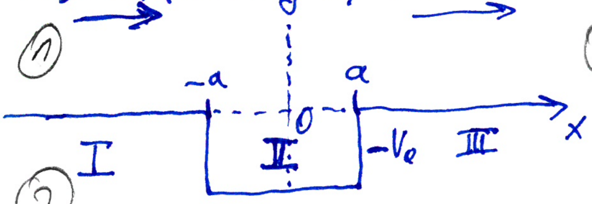
# Quantum scattering in 1D: U. Fano

- illustrates the elementary concepts of scattering theory:
- asymptotic phase-shifts, standing wave basis, use of symmetry

- scattering by a pot. well: we want sol. describing particle incoming from left
- this sol. defined by b.c. in I and III:

① 

③
$$\psi_{I}(x) = A\cdot e^{ikx} + Be^{-ikx},\quad x\le -a,\quad k=\sqrt{2mE}/\hbar,\ E>0,$$
$$\psi_{II}(x) = \alpha\cdot e^{ik_0x} + \beta e^{-ik_0x},\quad |x|<a,\quad k_0=\sqrt{2m(E+V_0)}/\hbar,$$
$$\psi_{III}(x) = C\cdot e^{ikx},\quad x\ge a.$$

general sol. in region II; only the transmitted wave here

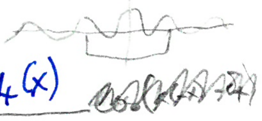
②
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi_E(x) = E\cdot\psi_E(x),$$
$$V(x) = \begin{cases}-V_0, & |x|<a \\ 0, & |x|\ge a,\quad V_0>0.\end{cases}$$

- we want the prob. of transmission and reflection: $T=\left|\frac{C}{A}\right|^2$ and $R=\left|\frac{B}{A}\right|^2$
- found by matching the solution at $x=\pm a$: ④ TRADITIONAL APPROACH

$$\psi_I(-a)=\psi_{II}(-a),\quad \psi_{III}(a)=\psi_{II}(a),$$
$$\psi_I'(-a)=\psi_{II}'(-a),\quad \psi_{III}'(a)=\psi_{II}'(a).$$
$\Rightarrow A, B, \alpha, \beta, C$ (normalization is arb.)

- drawbacks: makes no use of symetry, matching needs to be repeated when b.c. change.
- scattering theory: we know that $V(x)=V(-x) \Rightarrow$ take advantage of symmetry.

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x),\quad V(x)=V(-x)\Rightarrow [\hat{H},\hat{P}]=0,$$ where the parity operator:
$$\hat{P}\psi(x)=\psi(-x)$$ $\Rightarrow$ there exists a basis of our Hilbert space which simultaneously diagonalizes $\hat{H}$ and $\hat{P}$:

SYMMETRIC SOLUTIONS: 

$$Hu_+(x)=Eu_+(x),\quad Pu_+(x)=+1u_+(x)$$
$$u_+(x) = N_E\cos[kx-\delta_+],\quad x\le -a,$$
$$= A\cdot\cos[k_0 x],\quad |x|<a,$$
$$= N_E\cdot\cos[kx+\delta_+],\quad x\ge a.$$
required due to SYMMETRY

ANTISYMMETRIC SOLUTIONS: 

$$Hu_-(x)=Eu_-(x),\quad Pu_-(x)=-1u_-(x)$$
$$u_-(x) = -N_E\cdot\cos[kx-\delta_-],\quad x\le -a,$$
$$= B\cdot\sin[k_0x],\quad |x|<a,$$
$$= N_E\cdot\cos[kx+\delta_-],\quad x\ge a.$$

- the real wavefunctions $u_+(x), u_-(x)$ are called standing wave basis (they contain $k$ and $-k$ waves in equal amount)
- $\delta_+, \delta_-$ are the asymptotic ~~phase~~ partial-wave phase-shifts: they cary all information about the collision complex in region II which can be determined experimentally.
- $N_E, A, B, (\delta_\pm)$ found by matching the log-derivatives of the wavefunctions at the boundary:

$x=+a$:
$$\frac{u_+'(a)}{u_+(a)}:\quad k_0\cdot\tan[k_0a]=k\cdot\tan[ka+\delta_+],$$
$$\underbrace{A\cdot\cos[k_0a]}_{u_+^{II}(a)} = \underbrace{N_E\cos[ka+\delta_+]}_{u_+^{III}(a)}$$

$x=-a$:
$$\frac{u_-'(a)}{u_-(a)}:\quad k_0\cot[k_0a]=-k\cdot\tan[ka+\delta_-],$$
$$B\cdot\sin[k_0a]=N_E\cdot\cos[ka+\delta_-].$$

$\boxed{N_E \text{ is not needed to find } \delta_+, \delta_- \text{ !}}$

- Since $u_+$ and $u_-$ form a basis, any other solution can be expanded in them (2)

$\boxed{\psi(x) = c_+ u_+(x) + c_- u_-(x)}$, $|c_+|^2+|c_-|^2=1$,

- but $\psi(x)$ is not necessarily an eigenstate of parity (i.e. it can break the sym.) as in the first example
- We can form the following types of solutions: SHOW THE PICTURE WITH 4 WP-PACKETS

1) standing-wave states for which $c_+/c_-$ is real, so that $\psi(x)$ is real (up to a phase).

$\exp[ikx-\omega t] \Rightarrow ikx-\omega t=0 \to x=\frac{\omega}{k}t \Rightarrow$ outgoing ... incoming to the well at negative times

2) travelling-wave (scattering) solutions: $\boxed{u^{(+)}}$ put $\sin(y)=\frac{e^{iy}-e^{-iy}}{2i}$, $\cos(y)=\frac{e^{iy}+e^{-iy}}{2}$

for $x\geq a$: $\psi(x)=\frac{1}{2}N_E\Big[\underbrace{(c_+e^{i\delta_+}+c_-e^{i\delta_-})}_{A_>}e^{ikx}+\underbrace{(c_+e^{-i\delta_+}+c_-e^{-i\delta_-})}_{B_>}\cdot e^{-ikx}\Big]$, $x>a$,

$$=\frac{1}{2}N_E\Big[\underbrace{(c_+e^{-i\delta_+}-c_-e^{-i\delta_-})}_{A_<}e^{ikx}+\underbrace{(c_+e^{i\delta_+}-c_-e^{i\delta_-})}_{B_<}\cdot e^{-ikx}\Big],\ x<a.$$

scattering; half-scattering; in the final channel

- these are the physical solutions (particle has a well-defined momentum $-i\hbar\frac{d}{dx}\psi(x)=k\psi(x)$)

$\exp[ikx-i\omega t] \Rightarrow x=\frac{\omega}{k}t$ (for $t<0 \Rightarrow x<0$)

A) Particle approaching the well from $x=-\infty \Leftrightarrow B_> \equiv 0 = c_+e^{-i\delta_+}+c_-e^{-i\delta_-}$

WE SEE THAT $N_E$ IS IRRELEVANT

$$T=\left|\frac{A_>}{A_<}\right|^2=\left|\frac{c_+e^{i\delta_+}+c_-e^{i\delta_-}}{c_+e^{-i\delta_+}-c_-e^{-i\delta_-}}\right|^2=\left|\frac{\frac{c_+}{c_-}e^{i\delta_+}+e^{i\delta_-}}{\frac{c_+}{c_-}e^{-i\delta_+}-e^{-i\delta_-}}\right|^2\overset{\frac{c_+}{c_-}=}{=}\left|\frac{-e^{i(\delta_+-\delta_-)}\cdot e^{i\delta_+}+e^{i\delta_-}}{-e^{i(\delta_+-\delta_-)}\cdot e^{-i\delta_+}-e^{-i\delta_-}}\right|^2=$$

$$=\left|\frac{e^{i(\delta_+-\delta_-)}-e^{-i(\delta_+-\delta_-)}}{2}\right|^2=\boxed{\sin^2[\underbrace{\delta_+-\delta_-}_{\text{eigenphase sum}}]}$$

$\delta_+=\delta_+(E)$, $\delta_-=\delta_-(E)$,

QUESTION: WHAT IS R?

ANSWER: $R=\left|\frac{B_<}{A_>}\right|^2=\cos^2(\delta_+-\delta_-)$ so that T+R=1

- Key result which establishes the role of phase-shifts as quantities in terms of which all observables are determined!

B) Particle approaching the well from $x=+\infty \Leftrightarrow A_< \equiv 0 = c_+e^{-i\delta_+}-c_-e^{-i\delta_-}$

$T=\left|\frac{B_<}{B_>}\right|^2=\dots=\sin^2[\delta_+-\delta_-]$ as expected (i.e. identical phys. situation to A)

$R=\left|\frac{A_>}{B_>}\right|^2=\dots=\cos^2[\delta_+-\delta_-]$

outgoing from the well at positive times

3) Particle escape from the well ("half-scattering" solutions) $\boxed{u^{(-)}}$

A) escape in the direction $x=-\infty \Leftrightarrow A_> \equiv 0 = c_+\cdot e^{+i\delta_+}+c_-e^{+i\delta_-}$ must be zero $\Rightarrow A_>=0$

(at positive times the outgoing part in direction ...)

$\to \frac{c_+}{c_-}$ is complex conjugate of the same ratio from (2A). Q: WHAT DOES IT TELL US ABOUT THIS SOLUTION? A: IT IS A TIME-REVERSED SOL.

B) escape in the direction $x=+\infty \Leftrightarrow B_< \equiv 0 = c_+e^{i\delta_+}-c_-e^{i\delta_-}$

Q: ARE $u_+$ AND $u_-$ TIME-REVERSED VERSIONS OF EACH OTHER? A: NO BECAUSE THEY ARE REAL SO COMPLEX CONJ. DOES NOTHING.

$\to \frac{c_+}{c_-}$ is complex conjugate of the ratio from (2B).

$\to$ used in photoionization using weak (compared to binding pot.) and long monochromatic pulses:

Ionization amplitude: $\langle\psi^{(-)}|\hat{r}|\phi_g\rangle$ (REMEMBER BORN, I.E. 1st order PT)

$\hookrightarrow$ laser-atom potential: $\vec{E}=E_0\cdot\vec{r}\cdot\cos(\omega t)$

cf. $f=\langle k|V|\psi^{(+)}\rangle$

$\to$ The b.c. 3A; 3B are called "incoming-wave" b.c.

PHILOSOPHY OF THE PW APPROACH (I.E. MOST METHODS USED IN PRACTICE)

I. Determine a complete set of commuting operators for the given problem ($\hat{H}$)

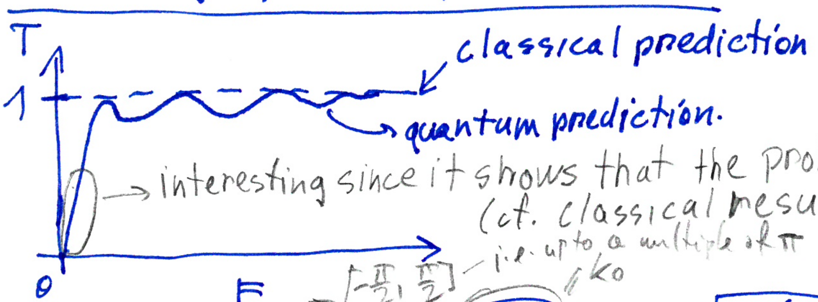
II. Find real-valued (standing-wave) solutions (basis) which simultaneously diagonalizes the commuting operators

III. Find the asymptotic phase shifts wrt. free solution.

IV. Form the desired physical solution ($\psi(x)=c_+u_+(x)+c_-u_-(x)$) and use it to compute the observables.

## Scattering by a 1D pot. well :






$$\delta_+(E) = \mathrm{ArcTan}\Big[\frac{\sqrt{E+V_0}}{\sqrt{E}}\cdot \mathrm{Tan}\big[\sqrt{2m\cdot(E+V_0)}\cdot a\big] - \sqrt{2mE} + n\cdot\pi \;,\; n=0,1,2,\dots$$

$\left[-\frac{\pi}{2},\frac{\pi}{2}\right]$ – i.e. up to a multiple of $\pi$; $k_0$; $\sqrt{E} = k_0$

$$\delta_-(E) = \mathrm{ArcTan}\Big[-\frac{\sqrt{E+V_0}}{\sqrt{E}}\cdot \mathrm{Cot}\big[\sqrt{2m(E+V_0)}\cdot a\big] - \sqrt{2m\cdot E} + k\cdot\pi \;,\; k=0,1,2,\dots$$

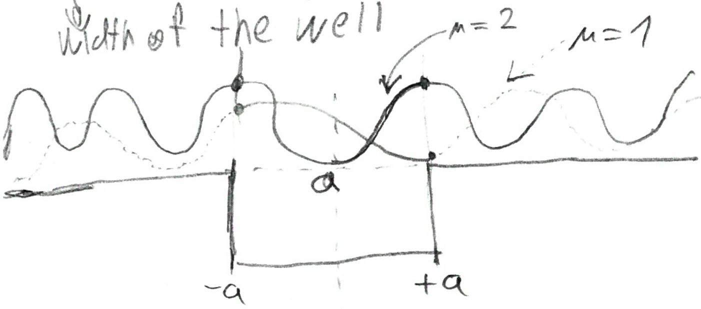
"Resonances": $\boxed{R-T \text{ minima}}$

– perfect transmission for $\delta_+ - \delta_- = j\cdot\frac{\pi}{2}$, $j = 0,1,2,\dots$ ($T = \sin^2[\delta_+ - \delta_-] = 1$) $\mathrm{ArcTan}\left[\frac{x-y}{1+xy}\right]$

$\boxed{2a = n\cdot\frac{\lambda}{2}}$, $\lambda = \frac{2\pi}{k_0}$ (de Broglie wavelength inside the well) ||

can be found using formulas for $\mathrm{ArcTan}[x] - \mathrm{ArcTan}[y] = \mathrm{ArcTan}[z]$

width of the well




- for $n=2$: phase at $x=-a$: 0
  phase at $x=+a$: 0 ($+2\pi$)
  ⇒ no asymptotic phase shift (up to a multiple of $\pi$)
- for $n=1$: phase at $x=+a$ is larger than at $x=-a$ by $\pi$ but the phase-shift is defined only up to a multiple of $\pi$! The particle is transmitted as if the well did not exist!

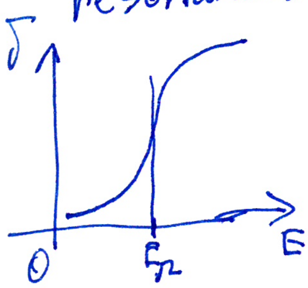
Transparency of rare gases to electrons (show the R-T experiments and pyrazine calculations)

1) PLOT THE CASE $V_0 = 0$ AND OBSERVE THAT $\delta_+ - \delta_- = \frac{\pi}{2}$ $(T=1)$ AND $\delta_+ = 0$, $\delta_- = -\frac{\pi}{2}$

2) The R-T minima is an effect that is very different to resonances : phase-shift ~~jumps~~ jumps by $\pi$

poles of the S-matrix in complex plane

– these states (resonances) are quasibound states (the wf has a large amplitude inside a barrier compared to the outside ⇝ small coupling to the continuum).




3) WE SEE THE CRUCIAL ROLE OF PHASE-SHIFTS AND THEIR ENERGY DEPENDENCE!


~~4) The larger the m~~ 4) Q: WHY DO WE GET MORE PEAKS FOR A LARGER MASS? A: $\lambda = \frac{h}{p}$ becomes SMALLER.