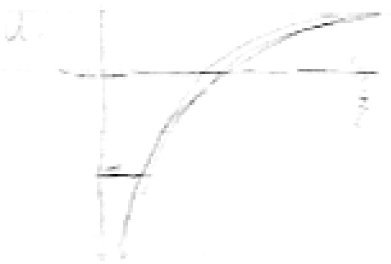


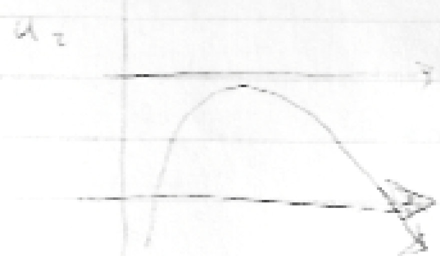
tunneling along η only!

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 $\Rightarrow m = 0$





$\xi_e \approx 0 = r + z_e \quad \eta_e = r - z_e$

$r \approx -z_e$

i.e. the displacement $\eta_e \approx -2z_e$ is essentially along z! (@ exit point)

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

Where we get η_e by solving:

$\frac{1}{2}E + \frac{\beta_2}{\eta} - \frac{1}{4\eta^2} + \frac{1}{4}F\eta = 0$ where $\beta_2 = \beta_1 = \frac{1}{2}$ for S=1 He

$2(E_2 - V_2(\eta_e)) = 0$

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

Compare to cartesian coords

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

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

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

$\Rightarrow z_e = \frac{I_p + \sqrt{I_p^2 - 4F}}{2F} < \frac{I_p}{F}$ (triangular approx)

For $F \approx 1$ au   7.7 au ≈ 9 au

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

$\Rightarrow$ cubic eqn $F\eta^3 + 2\overset{I_p}{E}\eta^2 - 2\eta + 1 = 0$

$R_e \approx \frac{\eta_e}{2} \approx \frac{16.8}{2} \approx 8.4$ a.u

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

7.7au < 8.4au < 9au

cartesian parabolic triangular approx.