Recap / Outline

atoms in strong laser fields ⇒ tunneling ionization

$V_L = -eEx$

Full Hamiltonian: $\hat{H}(t) = \underbrace{(\hat{p} - \frac{q}{c} A(t))^2}_{\text{laser field}} + \underbrace{V(r)}_{\text{atomic}}$

Today: Using SFA to estimate tunnel ionization probability as a function of I_p & $\vec{E}$

① Non-relativistic QM ⇒ Solving the Schrodinger Eqn.: $i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$

⇒ autonomous Hamiltonian

⇒ general case

② SFA assumptions: 1) Neglects laser field on $|\psi\rangle$ evolution while bound

2) Neglects Coulomb potential after ionization ⇒ Volkov states

Schrodinger Eqn.: $i\hbar \frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$ PDE: $\frac{\partial}{\partial t}$, ∇^2

$$\hat{H} = \hat{T}_k + V(\vec{r},t) = \underbrace{\frac{\hbar^2}{2m}\nabla^2}_{KE} + \underbrace{V(r,t)}_{PE}$$

$\Rightarrow$ Try $\Psi(r,t) = \psi(\vec{r})\cdot\varphi(t)$ as a solution

$$\frac{i\hbar\,\psi(r)\cdot\frac{\partial\varphi(t)}{\partial t}}{\Psi(r,t)} = \frac{\varphi(t)\,\hat{H}\,\psi(\vec{r})}{\Psi(r,t)}$$ ← dividing both sides by $\Psi(r,t)$

$$\underbrace{i\hbar\cdot\frac{1}{\varphi(t)}\cdot\frac{\partial\varphi(t)}{\partial t}}_{G(t)\text{ only}} = \underbrace{\frac{1}{\psi(\vec{r})}\cdot\hat{H}\,\psi(\vec{r})}_{F(\vec{r})\text{ only}} = E,$$ where E can be any constant

$\Downarrow$ $\qquad\qquad$ $\Downarrow$

$i\hbar\frac{\partial\varphi}{\partial t} = E\,\varphi(t)$ $\qquad$ $\hat{H}\,\psi(\vec{r}) = E\,\psi(\vec{r})$

$\varphi_E(t) = e^{-iEt/\hbar}\cdot\varphi_0$ $\qquad$ solve for $\psi_E(\vec{r})$, where $\hat{H} = \frac{\hbar^2}{2m}\nabla^2 + V(r)$

$$\Psi_E(r,t) = \varphi_E(t)\cdot\psi_E(\vec{r}) = \psi_E(\vec{r})\cdot e^{-iEt/\hbar}\varphi_0$$

E = energy: autonomous Hamiltonian = conserved E
(no time dependence in $V(r)$: $V(r,t) = V(r)$)

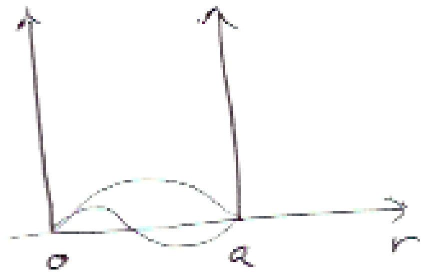
$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$ $\Rightarrow$ linear PDE

General solution for E = const: (linear combination of all possible solutions)

<u>Continuous case:</u> $\Psi(r,t) = \int_{-\infty}^{\infty} dE\, a(E)\,\psi_E(r)\cdot e^{-iEt/\hbar}$

discrete E values determined by boundary conditions on $\psi(r)$

Example: infinite potential well:



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

for $0<r<a$ $\quad \psi''(r) = -\frac{2mE}{\hbar^2}\psi(r)$ $\quad$ (same as SHO eqn.)

$$\psi(r) = A\cos(kx) + B\sin(kx) \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar} = \underbrace{\frac{2\pi n}{a}}_{\text{boundary condition!}}$$

Solution: $\psi_n(r) = B\sin(kx) = B\cdot\sin\left(\frac{2\pi n}{a}x\right)$

$$E_n = \left(\frac{2\pi n\hbar}{a}\right)^2 / 2m$$

discrete solution: $\quad \Psi(r,t) = \sum_{n=0}^{\infty} B_n \cdot \psi_n(r) \cdot e^{-iE_nt/\hbar}$

What about time-dependent Hamiltonians?

$\hat{H}(t) = \left(\hat{p} - \frac{q}{c}A(t)\right)^2 + V(r) \Rightarrow$ atom in laser field

General solution for $\hbar i \frac{\partial|\Psi\rangle}{\partial t} = \hat{H}(t)|\Psi\rangle$

$$\Rightarrow |\Psi(t)\rangle = \underbrace{e^{-i\int_{t_0}^{t}\hat{H}(t')dt'}}_{\substack{\text{propagator} \\ = \text{time evolution operator}: \ \hat{u}(t,t_0)}} |\Psi_i\rangle \quad \text{where } |\Psi_i\rangle = |\Psi(t=t_0)\rangle$$

$$\hat{u}(t,t_0) = \hat{u}(t,t')\cdot\hat{u}(t',t_0)$$

adjoint: $\langle\Psi(t)| = \langle\Psi_i|\hat{u}^{+}(t,t_0) = \langle\Psi_i| e^{+i\int_{t_0}^{t}\hat{H}(t')^{+}dt'}$

$$\langle \psi(t) | \psi(t) \rangle = \underbrace{\langle \psi_i | e^{+i\int_{t_0}^{t} \hat{H}^{+}(t')\,dt'}}_{\langle \psi |} \underbrace{e^{-i\int_{t_0}^{t} \hat{H}(t')\,dt'} | \psi_i \rangle}_{| \psi \rangle}$$

$= \langle \psi_i | \psi_i \rangle$ if $\hat{H}^{+} = \hat{H}$ ($\hat{H}$ is Hermitian)

$\Rightarrow \hat{u}^{+} = \hat{u}^{-1}$

Strong Field Approximation: SFA

$$\hat{H}(t) = \underbrace{\hat{H}_0}_{\text{field-free Hamiltonian}} + \underbrace{\hat{V}}_{\text{interaction with laser field}}$$

$\hat{V} = \frac{\hat{p}}{c}\vec{A} + \frac{1}{2c^2}\vec{A}^2$ (or in length gauge: $\hat{V}_L = -e\vec{r}\cdot\vec{E}$)

Approximations: Can use $\psi(r,t) = \psi(r)\cdot\varphi(t)$ for sufficiently slowly changing $\vec{E}(t)$: where $\underbrace{\omega_L}_{\text{laser frequency}} \ll \underbrace{\omega_B}_{\text{bounce frequency of electron}}$

$\Rightarrow$ Quasi-static potential: $V(\vec{r}) = V_{atom}(r) - e\vec{r}\cdot\vec{E}$

SFA Solution $|\Psi(t)\rangle = e^{-i\int_{t_0}^{t} \hat{H}(t')\,dt'} |\psi_i\rangle =$

$$|\Psi(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}(t') \underbrace{|\Psi\rangle}_{\text{need to know } |\Psi(t')}$$

Approximation (exact as $t \to 0$):

$$|\Psi(t)\rangle = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \left[e^{-i\int_{t'}^{t} \hat{H}(t'')\,dt''} \right] \cdot \hat{V}(t')$$

$$\times\, e^{-i\int_{t_0}^{t'} \hat{H}_0(t'')\,dt''} \cdot |\psi_i\rangle + e^{-i\int_{t_0}^{t} H_0(t'')\,dt''} |\psi_i\rangle$$

substituting into: $i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$

$$\Rightarrow i\frac{\partial |\psi(t)\rangle}{\partial t} = \underbrace{(H_0 + \hat{V})}_{\hat{H}} \cdot e^{-i\int_0^t H_0(t'')dt''} |\psi_i\rangle$$

Project onto velocity basis $|\vec{v}\rangle$ (continuum eigenstates $\Rightarrow$ plane waves $e^{i\vec{k}\cdot\vec{r}}$ as $|\vec{r}| \to \infty$)

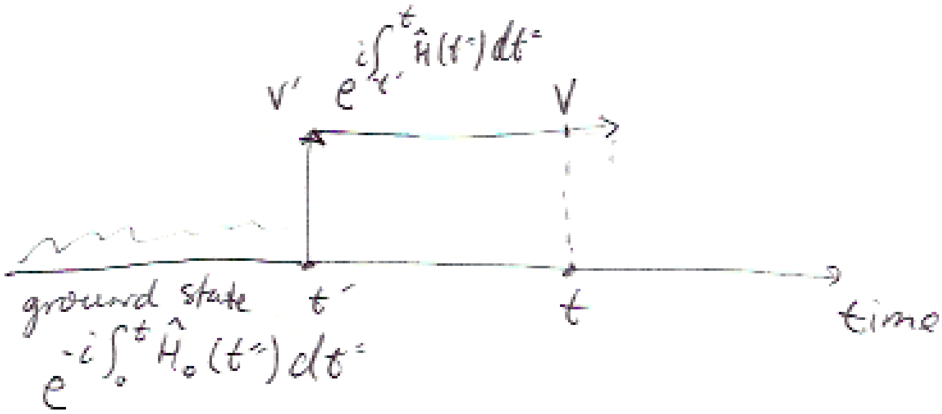
$$\langle \vec{v}|\psi(t)\rangle = \psi(v,t) = -i\int_0^t dt' \langle \vec{v}| e^{-i\int_{t'}^t \hat{H}(t'')dt''} \hat{V}(t') e^{-i\int_0^{t'} \hat{H}_0 dt''} \times |\psi_i\rangle$$

$|\psi_i\rangle = |\psi_g\rangle$ (ground state inside atom)

$\Rightarrow |\psi_g(t)\rangle = e^{iI_p t} |\psi_i\rangle$ where $|\psi_i\rangle = |\psi_g(t=0)\rangle$

$\langle \vec{v}|\psi_g\rangle = 0$ (no projection of $|\psi_g\rangle$ onto continuum states)

$\langle \vec{v}|\psi(t)\rangle = a_v(t) \Rightarrow$ "time reversed S-matrix"



SFA assumption: after ionization, the electron sees only the laser field (strong fields!) : $\hat{H} = \hat{V} = \hat{H}_F$

$\Rightarrow$ Volkov propagator : $e^{-i\int_{t'}^{t} \hat{H}_F(t'')dt''}$

where $\hat{H}_F = \frac{1}{2m}\big(\underbrace{\hat{P} - \frac{e}{c}\vec{A}}_{m\vec{v}}\big)^2 = KE$

$$\hat{H}_F |v\rangle = \underbrace{\tfrac{1}{2} m v^2}_{KE} |v\rangle \Rightarrow |v\rangle \text{ are eigenfunctions of } \hat{H}_F$$

$$* \ \tfrac{1}{2} m V_x^2 = \frac{(P - \frac{q}{c} A(t))^2}{2m} = H_F = \frac{mv_\perp^2}{2}; \ \dot{P} = -\frac{\partial H_F}{\partial r} = 0$$

P = const (conserved canonical angular momentum)

$$V_x(t) = V_x = [P - \tfrac{q}{c} A(t)] / 2m$$

$$V_x(t') = V_x' = [P - \tfrac{q}{c} A'(t)] / 2m \quad \text{where } \vec{A}(t) = v_0 \sin(\omega t)\,\hat{x}$$

in a.u. $e/c = 1$; $m = 1$

$$V_x - A(t) = V_x' - A'(t') \Rightarrow V_x = V_x' - A'(t') + A(t)$$

$$E(t) = KE(t'') = \tfrac{1}{2} m [V(t'')]^2 = \tfrac{1}{2} m [V_x - \hat{A}(t) + A''(t)]^2$$

$$\langle \vec{v} | e^{-i\int_{t'}^{t} \hat{H}_F(t'')\,dt''} = e^{-i\int_{t'}^{t} \left(\frac{1}{2}(\underbrace{V_x - A(t) + A''(t'')}_{V_x''})^2 + \frac{1}{2}(V_\perp'')^2\right) dt''} \times \langle \vec{v}' |$$

$$\Psi(v,t) = -i \int_{t_0}^{t} dt' \langle \vec{v} | e^{-i\int_{t'}^{t} \hat{H}_F(t'')\,dt''} \hat{V}(t') e^{-i\int_{t_0}^{t'} \hat{H}_0\,dt''} |\Psi_i\rangle$$

$$\Psi(v,t) = -i \int_{t_0}^{t} dt' \underbrace{\langle v' | \hat{V}(t') | \Psi_i \rangle}_{\text{prefactor}} \cdot e^{-iS(t,t')}$$

$$S(t,t') = \tfrac{1}{2} \int_{t'}^{t} (V_x - A(t') + A''(t''))^2\,dt'' - \left(I_p t' + \frac{V_\perp^2}{2}(t - t')\right)$$

Saddle-point approx

S is ~~larger~~ large (strong fields)

solve $\dfrac{\partial S(t,t')}{\partial t'} = 0$ for $t' = t_a$

then $S_0 = S(t, t_a)$

$\Psi(v,t) \sim e^{iS_0}$

solve: $\frac{1}{2}\left(V_x - V_0 \sin(\omega t) + V_0 \sin(\omega t')\right)^2 + \underbrace{\left(I_p + \frac{1}{2}V_\perp^2\right)}_{V_\perp \text{ adds to } I_p} = 0$

(decreases ionization probability)

Interested in projection $\langle V | \Psi \rangle$, where

$V_\perp = 0$

$\Rightarrow \left(\frac{V_x}{V_0} - \sin(\omega t) + \sin(\omega t')\right)^2 + \gamma^2 = 0$

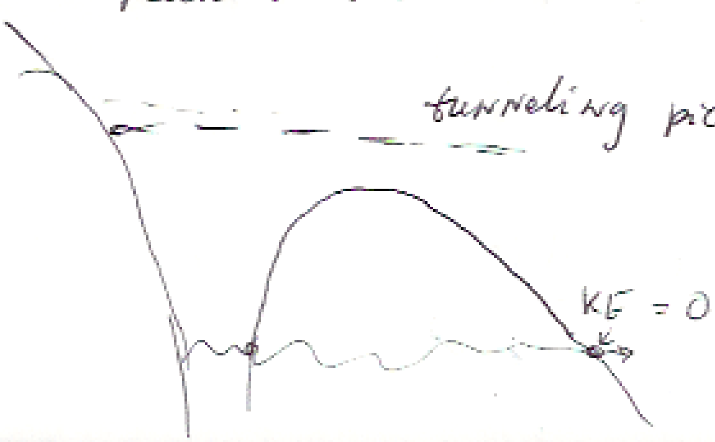
Ionization @ the peak of $\vec{E}$: $t = 0$

projection onto the likeliest state $\vec{V} = 0$

so ~~want to~~ want to find: $\langle 0 | \Psi(t=0) \rangle = \Psi(0,0)$

$\Rightarrow$ Probability of appearing in the continuum @ the peak of the field with $\vec{V} = 0$

tunneling picture:



$\Rightarrow \quad \sin^2(\omega t') = -\gamma^2 \qquad \sin(\omega t') = i\gamma$

for $\quad \omega t' \ll 1 \quad \Rightarrow \sin(\omega t') \approx \omega t' = i\gamma$

$$t' = i\,\frac{\gamma}{\omega} \qquad \text{where } \gamma = \tau_{kel}\cdot\omega = \frac{\sqrt{2I_p}}{F}\cdot\omega$$

$t' = i\,\tau_{kel} \quad \Rightarrow$ imaginary Keldysh time