Scattering of electrons from an interacting region

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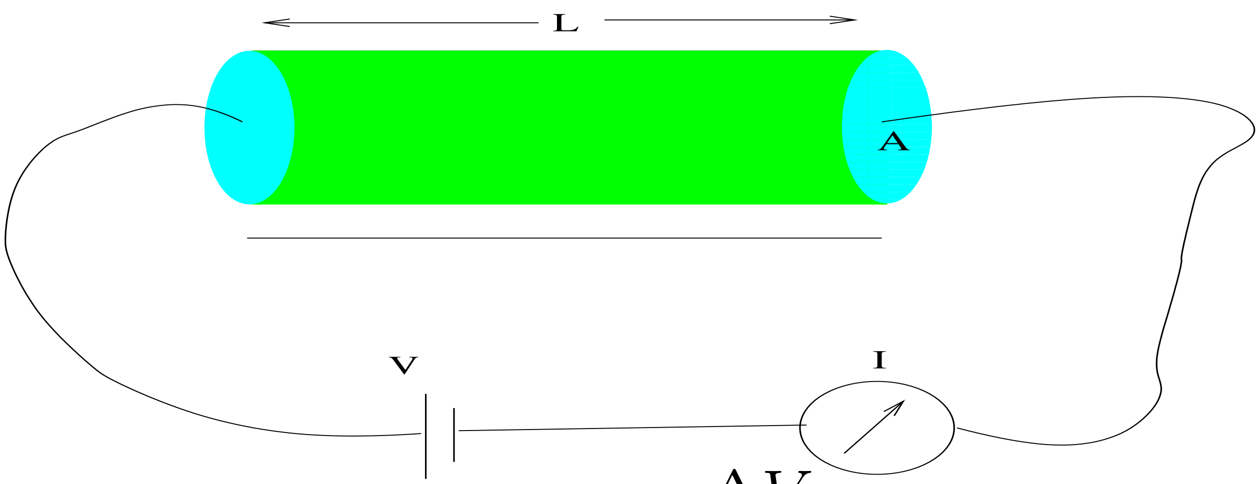
Phys. Rev. Lett. **101**, 066805 (2008)

The problem of transport



$$I = \frac{\Delta V}{R} = G\Delta V$$

$$G = \frac{1}{R} = \text{ conductance of system}$$

For macroscopic systems it is usual to define the resistivity and conductivity of the material

$$\rho = \frac{RA}{l} \quad \sigma = \frac{1}{\rho} \; .$$

Calculating conductivity

Microscopic theories for σ:

- Kinetic theory (Boltzmann transport theory). Think of diffusing electrons with mean collision time τ_c.

$$\sigma = \frac{ne^2\tau_c}{m}$$

.

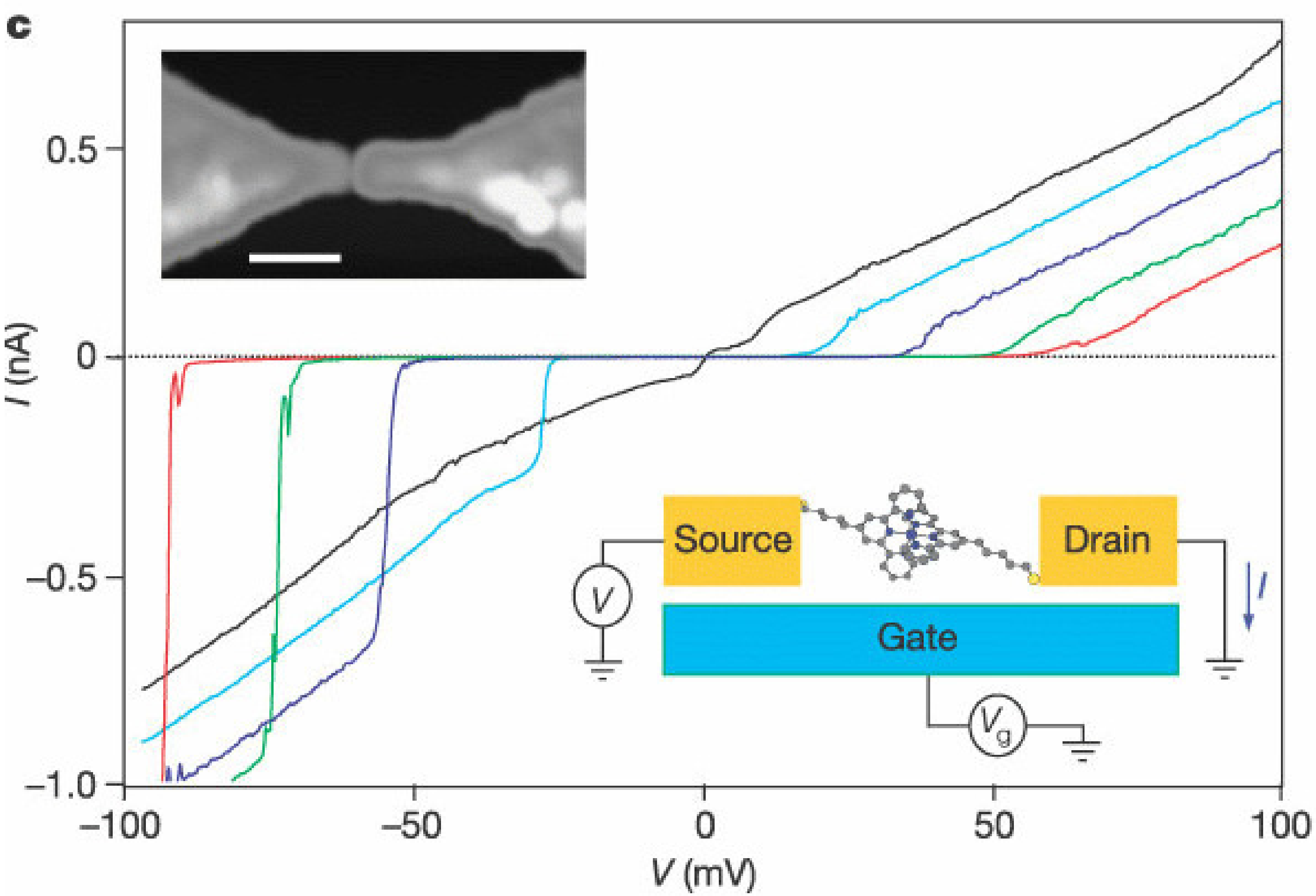
- Green-Kubo formula:

$$\sigma = () \lim_{\tau\to\infty} \lim_{L\to\infty} \int_0^{\tau} dt \langle J(0)J(t)\rangle$$

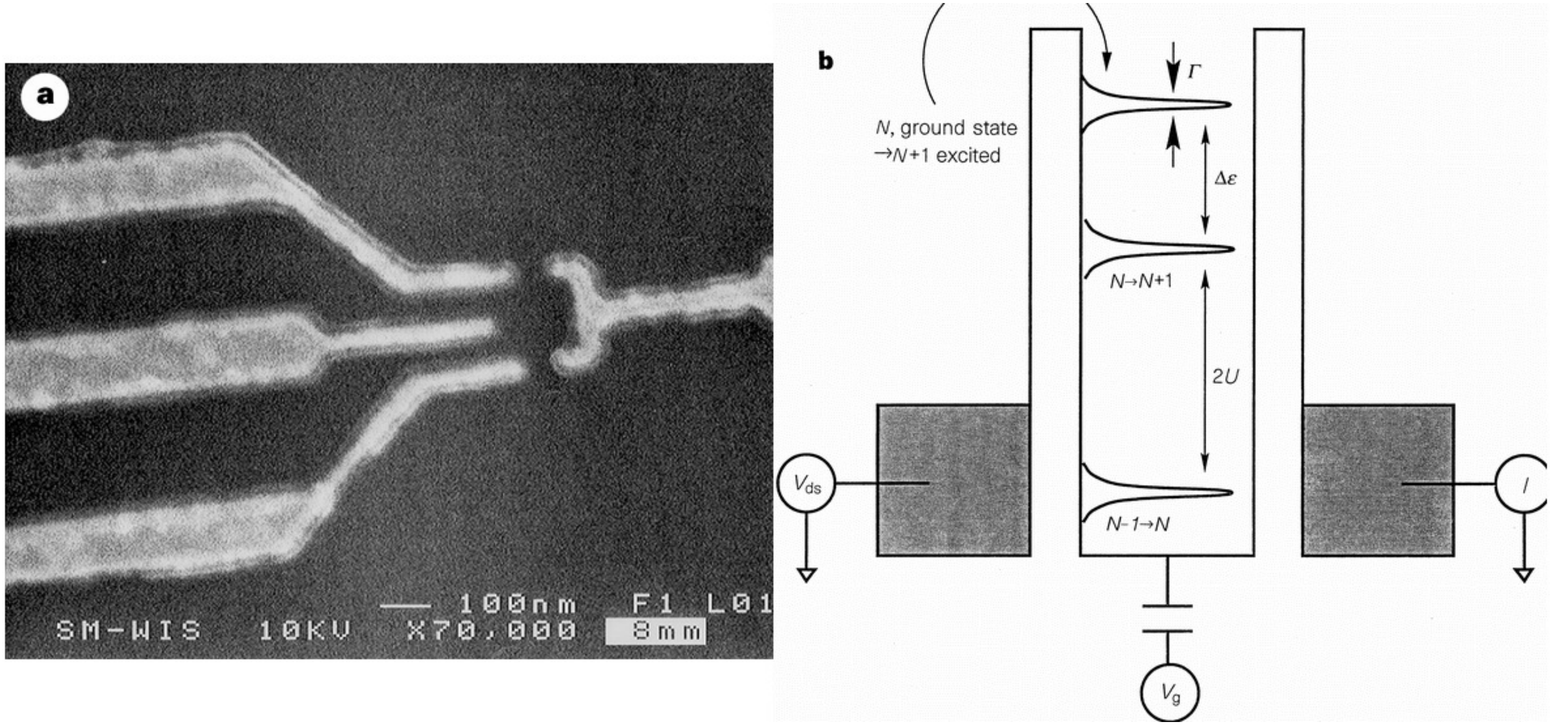
Infinite system size limit necessary.

Small systems

What about transport in mesoscopic systems and nanosystems ?



Small systems



Calculating conductance

Above theories are not directly applicable. It is not meaningful to talk of conductivity. Rather one is interested in the conductance:

$$G = \frac{I}{\Delta V}.$$

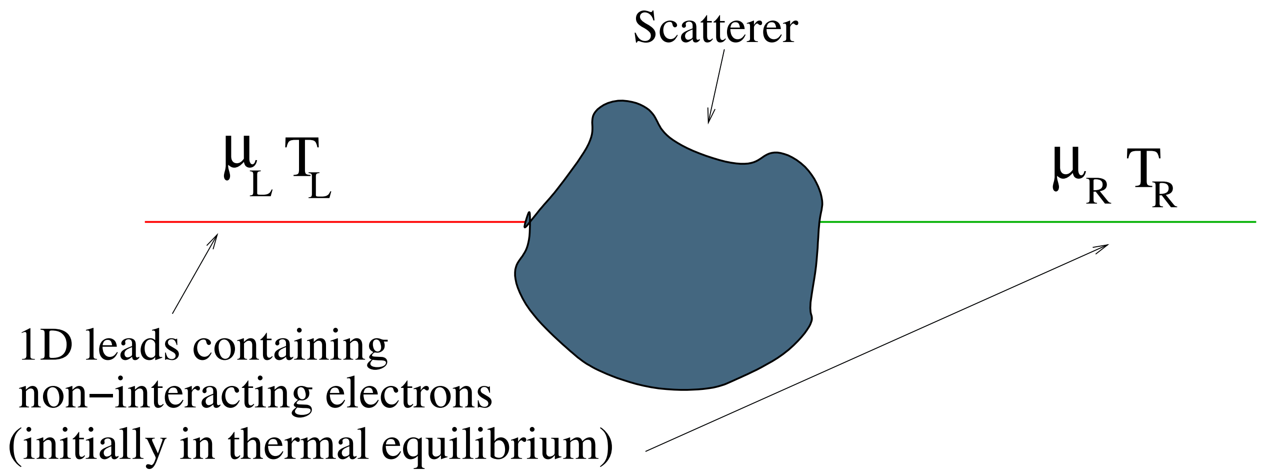
Main question: How do we calculate this?

Conductivity: Intrinsic property of system.

Conductance: Properties of reservoirs (leads) and contacts important and should be incorporated into calculation.

Non-interacting electrons: Landauer formalism

This is the most popular approach in mesoscopic physics. Views conduction as a quantum mechanical transmission problem. Simplest version:

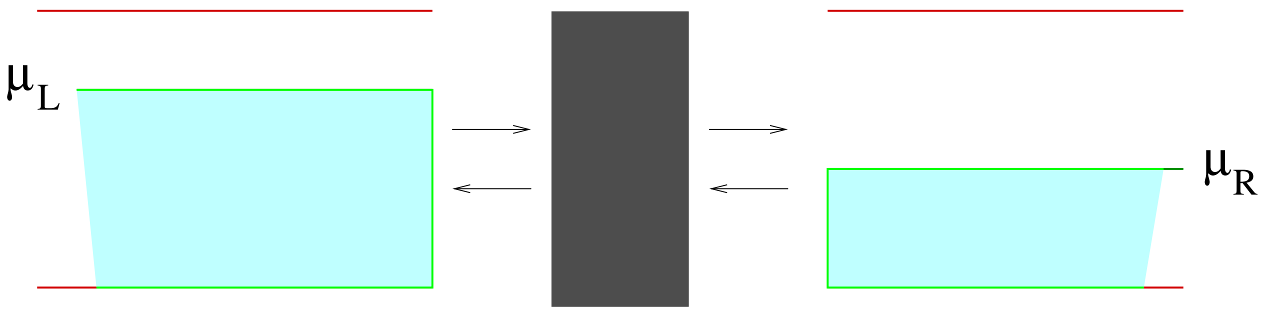


Electronic scattering states given by:

$$\begin{aligned} \psi_k(x) &= e^{ikx} + r_k e^{-ikx} \quad \text{left lead} \\ &= t_k e^{ikx} \quad \text{right lead} \end{aligned}$$

Transmission: $T(\epsilon_k) = |t_k|^2$.

Landauer formula



$$I = \frac{e}{2\pi\hbar}\int d\epsilon T(\epsilon)[f(\mu_L, T_L, \epsilon) - f(\mu_R, T_R, \epsilon)]$$

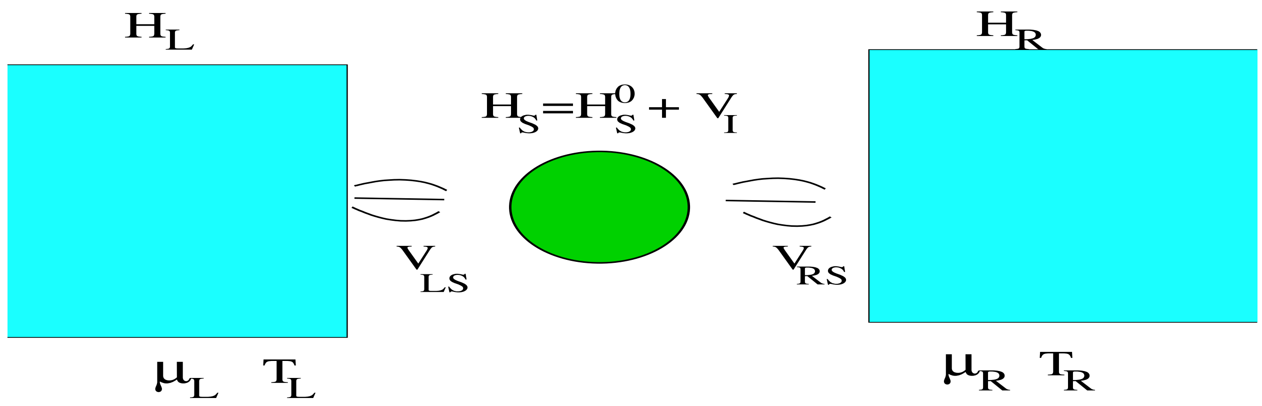
For $T_L = T_R = 0$:

$$\begin{aligned} I &= \frac{e}{2\pi\hbar}T(\epsilon_F)\Delta\mu = \frac{e^2}{2\pi\hbar}T(\epsilon_F)\Delta V \\ G &= \frac{I}{\Delta V} = \frac{e^2}{h}T(\epsilon_F)\ . \end{aligned}$$

The Landauer formula. →Keldysh formalism, quantum Langevin equations also give this.

Interacting electrons

What happens when electrons DO NOT interact while in the leads, but DO interact in the sample region. This is a harder problem.



$H_S^0 + H_L + H_R$ is non-interacting (quadratic Hamiltonian).

Coupling $V_C = V_{LS} + V_{RS}$ is also quadratic.

V_I is non-quadratic and represents interactions in sample.

General approach

Finding density matrix of nonequilibrium steady state (NESS): Solution in two stages.

- Start with $V_C = V_I = 0$ and

$$\rho(t=0) = \rho_L^{eq}(\mu_L, T_L) \otimes \rho_S \otimes \rho_R^{eq}(\mu_R, T_R)$$

- Let $H_0 = H_S^0 + H_L + H_R + V_C$. Evolve for infinite time using H_0 and find ρ_0^{NESS}.
- Start with ρ_0^{NESS}. Evolve again for an infinite time using $H_0 + V_I$ and find ρ_I^{NESS}.

Calculate: $J = Tr[\hat{J}\rho_I^{NESS}]$.

Our contribution: Solving this problem at zero temperature .

Zero temperature case

In this case $\rho_0^{NESS} \to |\phi\rangle$ which is a many-particle state satisfying:

$$H_0|\phi\rangle = E|\phi\rangle \ .$$

The state $|\phi\rangle$ is known exactly. It is formed of single particle states, $|\phi\rangle = |k_1, k_2, ...k_N\rangle$, and consists of right moving states $(k > 0)$ filled up to μ_L and left moving states $(k < 0)$ filled up to μ_R.
With this as the "incident" state we try to find the "scattering state" $|\psi\rangle$ satisfying the equation:

$$(H_0 + V_I)|\psi\rangle = E|\psi\rangle \ .$$

$|\psi\rangle$ corresponds to ρ_I^{NESS} and we calculate the current using $\langle\psi|\hat{J}|\psi\rangle$.

Lippman-Schwinger theory

$$(H_0 + V)|\psi\rangle = E|\psi\rangle$$

For "incident" state $|\phi\rangle$ the solution is given by:

$$\begin{aligned}
|\psi\rangle &= |\phi\rangle + \frac{1}{E + i\eta - H_0} V_I |\psi\rangle \\
&= |\phi\rangle + G_0 V_I |\psi\rangle \\
&= |\phi\rangle + G_0 V |\phi\rangle + G_0 V_I G_0 V_I |\phi\rangle + \ldots ,
\end{aligned}$$

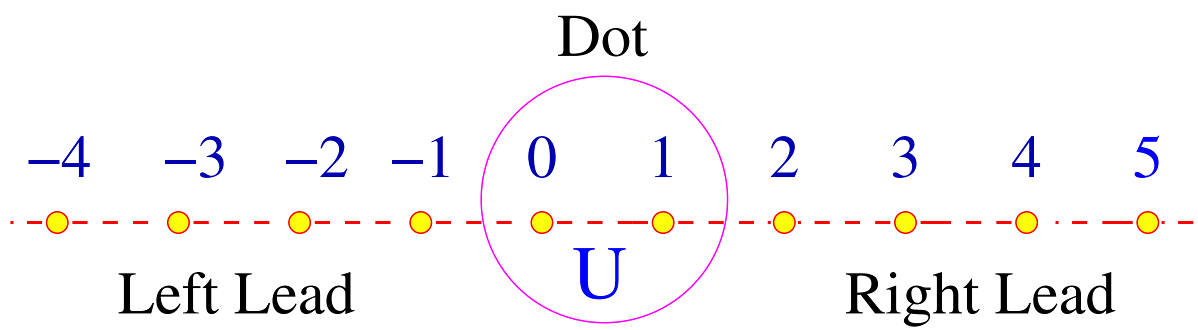
where $G = \frac{1}{E+i\eta-H_0}$ is the non-interacting Green's function.

Can find scattering state (and thus the nonequilibrium steady state) perturbatively.

Earlier work

- Mehta and Andrei, PRL (2006)
  For particular model with δ-function interaction find exact many-particle scattering state by Bethe-Ansatz. Find a solution corresponding to the correct incident state. Use this to find exact steady state current.
- Goorden and Buttiker, PRL (2007)
  Find two-particle scattering state in a two channel problem with interactions in a local region.
- Nonequilibrium Kondo problem: Results from nonequilibrium Green's function, Numerical RG, Density Matrix RG.

Model of 1D spinles Fermions



- Hamiltonian of the model,

$$H_L = -\sum_{x=-\infty}^{\infty} (c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x),$$
$$V_I = U n_0 n_1,$$

- Single particle state: $\phi_k(x) = e^{ikx}$
  Energy $\epsilon_k = -2\cos k$ and $-\pi < k \leq \pi$.

Two particles

- Two particle incoming state specified by $\mathbf{k} = (k_1, k_2)$ given by:

$$\phi_{\mathbf{k}}(\mathbf{x}) = e^{i(k_1 x_1 + k_2 x_2)} - e^{i(k_2 x_1 + k_1 x_2)}$$

$$E_{\mathbf{k}} = \epsilon_{k_1} + \epsilon_{k_2}.$$

- Two-particle scattering state can be found exactly. Let $\mathbf{0} = (1, 0)$.

$$\begin{aligned} \psi_{\mathbf{k}}(\mathbf{x}) &= \phi_{\mathbf{k}}(\mathbf{x}) + U K_{E_{\mathbf{k}}}(\mathbf{x}) \psi_{\mathbf{k}}(\mathbf{0}) \\ \text{where } K_{E_{\mathbf{k}}}(\mathbf{x}) &= \langle \mathbf{x} | G_0^+(E_{\mathbf{k}}) | \underline{0} \rangle \\ \psi_{\mathbf{k}}(\underline{0}) &= \frac{\phi_{\mathbf{k}}(\underline{0})}{[1 - U K_{E_{\mathbf{k}}}(\underline{0})]} \end{aligned}$$

Two particle S-matrix

- Two electrons from the noninteracting leads with initial momenta (k_1, k_2) emerge, after scattering, with momenta (k_1', k_2'). At $\mathbf{x} = (x_1, x_2)$ one has

$$\frac{x_1}{\sin(k_1')} = \frac{x_2}{\sin(k_2')} \; .$$

- Energy is conserved, i.e., $E_{\mathbf{k}} = E_{\mathbf{k}'}$; but momentum is not conserved because the interaction term $U n_0 n_1$ breaks translation invariance.
- Probably not solvable by Bethe-Ansatz.
- Bound states.

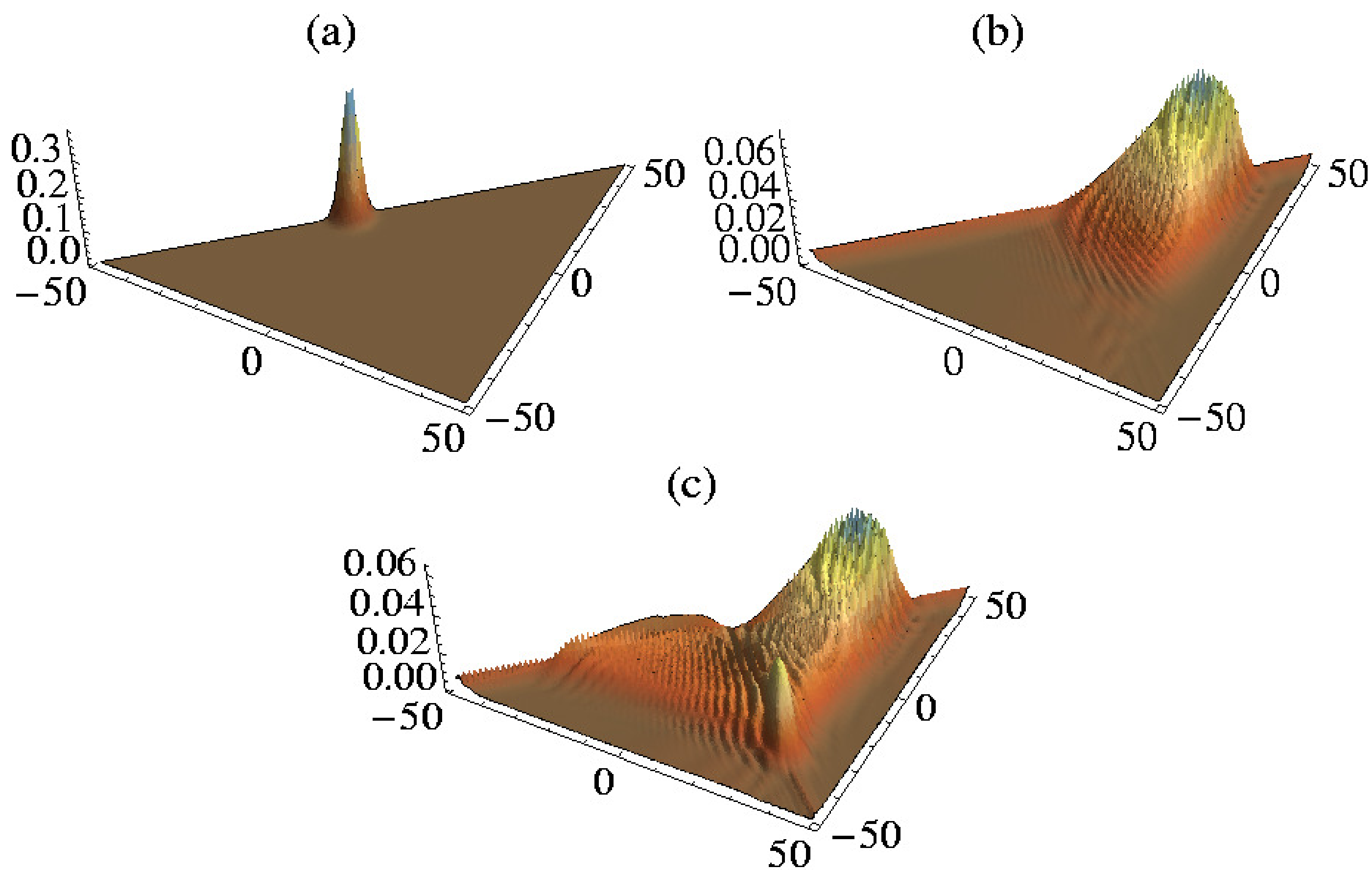
Wavepacket dynamics

- We numerically study time evolution of a two-particle wave-packet which passes throught the interacting region.
- We form the wave-packet with the complete set of the exact two-particle scattering eigenstates and determine their time-evolution through:

$$\Psi(\mathbf{x},t) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dq_1 \int_{-\pi}^{q_1} dq_2\; a(\mathbf{q})\psi_{\mathbf{q}}(\mathbf{x})\; e^{-iE_{\mathbf{q}}t},$$

$$\text{where}\;\; a(\mathbf{q}) = \sum_{x_1>x_2} \Psi(\mathbf{x},t=0)\;\psi^*_{\mathbf{q}}(\mathbf{x}).$$

Wavepacket dynamics



(a) incident wave-packet, (b) after passing through the origin with $U = 0$, (c) after passing through the origin with $U = 2$.

Two-particle current.

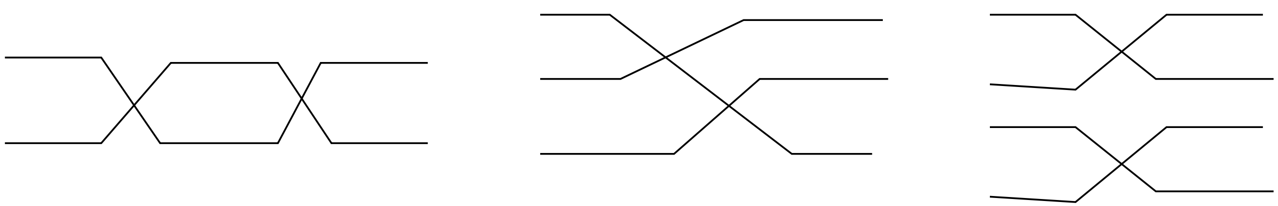
- Current is given by the expectation value of the operator $j_x = -i(c_x^\dagger c_{x+1} - h.c.)$ in the scattering state $|\psi_\mathbf{k}\rangle = |\phi_\mathbf{k}\rangle + |S_\mathbf{k}\rangle$.
- Current in the incident state is given by $\langle\phi_\mathbf{k}|j_x|\phi_\mathbf{k}\rangle = 2[\sin(k_1) + \sin(k_2)]\mathcal{N}$, $\mathcal{N} =$ total number of sites in the entire system.
- Change in current due to scattering,

$$
\begin{aligned}
\delta j(k_1, k_2) &= \langle S_\mathbf{k}|j_x|S_\mathbf{k}\rangle + \langle S_\mathbf{k}|j_x|\phi_\mathbf{k}\rangle + \langle\phi_\mathbf{k}|j_x|S_\mathbf{k}\rangle \\
&= \frac{2|\phi_\mathbf{k}(\underline{0})|^2 Im[K_{E_\mathbf{k}}(\underline{0})]}{|1/U - K_{E_\mathbf{k}}(\underline{0})|^2} [sgn(k_1) + sgn(k_2)]
\end{aligned}
$$

where $sgn(k) \equiv |k|/k$. $\delta j \sim U^2$.

N-particle generalisation

- For incident state $|\phi_{\mathbf{k_N}}\rangle = |k_1, k_2, ...k_N\rangle$ we cannot find $|\psi_{\mathbf{k_N}}\rangle$ exactly for $N \geq 3$.
- Scattered wave is given by $|\psi_{\mathbf{k_N}}\rangle = |\phi_{\mathbf{k_N}}\rangle + |S_{\mathbf{k_N}}\rangle$. Do second order perturbation theory $|S_{\mathbf{k_N}}\rangle = G_0 V_I |\mathbf{k_N}\rangle + G_0 V_I G_0 V_I |\mathbf{k_N}\rangle + ...$
- Three processes at $O(U^2)$.



- Consider only two-particle scattering.

Change in Landauer current

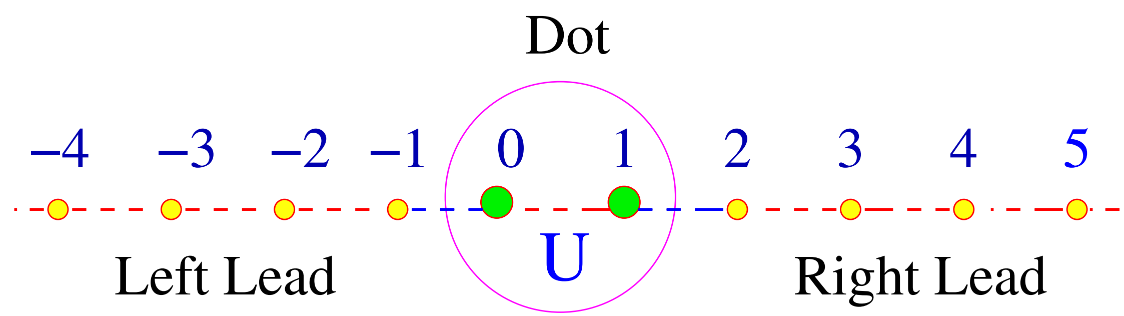
- $\langle \mathbf{k_N} | \hat{j} | \mathbf{k_N} \rangle$ gives the Landauer current.
- Change in current value is given by:

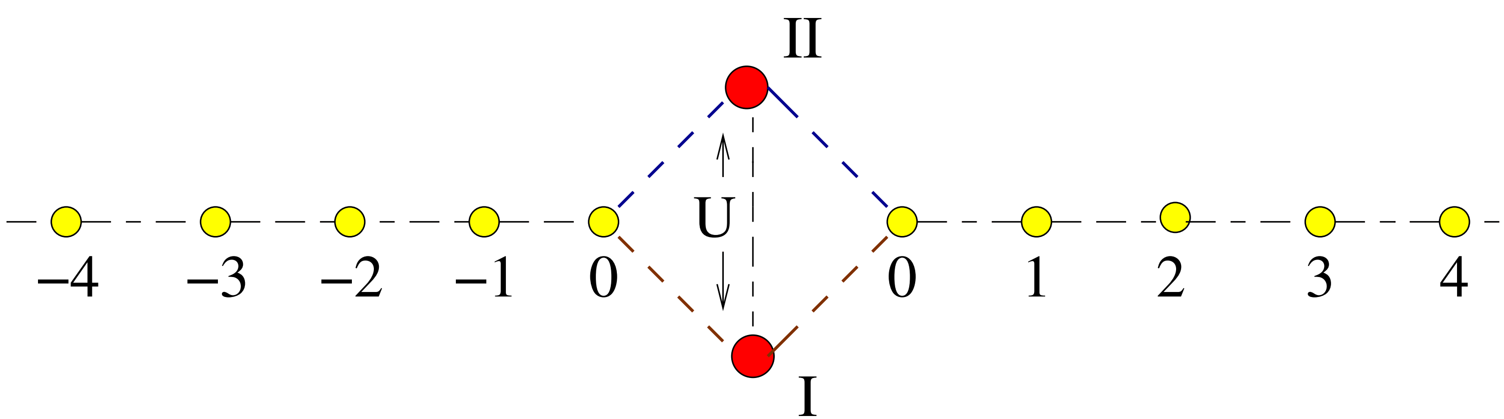
$$\begin{aligned} \delta j_N &= \langle \psi_{\mathbf{k_N}} | \hat{j} | \psi_{\mathbf{k_N}} \rangle - \langle \mathbf{k_N} | \hat{j} | \mathbf{k_N} \rangle \\ &= \frac{1}{2(2\pi)^2} \int dk_1 \int k_2 \delta j(k_1, k_2) \; . \end{aligned}$$

We find that the Landauer current e^2/h is reduced by a term of order U^2. In the presence of impurities reduction is $O(U)$.

Other applications

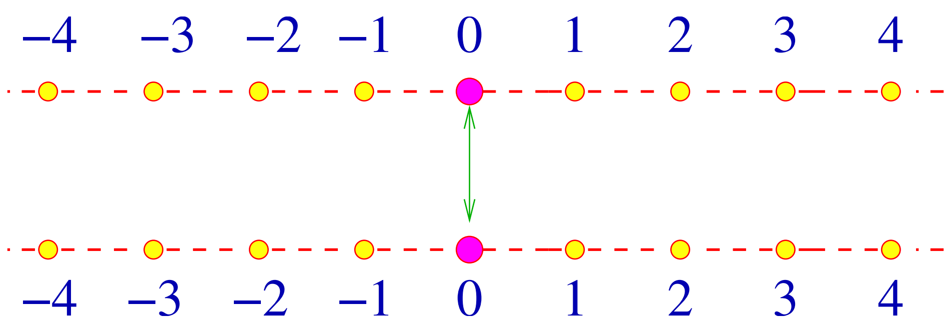
- More general dot with applied gate voltage.
- Study of resonance behaviour in systems like parallel and series double dots.





Other applications

- Parallel conductors in proximity to each other and interacting in some localised region.



- Electrons with spin, interactions on more sites.
- Entanglement by interactions.

Lippman-Schwinger scattering theory provides a nice framework to study zero temperature nonequilibrium steady states of electrons driven across an interacting region by a finite chemical potential bias.