Lecture 4: Resonant Scattering

Sep 16, 2008

Fall 2008 8.513 "Quantum Transport"

- Analyticity properties of S-matrix
- Poles and zeros in a complex plane
- Isolated resonances; Breit-Wigner theory
- Quasi-stationary states
- Example: $S(E)$ for inverted parabola
- Observation of resonances in transport
- Fabry-Perot vs. Coulomb blockade

Symmetries and analytic properties of S-matrix

Causality: $S(E)$ analytic in the complex half-plane $\mathrm{Im}\,E > 0$.

Example: S-matrix for a delta function; $E\psi = -\frac{1}{2}\psi'' + u\delta(x)\psi$

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \begin{pmatrix} \frac{z}{1-z} & \frac{1}{1-z} \\ \frac{1}{1-z} & \frac{z}{1-z} \end{pmatrix}, \quad z = \frac{u}{2ik} = \frac{u}{2\sqrt{-2E}}$$

Unitary for real $E > 0$; analytic in the complex E plane; branch cut at $E > 0$ (convention).

General decomposition: scattering channels and phases:

$$S(E) = \sum_n e^{2i\delta_n} |n\rangle\langle n|$$

Symmetries in the plane of complex k:

For central force problem, there are two asymptotic solutions $\chi_{kl}^{(\pm)}(r) \propto e^{i(kr-\pi l/2)}$. Consider a solution which is regular near $r=0$:

$$\psi(r) = a_l(k)\chi_{kl}^{(-)}(r) - b_l(k)\chi_{kl}^{(+)}(r) \quad (1)$$

Zero boundary condition at $r=0$ gives

$$\frac{b_l(k)}{a_l(k)} = \lim_{r\to 0} \frac{\chi_{kl}^{(-)}(r)}{\chi_{kl}^{(+)}(r)} \quad \text{hence} \quad S_l(k) = \frac{b_l(k)}{a_l(k)}$$

Consider symmetry $k \to -k$: S.E. unchanged (kinetic energy is $\sim k^2$); wavefunctions change as $\chi_{kl}^{(\pm)}(r) = (-1)^l \chi_{-kl}^{(\mp)}(r)$. Thus

$$\frac{b_l(k)}{a_l(k)} = \frac{a_l(-k)}{b_l(-k)}, \quad S_l(k) = S_l^{-1}(-k)$$

Next, from time reversal symmetry, complex conjugation transforms a solution of S.E. $\chi_{kl}(r)$ to another solution of the same S.E., $\chi_{kl}^*(r)$.

Combining with uniqueness of the solution (1), obtain

$$\frac{a_l(k)}{b_l(k)} = \frac{b_l^*(k)}{a_l^*(k)}, \quad S_l(k) = \left(S_l^{-1}(k)\right)^*$$

(for real k). Extending k to the complex plane, we find

$$S_l(k) = \left(S_l^{-1}(k^*)\right)^*$$

This gives relations between $S_l(k)$ in the four quadrants:

$$S_l(k) = S_0, \quad S_l(k^*) = \frac{1}{S_0^*}, \quad S_l(-k^*) = S_0^*, \quad S_l(-k) = \frac{1}{S_0}$$

from k plane to E plane; prove analyticity at $\operatorname{Im} E > 0$ ... (see handout material online).

Resonances

Example: 1D motion with a hard wall at $x = 0$ and a delta function $U(x) = u\delta(x-a)$. One channel; S-matrix a 1×1 matrix, a c-number

Method 1. Solve S.E. $E\psi = -\frac{1}{2}\psi'' + u\delta(x-a)\psi$ for $x > 0$:

$$\psi(0 < x < a) = A\sin kx, \quad \psi(x > a) = e^{-ik(x-a)} + Se^{ik(x-a)}$$

Matching ψ values: $[\psi']_{a-}^{a+} = u\psi(a)$

$$1 + S = A\sin ka, \quad ik(S-1) - Ak\cos ka = u(1+S)$$

solved by $S = (\sin ka + (k/u)e^{ika})/(\sin ka + (k/u)e^{-ika})$ (explicitly unitary)

Method 2. Summing partial reflected waves (note the hard-wall minus sign):

$$r_{total} = r - t^2e^{2ika} + t^2re^{4ika} - t^2r^2e^{6ika} + ... = r - \frac{t^2e^{2ika}}{1 + re^{2ika}}$$

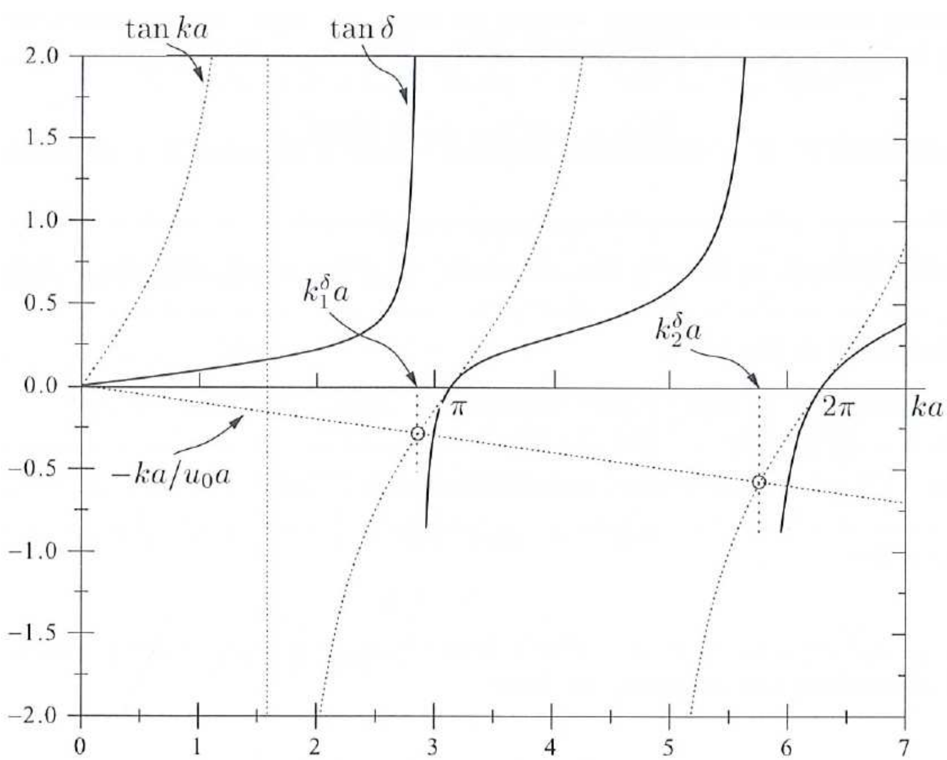
$$= -e^{2ika}\frac{1 + z - ze^{-2ika}}{1 - z + ze^{2ika}} = -e^{2ika}S = e^{2ika}e^{2i\delta}$$

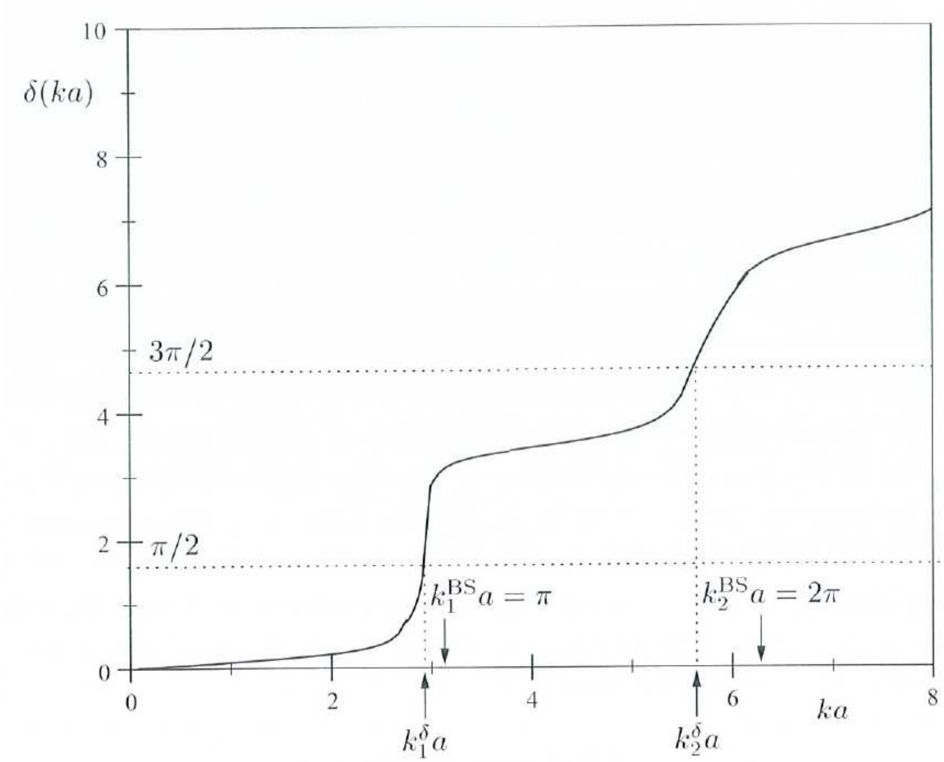
Phase shifts

$$S = -e^{2i\delta}, \quad \tan\delta = \frac{\tan ka}{1 + (u/k)\tan ka}$$

Sanity check: for $u = 0$ have $\delta = ka$, agrees with the wavefunction $\psi(x > 0) = \sin kx$.

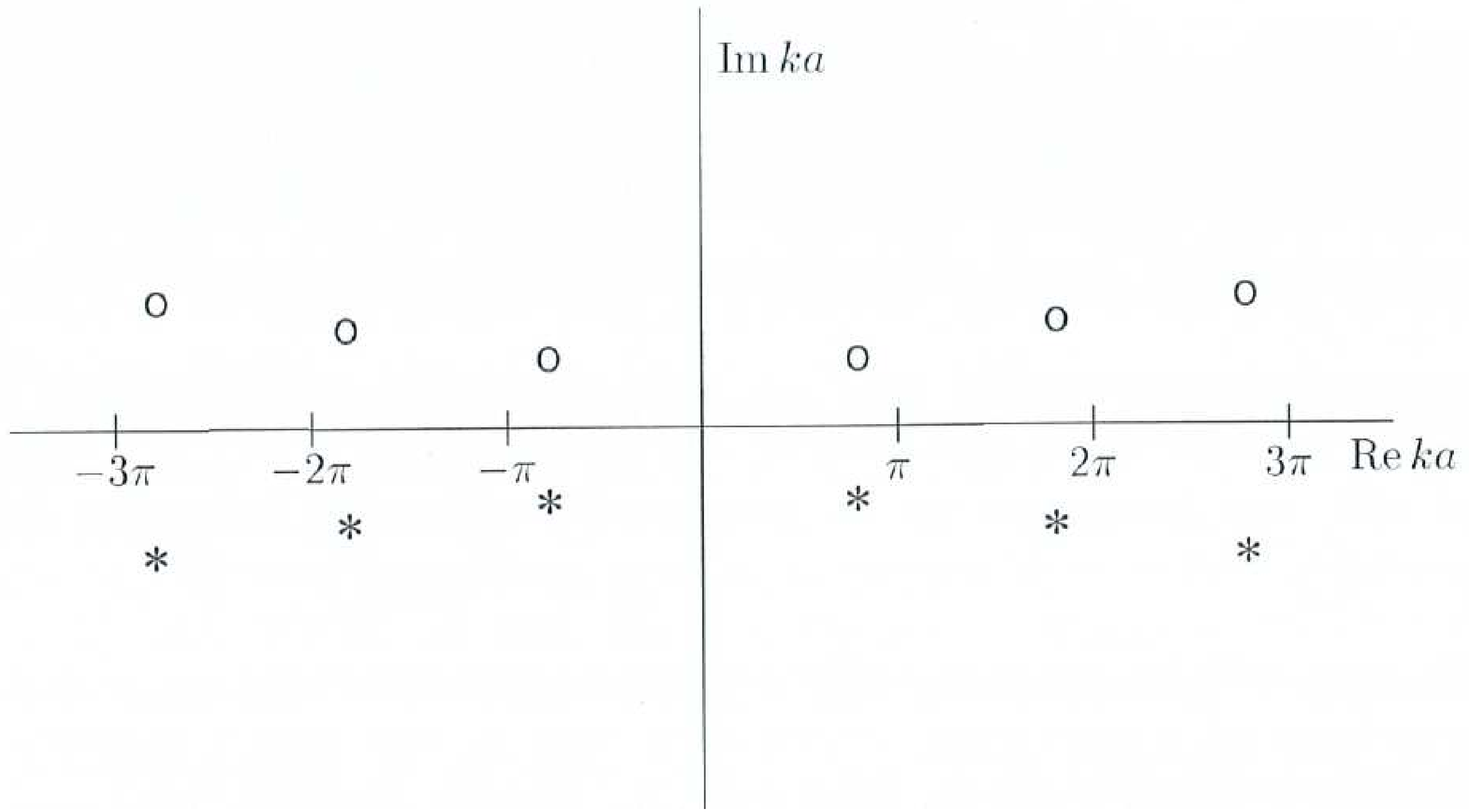
For $u > 0$, kinks in δ of size π located at $ka \approx \pi n$, $n > 0$.





Poles and zeros in the complex k plane

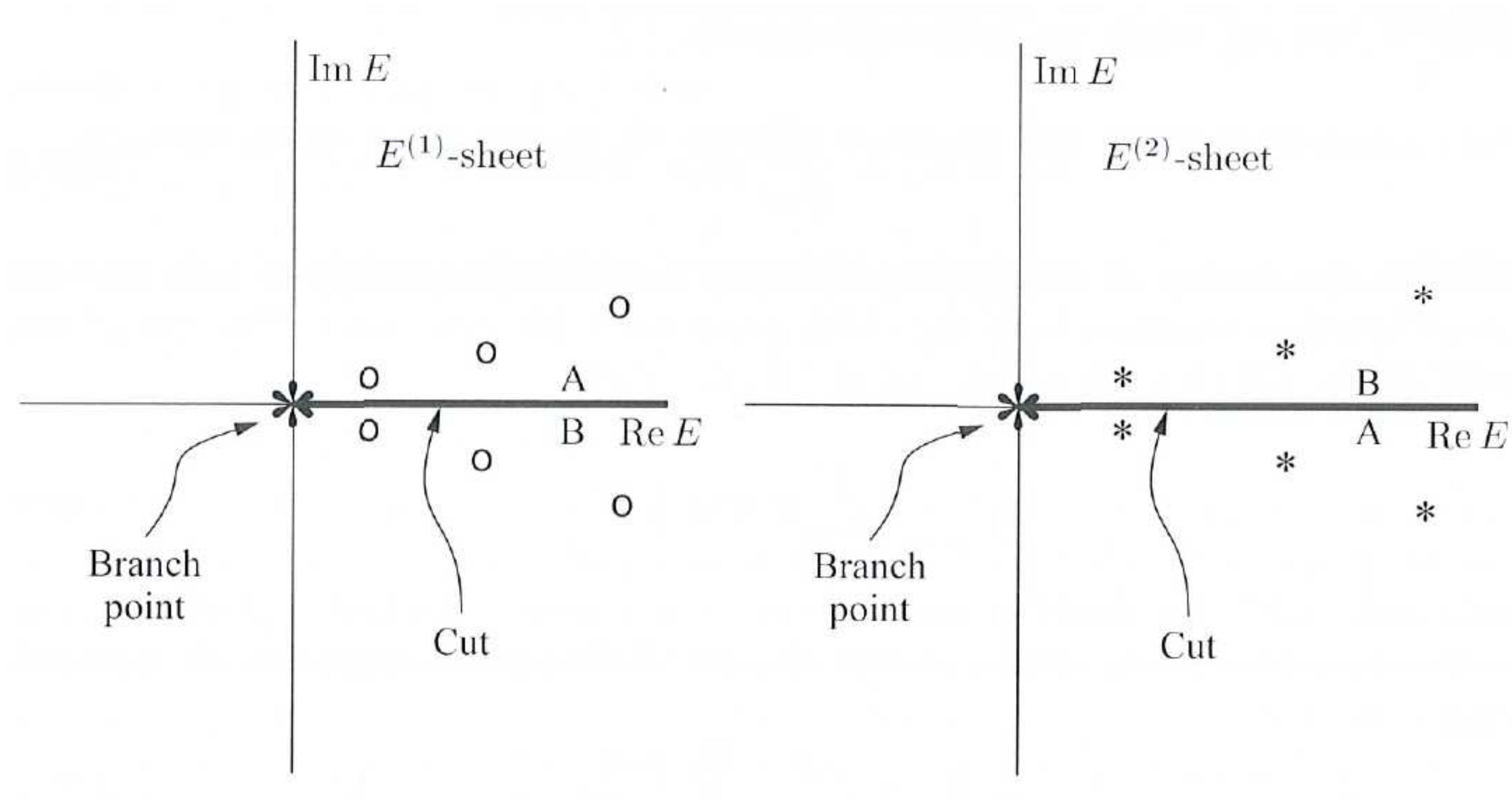
Quasibound states: near each resonance $S \approx \frac{k-k_n-i\kappa_n}{k-k_n+i\kappa_n}$ (true for strong barrier, $u/k_n \gg 1$). Schematically:



Zeros at $\mathrm{Im}\,k > 0$; poles at $\mathrm{Im}\,k < 0$; symmetrically arranged

Complex energy plane

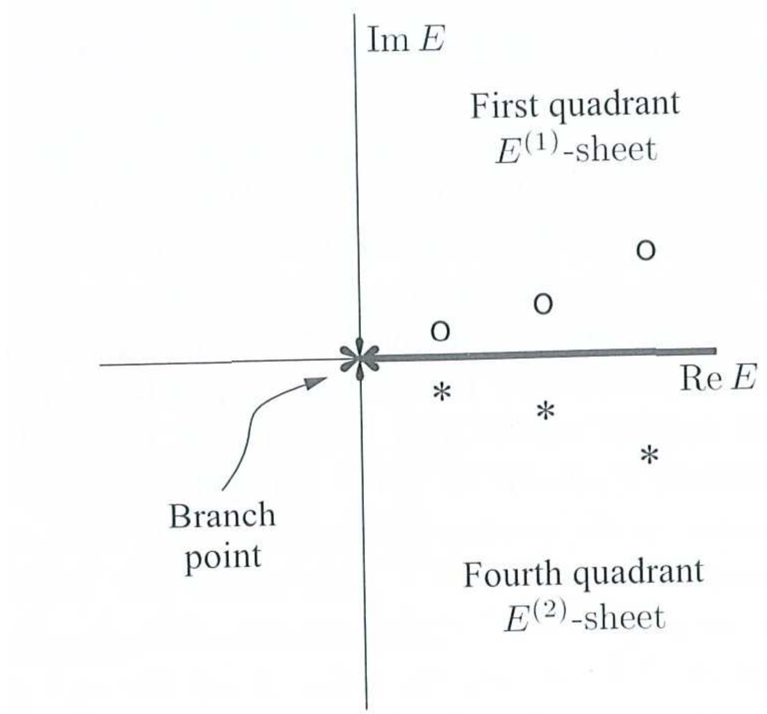
The S-matrix is defined on two Riemannian sheets: $E = k^2/2$.



$S(E)$ analytic on the $E^{(1)}$ sheet.

One-pole approximation

Analytical continuation from the 1st quadrant of $E^{(1)}$ to the 4th quadrant of $E^{(2)}$.



Breit-Wigner behavior near resonance:

$$S(E) \approx -\frac{E - E_n - i\gamma_n/2}{E - E_n + i\gamma_n/2}$$

Quasistationary states

Seek solution of S.E. $E\psi = -\frac{\hbar^2}{2m}\psi'' + U(x)$ with only an outgoing wave, no incoming wave:

$$\psi_{asym} = \psi_{in} + \psi_{out} = \psi_{in} + S(E)\psi_{in}, \quad S(E) \to \infty, \quad \psi_{in} \to 0$$

Unitarity violated, complex-valued energy eigenstates. Near a pole $S(E) \approx -\frac{E-E_0-i\gamma/2}{E-E_0+i\gamma/2}$ find solution $E = E_0 - i\gamma/2$

Time evolution $\psi(t) \propto e^{-iEt} = e^{-iE_0t}e^{-\frac{1}{2}\gamma t}$, thus γ is the decay rate. Generalization of Gamow's tunneling theory.

Example: S.E. on the semi-axis $x > 0$ with $U(x) = u\delta(x-a)$ (see above). Setting $S(E) = \infty$, have

$$1-z+ze^{2ika} = 0, \quad 2ika = \ln\left(1 - \frac{1}{z}\right) = 2\pi in - \frac{1}{z} - \frac{1}{2z^2} + O(z^{-3}), \quad z = \frac{u}{2ik}$$

weak tunneling, large u limit. Find $k = \pi n/a + \Delta k$, $\Delta k = \Delta k' - i\Delta k''$, $\Delta k'' = \frac{\hbar^4(\pi n/a)^2}{4am^2u^2}$. The decay rate is $\gamma = 2\mathrm{Im}\,E = 2\frac{\hbar^2}{m}k_n\Delta k''_n$

Scattering on an inverted parabola revisited

For the scattering problem $E\psi = -\frac{1}{2}\psi'' - \frac{1}{2}x^2\psi$ find quasi-energy states: (i) Try $\psi_0(x) = e^{ix^2/2}$ (pure outgoing wave), get $E_0 = -i/2$; (ii) Generalize to $\psi_n(x) = H_n(ix)e^{ix^2/2}$ (may need to change the mass sign, $m' = -m$!). Find the spectrum of quasi-energies: $E_n = -i(n + \frac{1}{2})$.

For a symmetric potential, the scattering matrix is diagonal in the basis of the even and odd wavefunctions:

$$S = e^{2i\delta_+}|+\rangle\langle+| + e^{2i\delta_-}|-\rangle\langle-| = \frac{1}{2}\begin{pmatrix} e^{2i\delta_+} + e^{2i\delta_-} & e^{2i\delta_+} - e^{2i\delta_-} \\ e^{2i\delta_+} - e^{2i\delta_-} & e^{2i\delta_+} + e^{2i\delta_-} \end{pmatrix}$$

Consider $f(E) = t(E)/r(E) = (e^{2i\delta_+} - e^{2i\delta_-})/(e^{2i\delta_+} + e^{2i\delta_-})$. Because $e^{2i\delta_+}$ has poles at E_n and zeros at $-E_n$ with n even, and $e^{2i\delta_-}$ has poles at E_n and zeros at $-E_n$ with n odd. Therefore:

$$f(E_n) = +1 \ (n = 2k), \quad f(-E_n) = -1 \ (n = 2k),$$

$$f(-E_n) = +1 \ (n = 2k+1), \quad f(E_n) = -1 \ (n = 2k+1),$$

An analytic function of E that takes these values at $\epsilon = E_n$ is $ie^{\pi\epsilon}$. Such a function is unique, thus $f(\epsilon) = t(\epsilon)/r(\epsilon) = ie^{\pi\epsilon}$.

Combining this with unitarity $|t(E)|^2 + |r(E)|^2 = 1$, obtain

$$|r(E)|^2 = \frac{1}{1+e^{2\pi E}}, \quad |t(E)|^2 = \frac{1}{1+e^{-2\pi E}}$$

in agreement with what we have found in Lecture 2.

Alternative route: use modified creation and annihilation operators $a = 2^{-1/2}(x+i\frac{d}{dx})$, $a^\dagger = 2^{-1/2}(x-i\frac{d}{dx})$, $[a, a^\dagger] = i$ to write the Hamiltonian as $H = -a^\dagger a - \frac{i}{2}$ etc.

Projecting Hamiltonian on the single-resonance subspace

Example: hard wall + a delta function (again!)

Suppose we are interested only in the energies near one resonance E_n (e.g. Fermi level is aligned with resonance). For a narrow resonance $\Gamma \ll \Delta E, E_F$ ($\Delta E = E_{n+1} - E_n$) we can write

$$H_{res} = -i\hbar v_F \frac{d}{dx} + E_n |n\rangle\langle n| + \lambda |x=0\rangle\langle n| + \lambda^* |n\rangle\langle x=0|$$

where $\langle x'|x=0\rangle = \delta(x-x')$. Here $-\infty < x < \infty$, i.e. the x-axis is unfolded.

For the wavefunction $\sum_x \psi(x)|x\rangle + \phi|n\rangle$ write S.E. as

$$E\psi(x) = -i\hbar v_F \psi'(x) + \lambda\delta(x)\phi, \quad E\phi = E_n\phi + \lambda^* \int dx \delta(x)\psi(x)$$

Generally $\psi(x)$ has a jump at zero, thus the 2nd equation must be understood as $(E - E_n)\phi = \frac{1}{2}\lambda^* \left(\psi(0+) + \psi(0-)\right)$.

Solving:

$$-i\hbar v_F\left(\psi(0+)-\psi(0-)\right)+\frac{|\lambda|^2}{2(E-E_n)}\left(\psi(0+)+\psi(0-)\right)$$

$$\psi(0+)\left(\gamma/2-i(E-E_n)\right)+\psi(0-)\left(\gamma/2+i(E-E_n)\right)=0,\quad \gamma=\frac{|\lambda|^2}{\hbar v_F}$$

$$\psi(0+)=\psi(0-)\frac{E-E_n-i\gamma/2}{E-E_n+i\gamma/2}$$

Phase shift changes by π across the resonance:

$$e^{2i\delta}=-\frac{E-E_n-i\gamma/2}{E-E_n+i\gamma/2},\quad \cot\delta=2(E-E_n)/\gamma$$

Lifetime of a resonance state coupled to continuum

Initial state: $\phi = 1$, $\psi_{in} = 0$.

$$(E - E_n)\phi = \frac{1}{2}\lambda^* \left(\psi(0+) + 0\right), \quad -i\hbar v_F \left(\psi(0+) - 0\right) + \lambda\phi = 0$$

Eliminate $\psi(0+)$ and write $(E - E_n)\phi = -i\frac{1}{2}\gamma\phi$ (note complex quasi-energy $E = E_n - \frac{i}{2}\gamma$).

In the time representation this gives

$$i\dot{\phi} = \left(E_n - \frac{i}{2}\gamma\right)\phi, \quad \phi(t) = e^{-E_n t} e^{-\frac{1}{2}\gamma t}$$

Generalization of Wigner-Weisskopf treatment of atom radiation.

Resonance coupled to two leads

Example: 1D S.E. with a potential $U(x) = u_1\delta(x+a/2) + u_2\delta(x-a/2)$.

Method 1. Summing partial waves in analogy with the Fabry-Perot interferometer problem:

$$t_{total} = t_1 t_2 + t_1 r_1 r_2 t_2 e^{2ika} + t_1 t_2 (r_2 t_2 e^{2ika})^2 + ... = \frac{t_1 t_2}{1 - r_1 r_2 e^{2ika}}$$

$$r_{total} e^{ika} = r_1 + t_1^2 r_2 e^{2ika} + t_1^2 r_2^2 r_1 e^{4ika} + ... = r_1 + \frac{t_1^2 r_2 e^{2ika}}{1 - r_1 r_2 e^{2ika}}$$

Check unitarity!

Method 2. Project on the resonance subspace ($x_{1,2} = x_{\mathrm{Left,Right}}$):

$$H_{res} = -i\hbar v_F \frac{d}{dx_1} - i\hbar v_F \frac{d}{dx_2} + E_n|n\rangle\langle n| + (\lambda_1|x_1 = 0\rangle + \lambda_2|x_2 = 0\rangle)\langle n| + \mathrm{h.c.}$$

Let $\lambda_1 = \lambda_2$. Define the even and odd states $\psi_\pm = 2^{-1/2}(\psi_+ \pm \psi_-)$. The resonant level couples to ψ_+ only:

$$H_{res} = -i\hbar v_F \frac{d}{dx_+} - i\hbar v_F \frac{d}{dx_-} + E_n|n\rangle\langle n| + \sqrt{2}\lambda|x_+ = 0\rangle\langle n| + \mathrm{h.c.}$$

Note $\lambda' = \sqrt{2}\lambda$. For scattering in the even and odd channels find $\psi_{+,out} = e^{2i\delta}\psi_{+,in}$, $\psi_{-,out} = \psi_{-,in}$ which gives

$$r + t = e^{2i\delta}, \quad r - t = 1 \quad \to \quad r = \frac{1}{2}\left(e^{2i\delta} + 1\right), \quad t = \frac{1}{2}\left(e^{2i\delta} - 1\right)$$

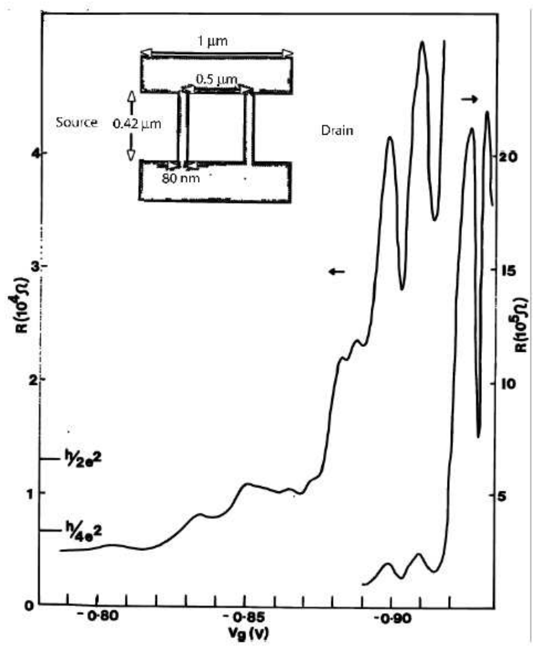
Lorentzian peak in transmission (Note perfect transmission on resonance):

$$T(E) = |t|^2 = \frac{1}{2}(1 - \cos 2\delta) = \frac{1}{4}\left[2 - \frac{E - E_n - i\gamma}{E - E_n + i\gamma} + \mathrm{h.c.}\right] = \frac{\gamma^2}{(E - E_n)^2 + \gamma^2}$$

Resonances in electron cavity

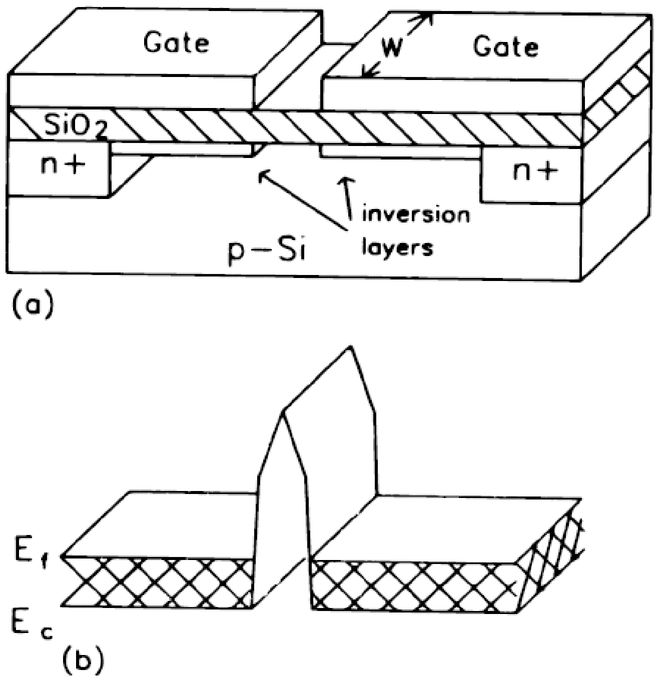
Resonance peaks in conductance:

$$G(E) = \frac{e^2}{h} \frac{\Gamma_L \Gamma_R}{(E - E_0)^2 + \frac{1}{4}(\Gamma_L + \Gamma_R)^2}$$

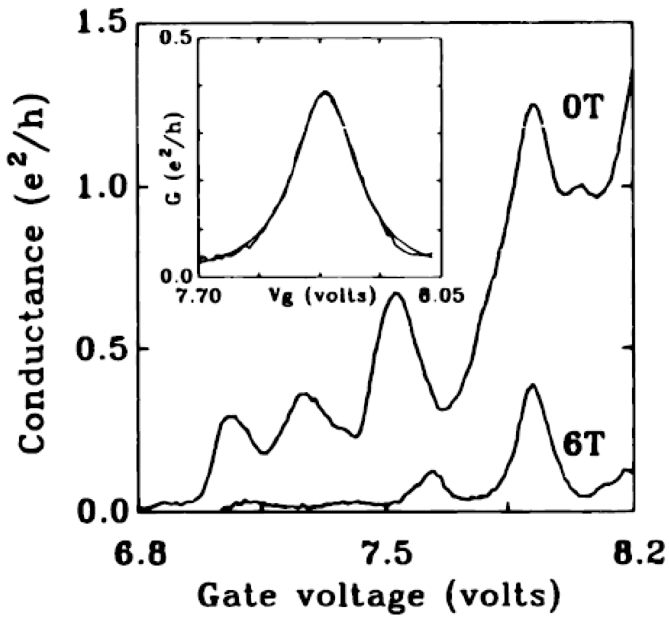


Resistance versus gate voltage of a cavity (defined by gates on top of a GaAs-AlGaAs heterostructure; see inset), showing plateau like features (for $R \lesssim h/2e^2$) and tunneling resonances (for $R \gtrsim h/2e^2$). The left- and right-hand curves refer to the adjacent resistance scales. Taken from C. G. Smith et al., Surf. Sci. **228**, 387 (1990).

Localized resonance levels in the tunnel barrier

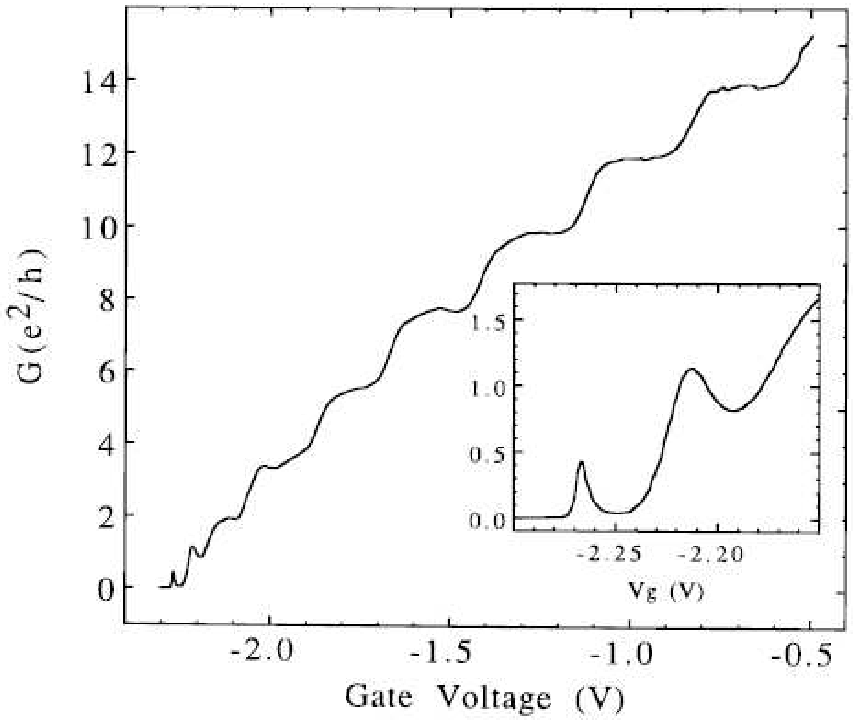


Schematic diagram of a Si MOSFET with a split gate (a), which creates a potential barrier in the inversion layer (b). Taken from T. E. Kopley et al. Phys. Rev. Lett. **61**, 1654 (1988).



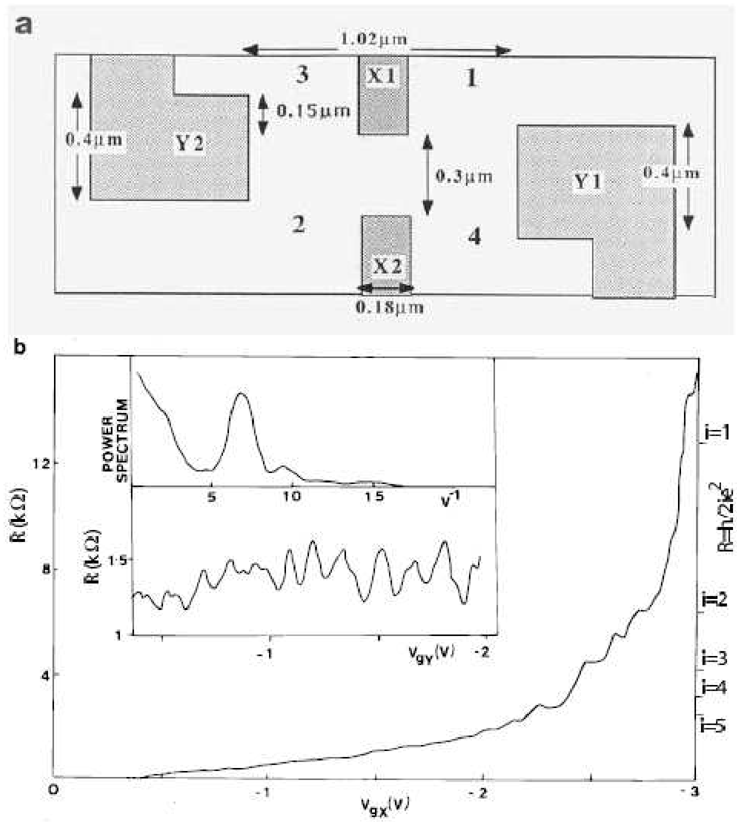
Oscillations in the conductance as a function of gate voltage at 0.5 K are attributed to resonant tunneling through localized states in the potential barrier. A second trace is shown for a magnetic field of 6 T (with a horizontal offset of $-0.04\,\mathrm{V}$). The inset is a close-up of the largest peak at 6 T, together with a Lorentzian fit. Taken from T. E. Kopley et al. Phys. Rev. Lett. **61**, 1654 (1988).

IN A QUANTUM POINT CONTACT



Conductance as a function of gate voltage for a quantum point contact at 0.55 K. The inset is a close-up of the low-conductance regime, showing peaks attributed to transmission resonances associated with impurity states in the constriction. Taken from P. L. McEuen et al., Surf. Sci. **229**, 312 (1990).

In a Fabry-Perot resonator



(a) Schematic diagram of a constriction with two adjustable external reflectors defined by gates on top of a GaAs-AlGaAs heterostructure. (b) Plot of the constriction resistance as a function of gate voltage with the external reflector gates (Y1, Y2) grounded. Inset: Fabry-Perot-type transmission resonances due to a variation of the gate voltage on the reflectors (Y1, Y2) (bottom panel), and Fourier power spectrum (top panel). Taken from C. G. Smith et al., Surf. Sci. **228**, 387 (1990).