A Crash Course in Quantum Transport: Coherent & Metallic Conduction

Kongju National University
Dept. of Physics Education

Sang-Jun Choi

Summer School of Mesoscopic Physics
@POSTECH, 2024. 5. 24

Overview

- **What is Mesoscopic Quantum Transport (MQT)**

  → What are we exploring?

- **What really happens at coherent & metallic conductions**

  → From perfect conductor to single impurity to Ohmic regime

  → MQT with multi-terminal transport

  → Finite voltage bias and temperature

- **Let us see MQT in action**

  → Examples & Applications from research papers

- **Theoretical machinery**: how to obtain S-matrix

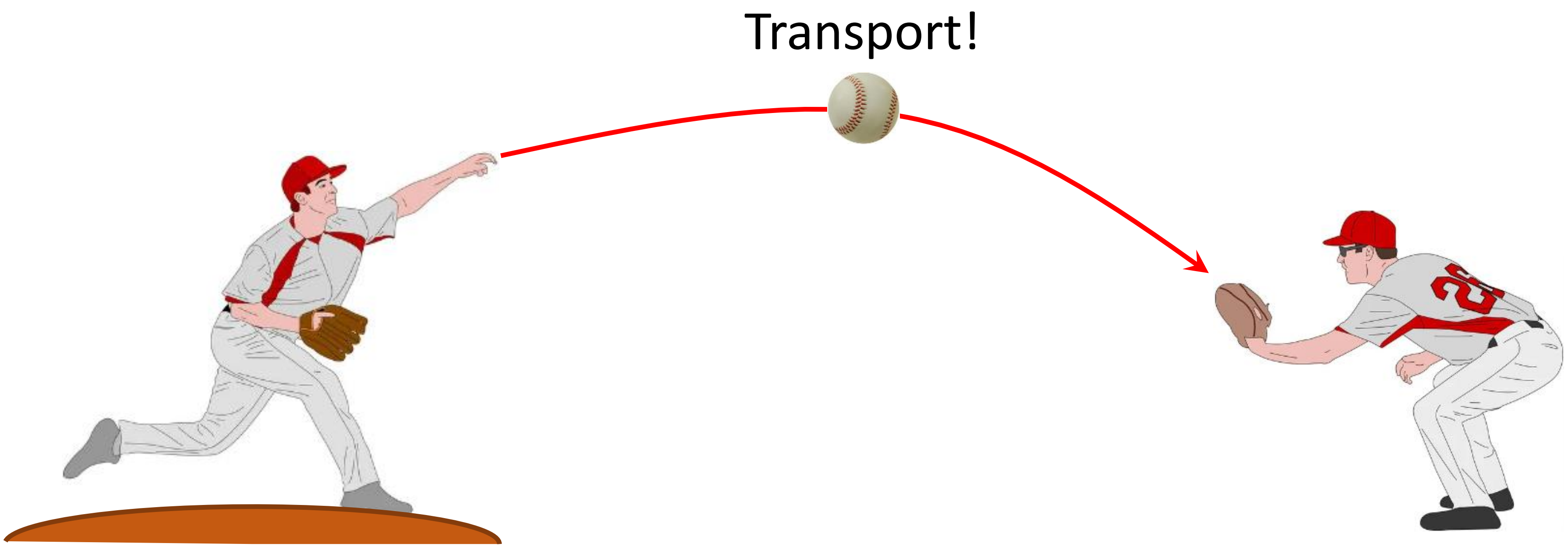
- **Beyond coherent & metallic conductions**

  → A lot more exciting things left for you!

Mesoscopic Quantum Transport in 2 hours!

What is Mesoscopic Quantum Transport

- **Mesoscopic quantum transport**?

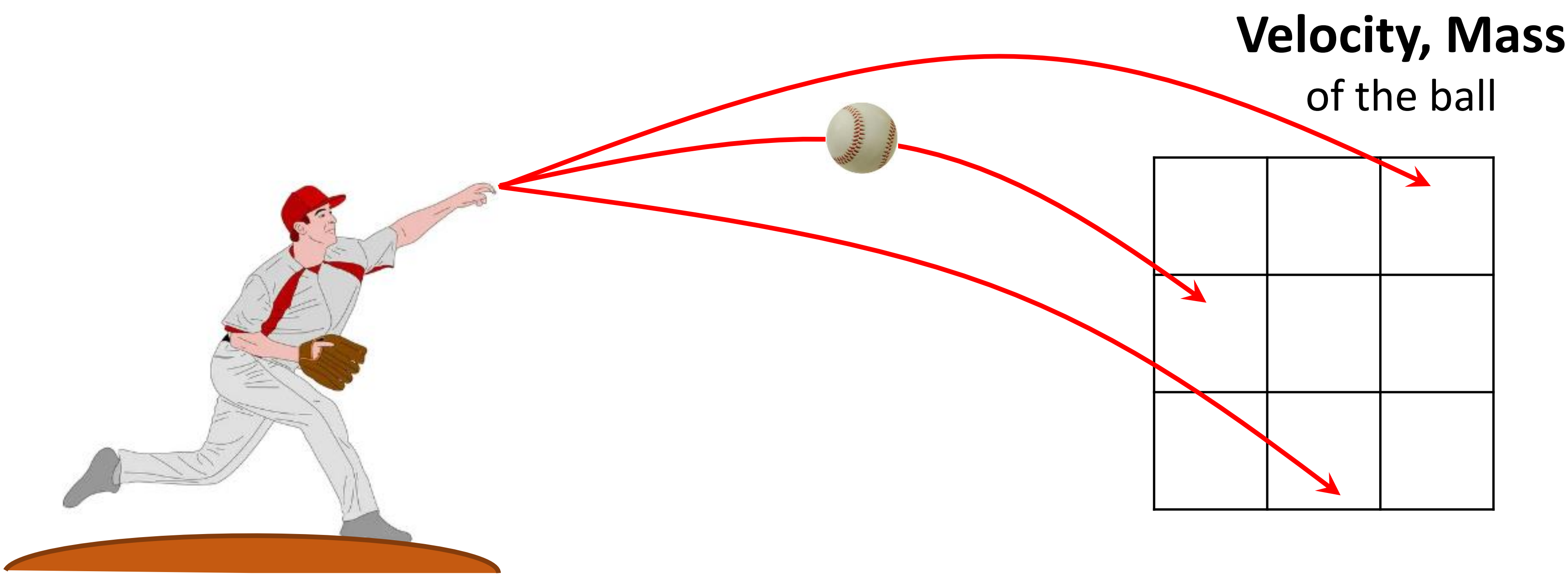


Figures from depositphotos.com

What is Mesoscopic Quantum Transport

- **Mesoscopic quantum transport?**
- **Why 'transport?'**

→ Transport reveals information of transported objects



Figures from depositphotos.com

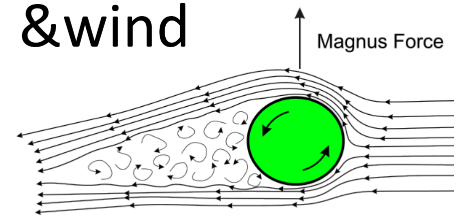
What is Mesoscopic Quantum Transport

- **Mesoscopic quantum transport**?

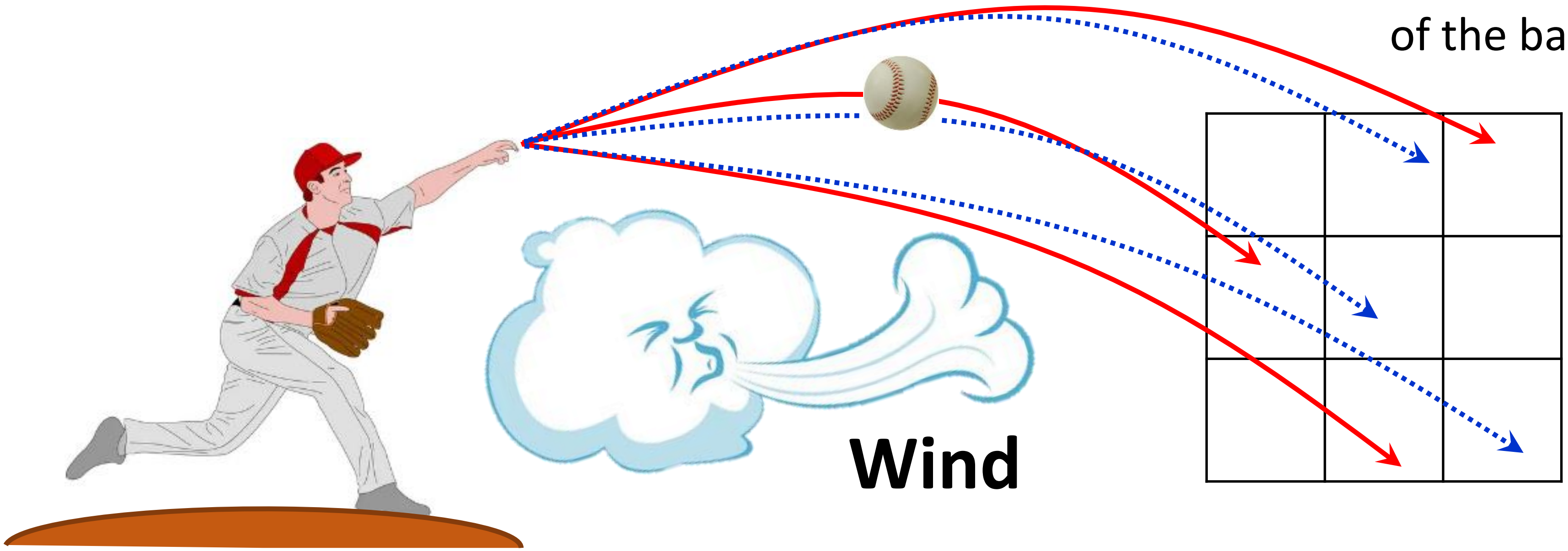
- **Why ‘transport?’**

  → Transport reveals <u>information</u> of transported objects

Interaction b/t ball &wind



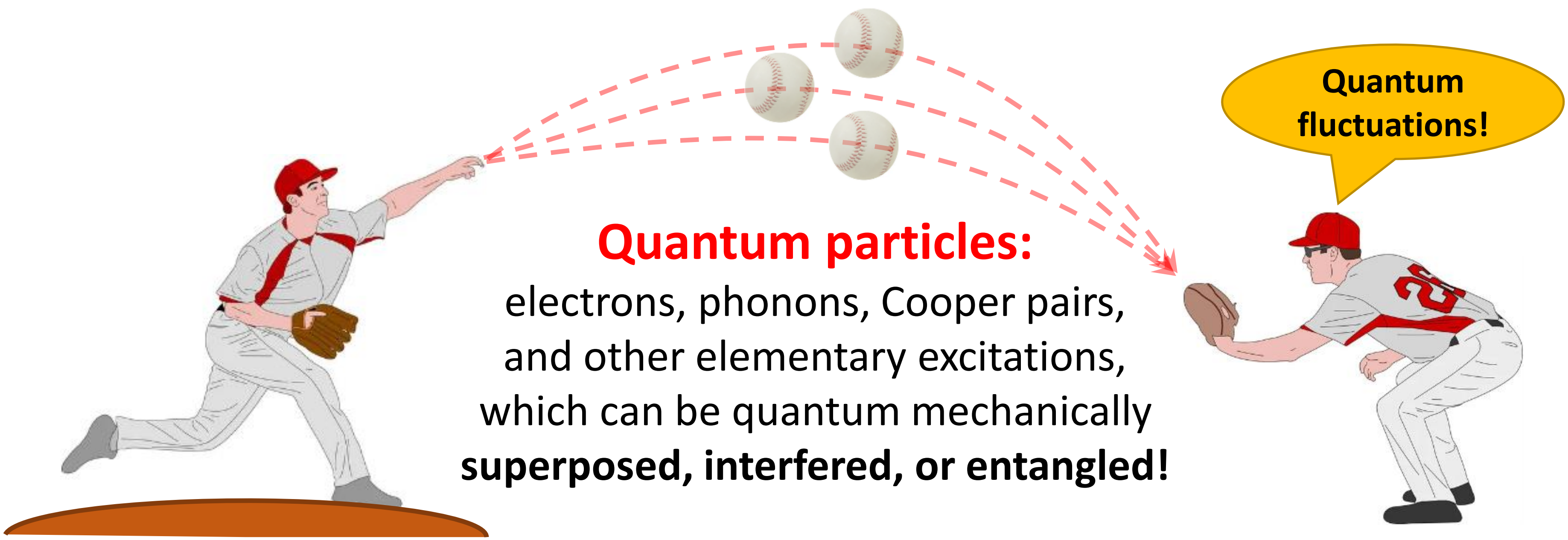
Spin of the ball



Figures from depositphotos.com

What is Mesoscopic Quantum Transport

- **Mesoscopic quantum transport**?
- **Why 'transport'**: Transport reveals information of transported objects
- **Which one is 'quantum'**: ptls are superposed, interfered, or entangled



Quantum particles:
electrons, phonons, Cooper pairs, and other elementary excitations, which can be quantum mechanically **superposed, interfered, or entangled!**

Figures from depositphotos.com

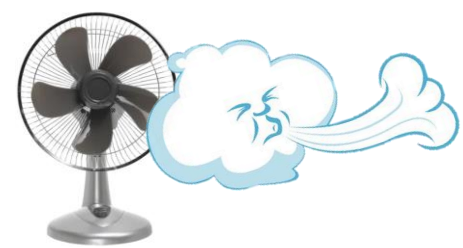
What is Mesoscopic Quantum Transport

- **Mesoscopic quantum transport**?
- **Why 'transport'**: Transport reveals information of transported objects
- **Which one is 'quantum'**: ptls are superposed, interfered, or entangled
- **What's meso-scopic systems**

→ **Playground** for **quantum** baseballs (not too large: macro-scopic)
but **well-controllable & designable** (not too small: micro-scopic)

Competition b/t **various scales matter**!

We can place **quantum** pitchers, catchers, fans on the field, **as we want!**



Physics of MQT: Ohm's law & Drude mode

- **Most well-known transport theory: Ohm's law & Drude model**

→ Ohm's Law: electric field accelerates charges generating current

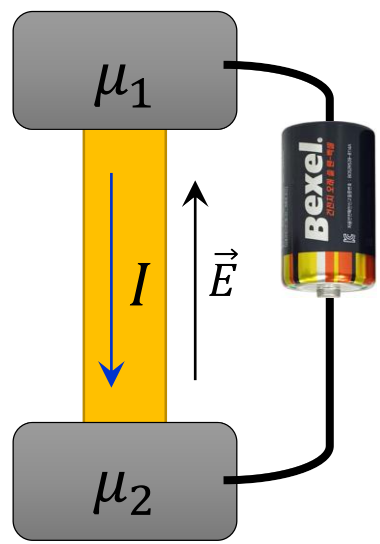
$$V = RI \text{ or } I = GV$$

Drude model

→ Impurities prevent charges from being accelerated indefinitely

$$G = \frac{\sigma A}{L}$$

$$JA = \frac{\sigma A}{L} V \Leftrightarrow J = \sigma E$$



$$V = (\mu_1 - \mu_2)/e$$

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

$$J = -nev_d = -ne\left(\frac{-eE\tau}{m}\right) = \frac{ne^2\tau}{m}E$$

Physics of MQT: Ohm's law & Drude mode

- **Most well-known transport theory: Ohm's law & Drude model**
  - → Ohm's Law: electric field accelerates charges generating current

$$V = RI \text{ or } I = GV$$

Drude model

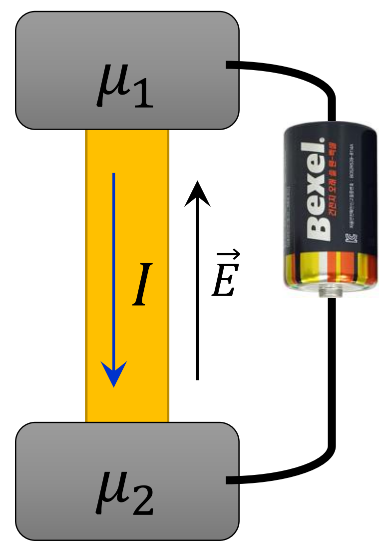
  - → Impurities prevent charges from being accelerated indefinitely

$$G = \frac{\sigma A}{L}$$

$$JA = \frac{\sigma A}{L} V \Leftrightarrow J = \sigma E$$

What if a <u>conductor is so small</u> that it contains <u>no impurity?</u>

Do we have $\sigma \to \infty$?
If not, what do we have?



$$V = (\mu_1 - \mu_2)/e$$

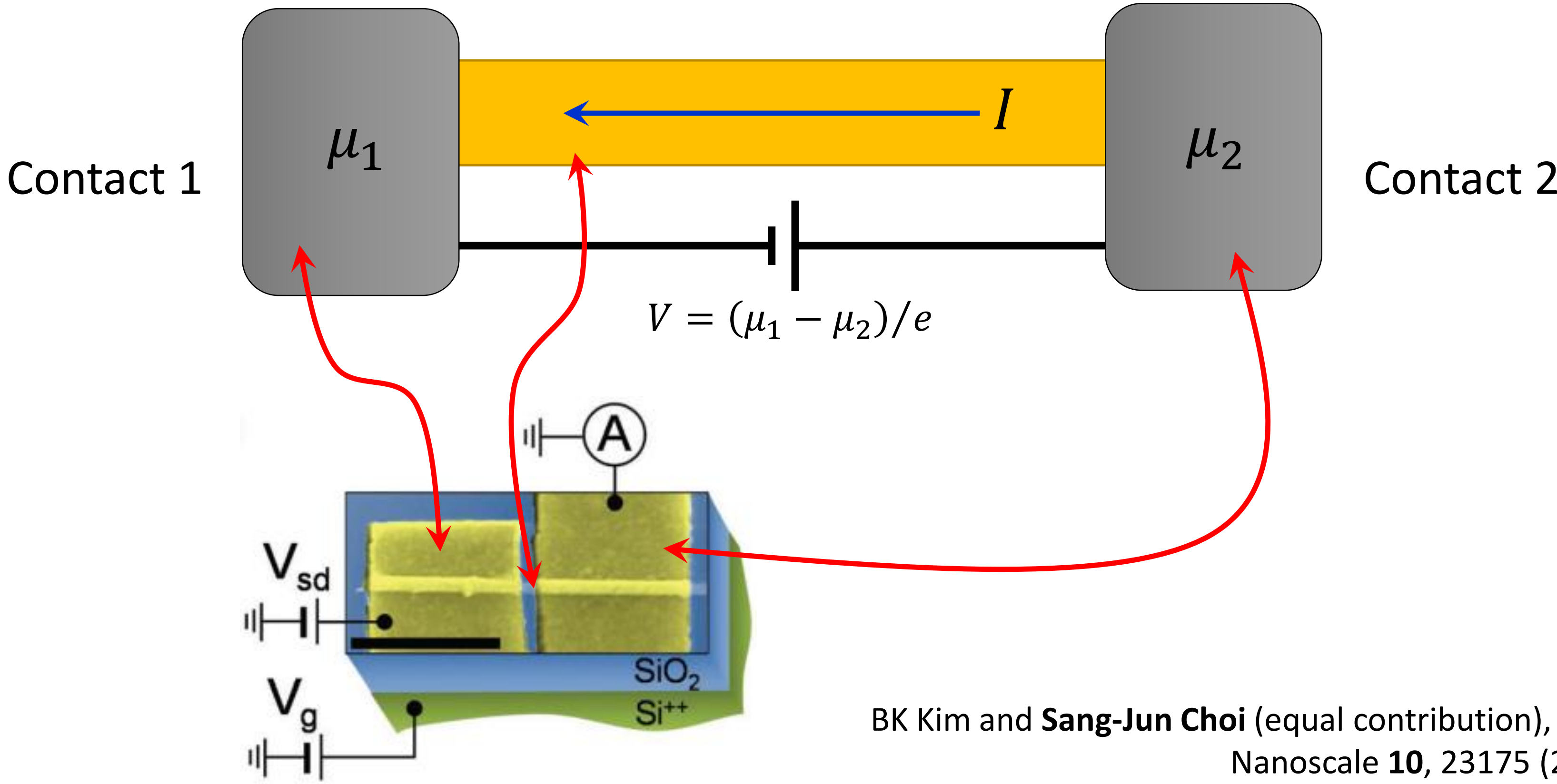
$$\sigma = \frac{ne^2\tau}{m}$$

$$J = -nev_d = -ne\left(\frac{-eE\tau}{m}\right) = \frac{ne^2\tau}{m} E$$

Physics of MQT: perfect conductor

- **Perfect conductor**

What is the conductance G of a perfect conductor?



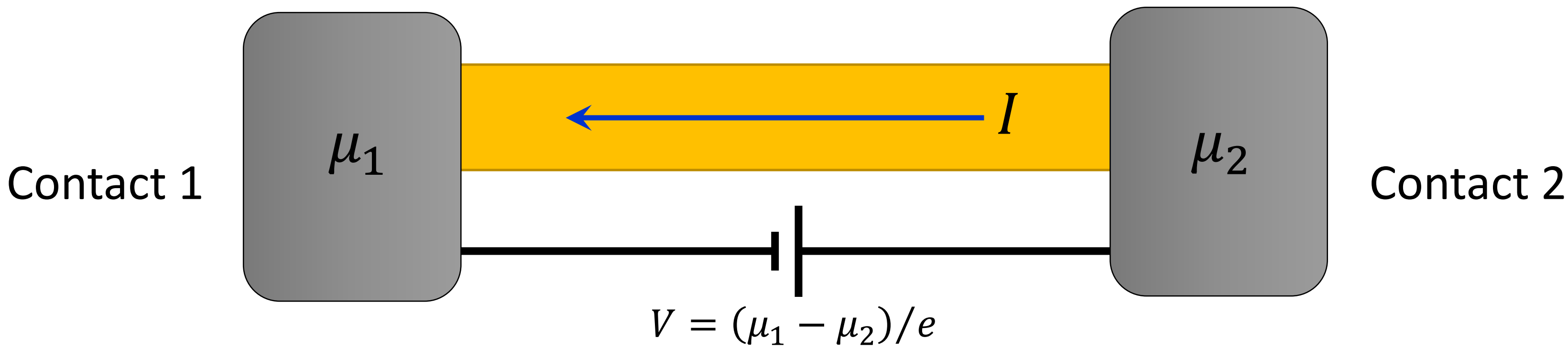
BK Kim and **Sang-Jun Choi** (equal contribution), et al., Nanoscale **10**, 23175 (2018).

Physics of MQT: perfect conductor

- **Perfect conductor**

  Mean free path | Phase relaxation length

  we assume: size of conductor, $L << L_{\mathrm{m}}, L_{\varphi}$.

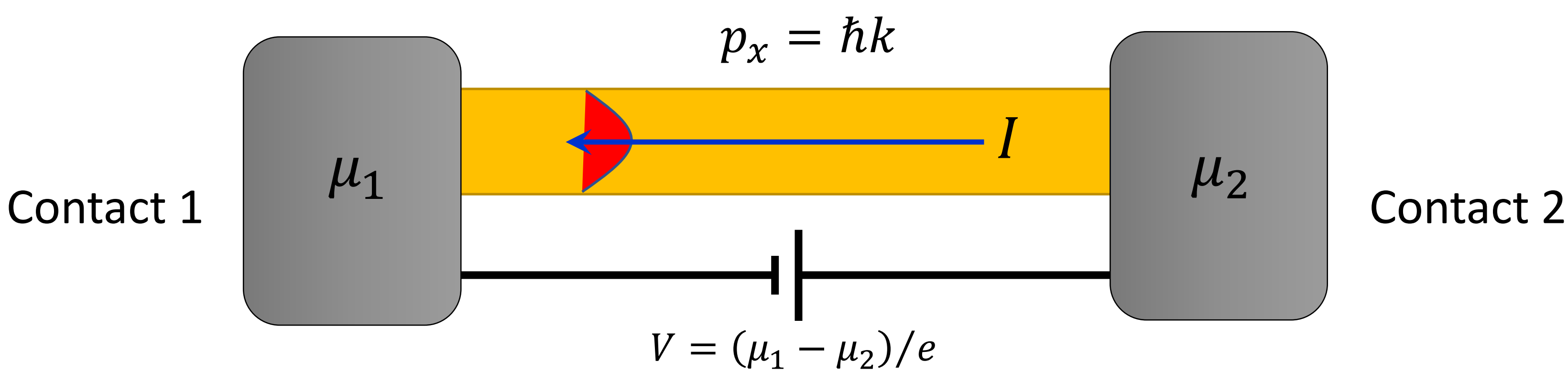


Physics of MQT: perfect conductor

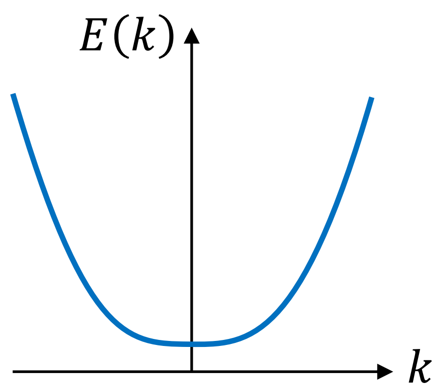
- **Perfect conductor**

Fermi wavelength

we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands



$$E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + U$$
$$= \frac{p_x^2}{2m} + \frac{n^2\pi^2\hbar^2}{2mW^2} + U$$

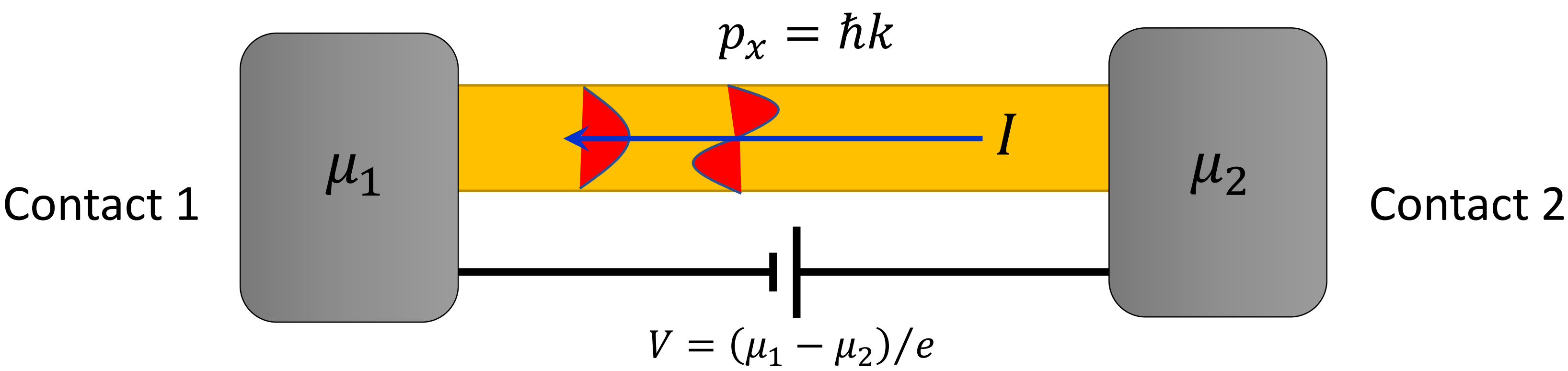


Physics of MQT: perfect conductor

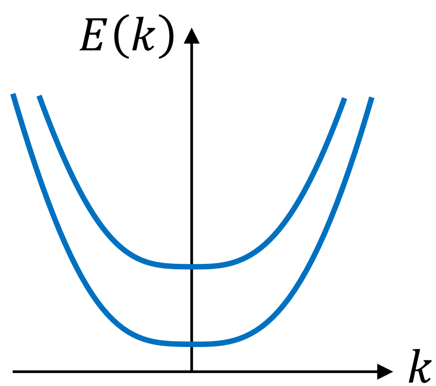
- **Perfect conductor**

Fermi wavelength

we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands



$$E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + U$$
$$= \frac{p_x^2}{2m} + \frac{n^2\pi^2\hbar^2}{2mW^2} + U$$

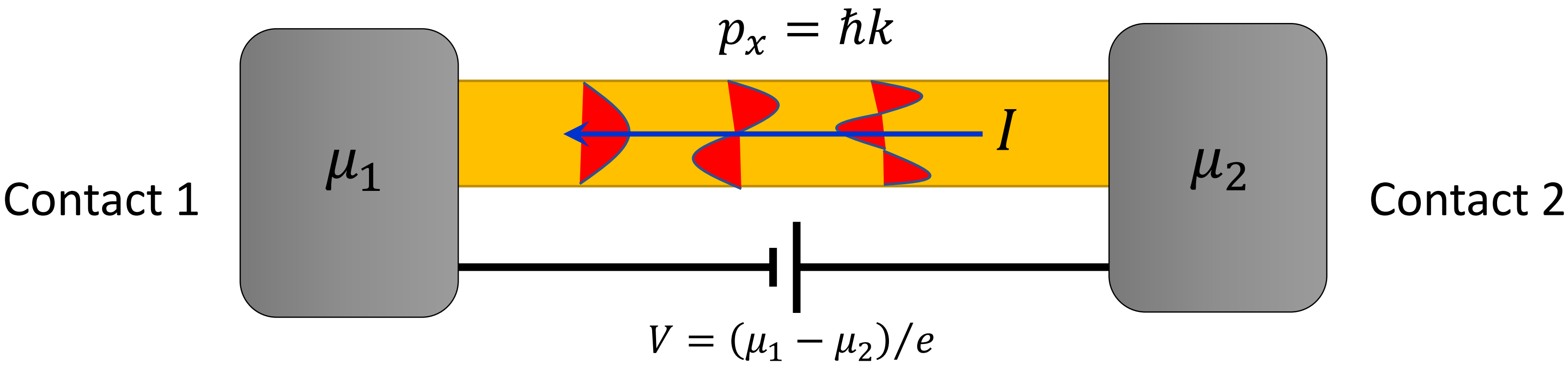


Physics of MQT: perfect conductor

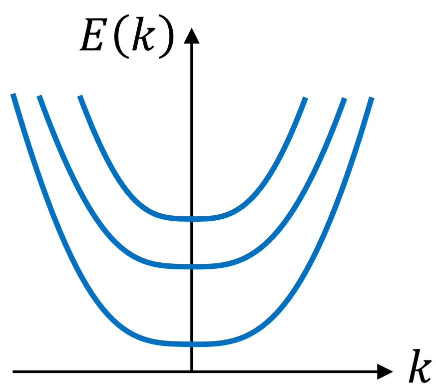
- **Perfect conductor**

we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

Fermi wavelength



$$E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + U$$
$$= \frac{p_x^2}{2m} + \frac{n^2\pi^2\hbar^2}{2mW^2} + U$$



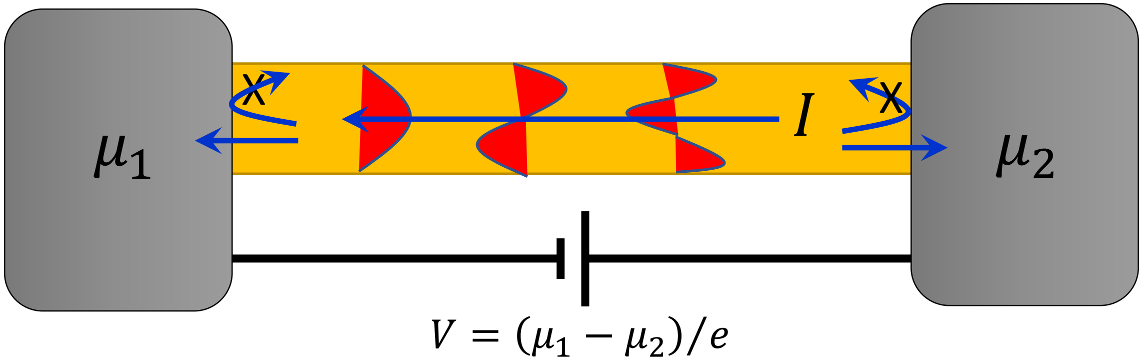
Physics of MQT: perfect conductor

- **Perfect conductor**

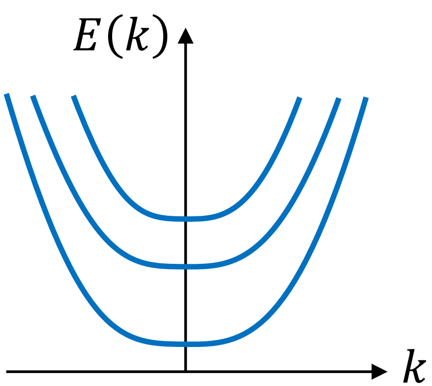
we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

Reflectionless contacts (no backscattering at contact)

Contact 1



Contact 2

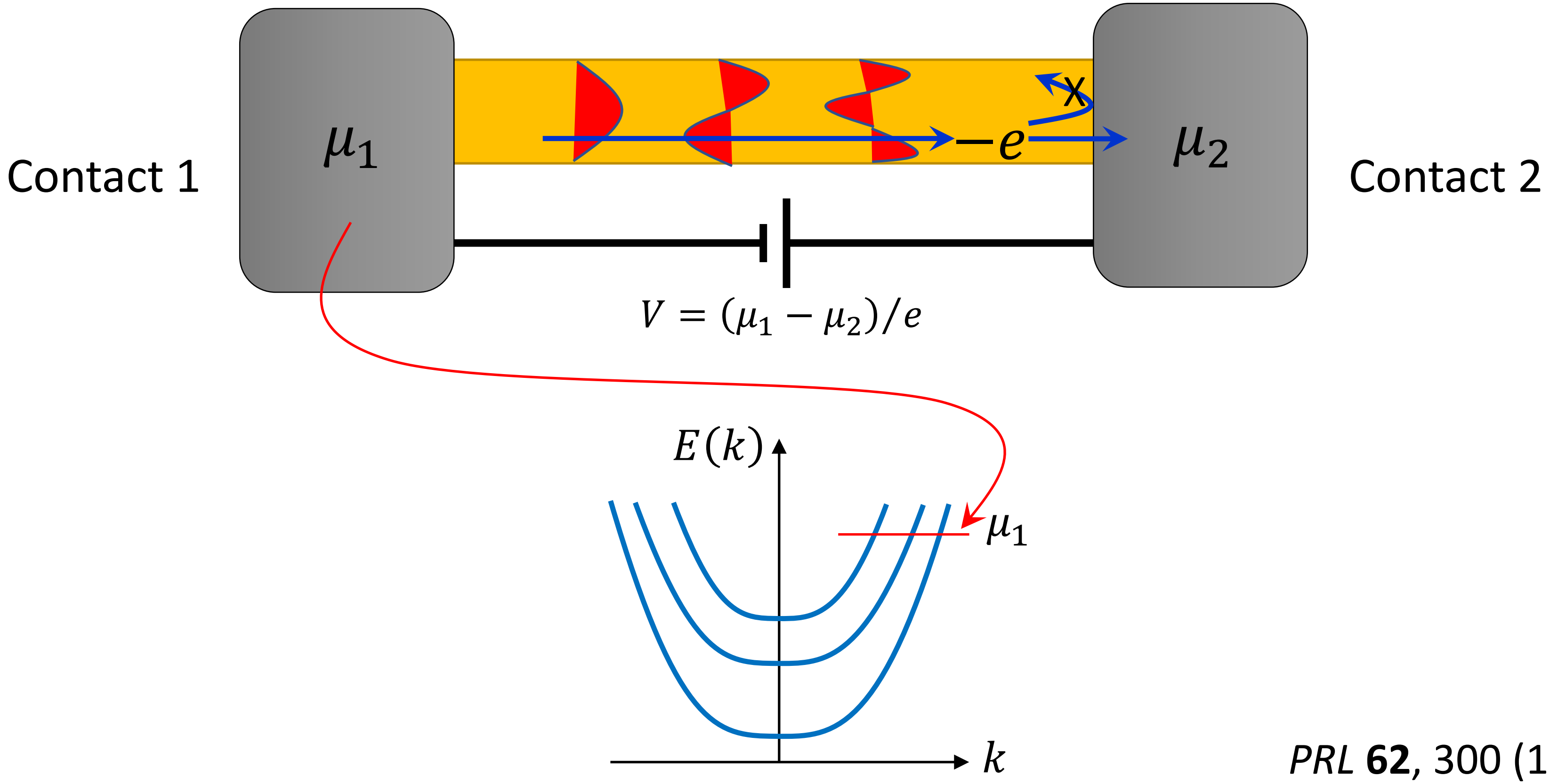


PRL **62**, 300 (1989)

Physics of MQT: perfect conductor

- **Perfect conductor**

we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands
Reflectionless contacts (no backscattering at contact)



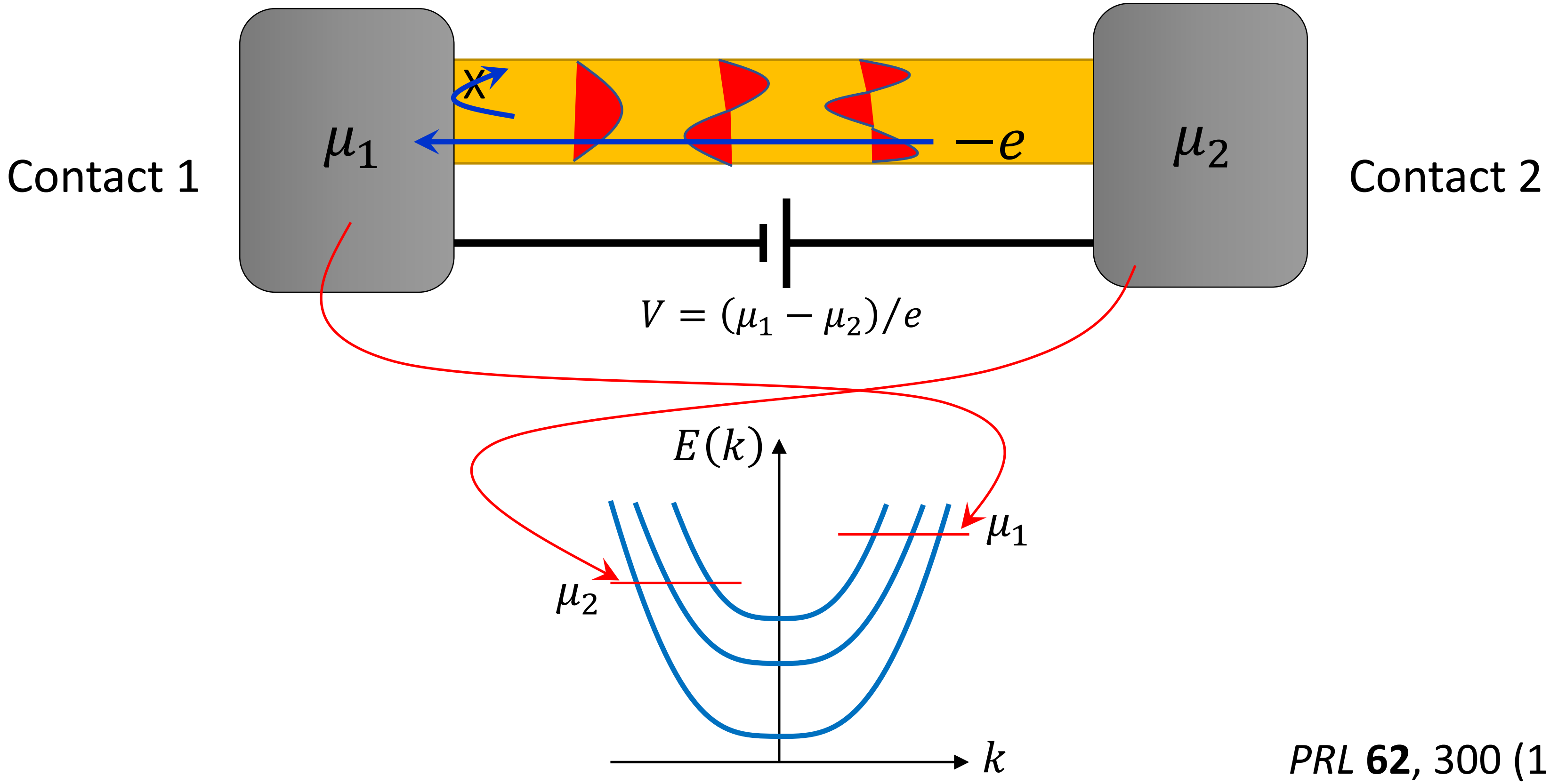
PRL **62**, 300 (1989)

Physics of MQT: perfect conductor

- **Perfect conductor**

we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

Reflectionless contacts (no backscattering at contact)



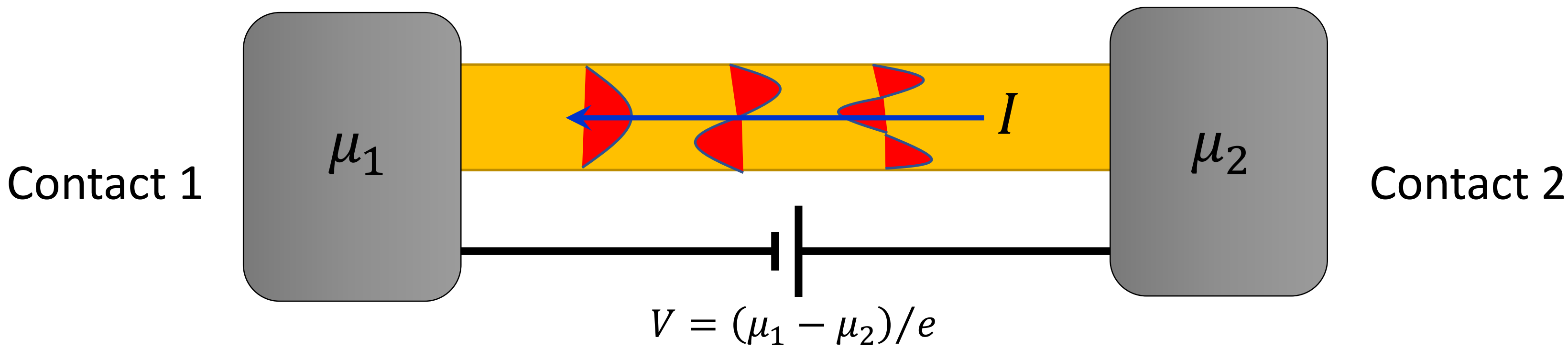
PRL **62**, 300 (1989)

Physics of MQT: perfect conductor

- **Perfect conductor**

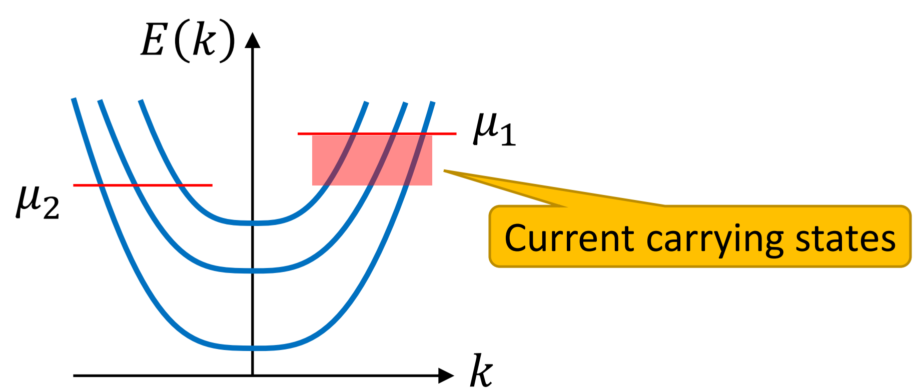
we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

Reflectionless contacts (no backscattering at contact)



What is the conductance G of a perfect conductor?

To answer, just calculate I for given $V = (\mu_2 - \mu_1)/e$



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

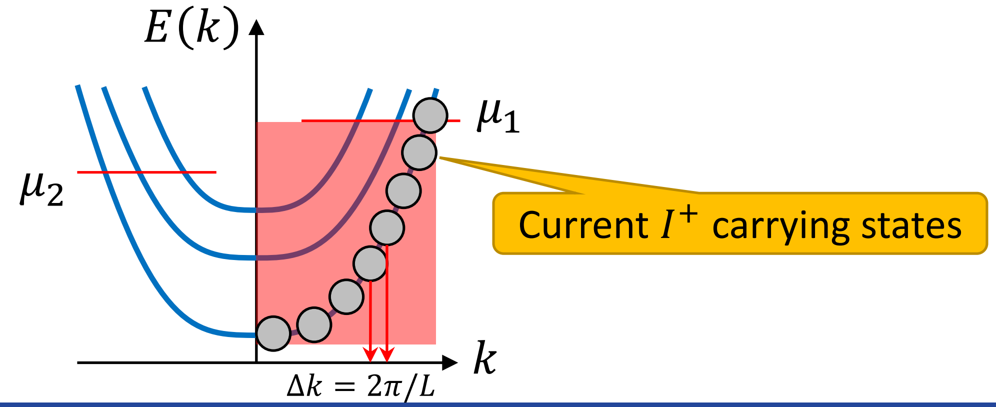
  Reflectionless contacts (no backscattering at contact)

- **Calculating the current**

Spin degeneracy

$$I^+ = env^+ = e\left(\frac{1}{L}\sum_k f^+(E_k)\right)\frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{e}{\hbar L}\left(\frac{2L}{2\pi}\int f^+(E_k)dk\right)\frac{dE}{dk}$$

$$= \frac{2e}{h}\int f^+(E)dE$$



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

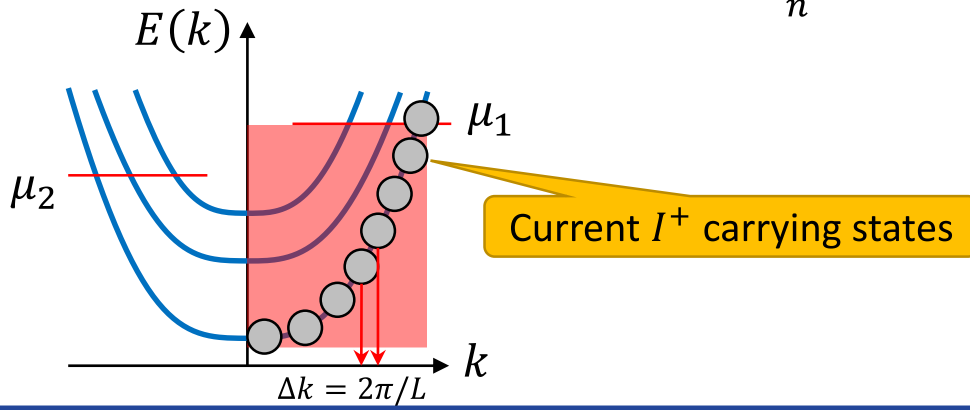
  Reflectionless contacts (no backscattering at contact)

- **Calculating the current**

Spin degeneracy

$$I^+ = env^+ = e\left(\frac{1}{L}\sum_k f^+(E_k)\right)\frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{e}{\hbar L}\left(\frac{2L}{2\pi}\int f^+(E_k)dk\right)\frac{dE}{dk}$$

$$= \frac{2e}{h}\int f^+(E)dE \Rightarrow \frac{2e}{h}\int f^+(E)M(E)dE \qquad M(E) = \sum_n \Theta(E - E_n)$$



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

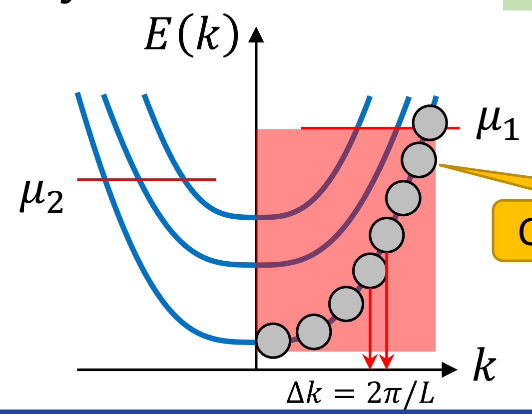
  Reflectionless contacts (no backscattering at contact)

- **Calculating the current**

Spin degeneracy

$$I^+ = env^+ = e\left(\frac{1}{L}\sum_k f^+(E_k)\right)\frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{e}{\hbar L}\left(\frac{2L}{2\pi}\int f^+(E_k)dk\right)\frac{dE}{dk}$$

$$= \frac{2e}{h}\int f^+(E)dE \Rightarrow \frac{2e}{h}\int f^+(E)M(E)dE \Rightarrow I^+ = \frac{2e}{h}M\mu_1 \quad \text{(zero temp.)}$$



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L \ll L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

  Reflectionless contacts (no backscattering at contact)

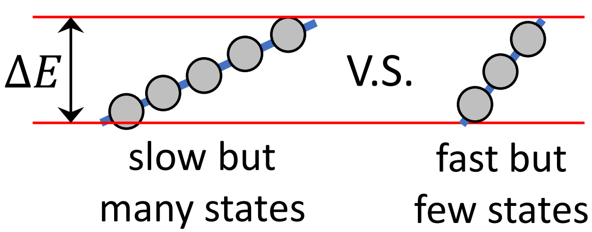
- **Calculating the current**

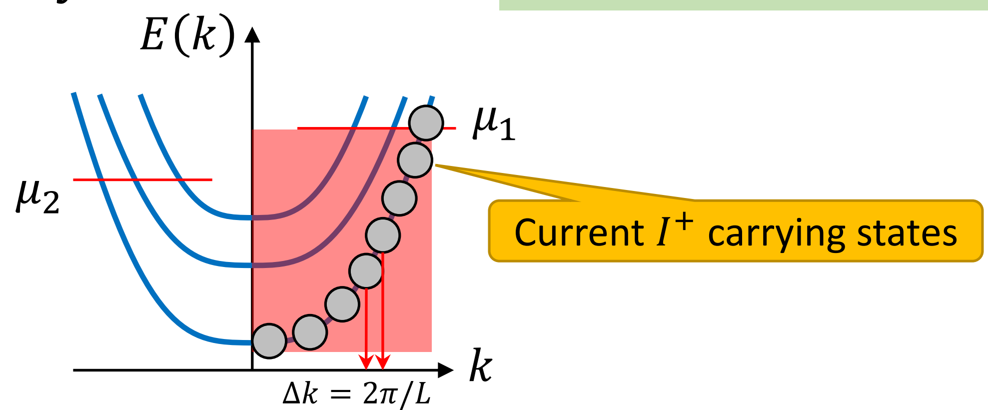
Spin degeneracy

$$I^+ = env^+ = e\left(\frac{1}{L}\sum_k f^+(E_k)\right)\frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{e}{\hbar L}\left(\frac{2L}{2\pi}\int f^+(E_k)dk\right)\frac{dE}{dk}$$

$$= \frac{2e}{h}\int f^+(E)dE \Rightarrow \frac{2e}{h}\int f^+(E)M(E)dE \Rightarrow I^+ = \frac{2e}{h}M\mu_1 \quad \text{(zero temp.)}$$

I^+, independent from group velocity?





Physics of MQT: perfect conductor

- **Perfect conductor**

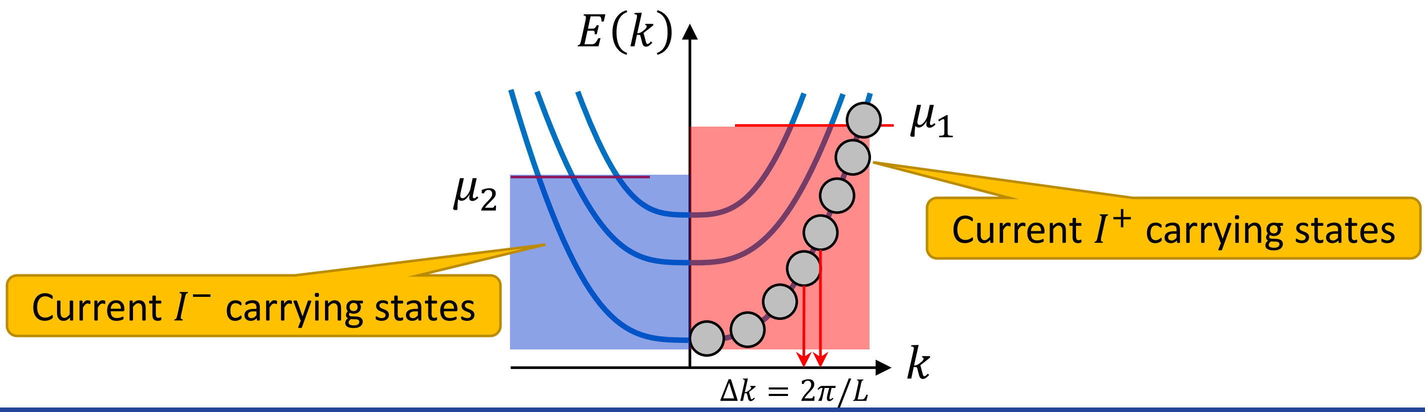
we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

Reflectionless contacts (no backscattering at contact)

- **Calculating the current**

(zero temp.) $$I^+ = \frac{2e}{h} M\mu_1 \;\&\; I^- = -\frac{2e}{h} M\mu_2$$

Opposite sign due to opposite group velocity



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L \ll L_m$, L_φ. But $\lambda_F < W$ w/ subbands

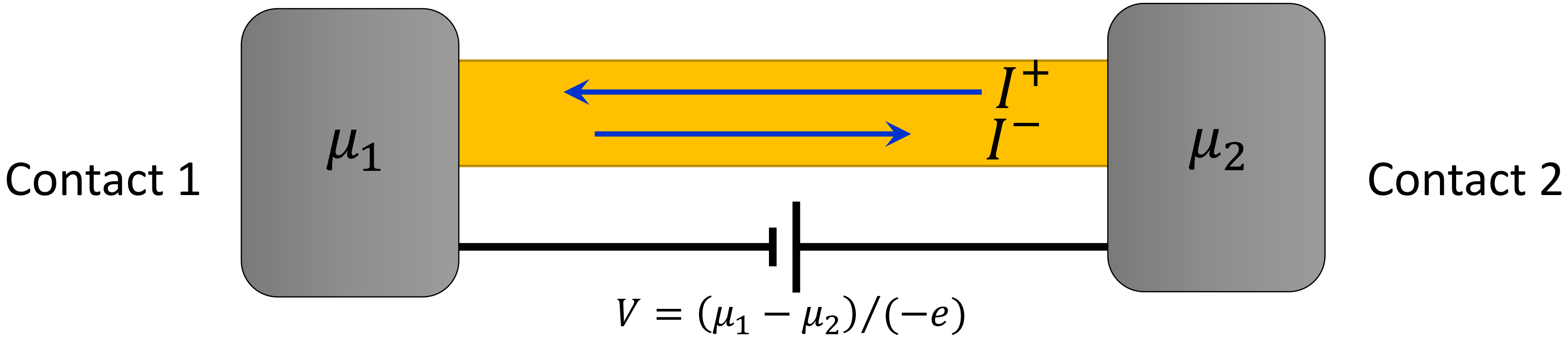
  Reflectionless contacts (no backscattering at contact)

- **Calculating the current**

(zero temp.) $$I^+ = \frac{2e}{h} M\mu_1 \ \& \ I^- = -\frac{2e}{h} M\mu_2$$

$$I = I^+ + I^- = \frac{2e}{h} M(\mu_1 - \mu_2) = \frac{2e^2}{h} M \frac{\mu_1 - \mu_2}{e} = \frac{2e^2}{h} MV$$

G of a perfect conductor = integer multiple of conductance quantum



Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

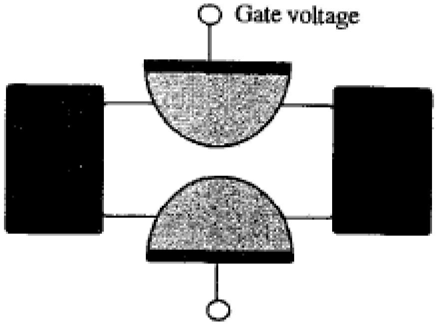
  Reflectionless contacts (no backscattering at contact)

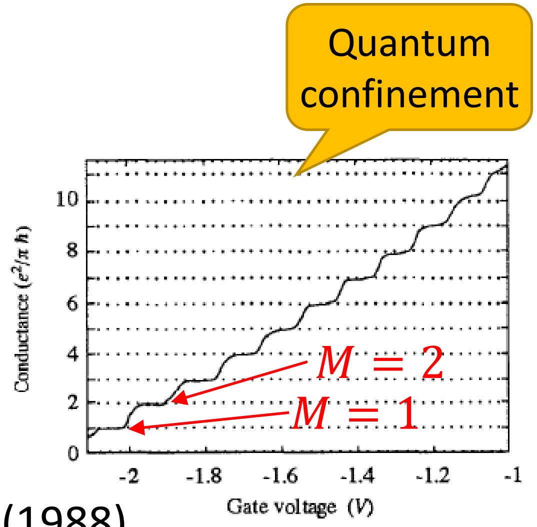
- **Conductance of a perfect conductor**

  (zero temp.) $$G = \frac{2e^2}{h} M$$

Conductance of a perfect conductor is quantized by $G = MG_Q$

(Conductance quantum $G_Q = \frac{2e^2}{h}$, **independent of geometry**)





PRL **60**, 848 (1988)

Physics of MQT: perfect conductor

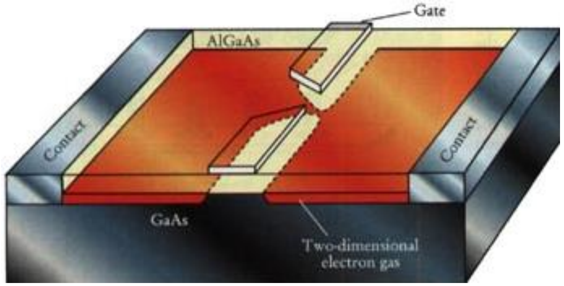
- **Perfect conductor**

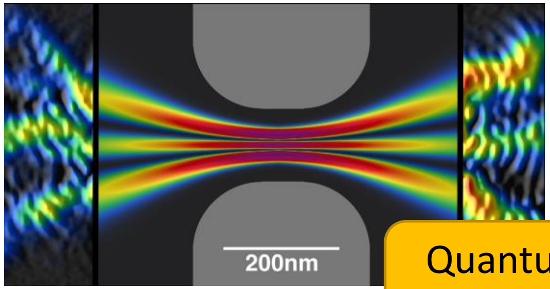
  we assume: size of conductor, $L << L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

  Reflectionless contacts (no backscattering at contact)

- **Quantized conductance**

$$G = \frac{2e^2}{h} M$$



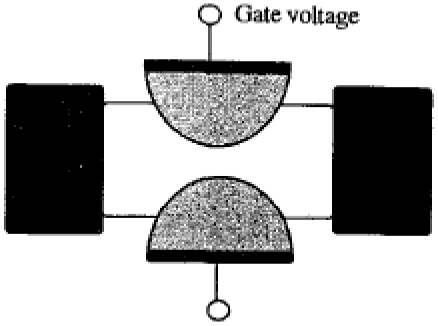


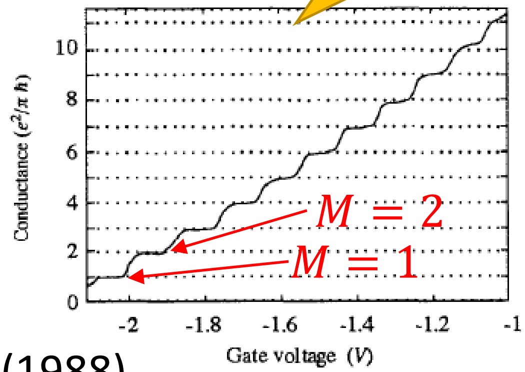
Quantum confinement

What is the source of resistance quantum, $R_Q = \frac{12.9}{M}\,\mathrm{k\Omega}$?

Conductance of a perfect conductor is quantized by $G = MG_Q$

(Conductance quantum $G_Q = \frac{2e^2}{h}$, **independent of geometry**)





PRL **60**, 848 (1988)

Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L << L_m$, L_φ. But $\lambda_F < W$ w/ subbands

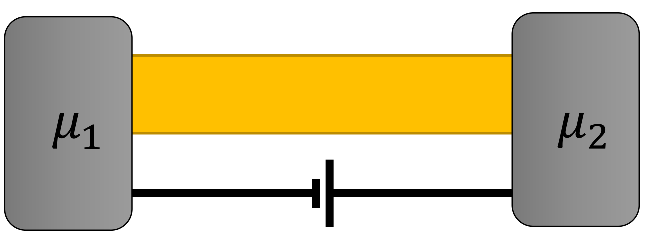
  Reflectionless contacts (no backscattering at contact)

- **Quantized conductance**

$$G = \frac{2e^2}{h} M$$

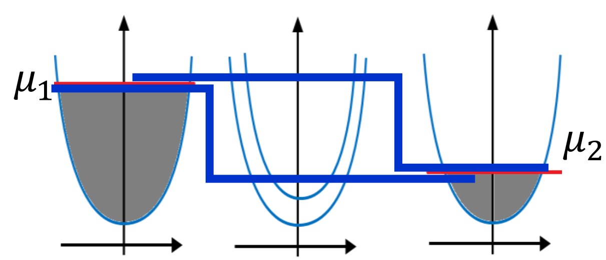
- **Where is the voltage drop?**

  Ans. at the contacts



Contact 1

Contact 2



We can define the voltage drop also with electrochemical potential

No matter how we define the voltage drop, it occurs **at the contacts**

Physics of MQT: perfect conductor

- **Perfect conductor**

  we assume: size of conductor, $L \ll L_m, L_\varphi$. But $\lambda_F < W$ w/ subbands

  Reflectionless contacts (no backscattering at contact)

- **Quantized conductance**

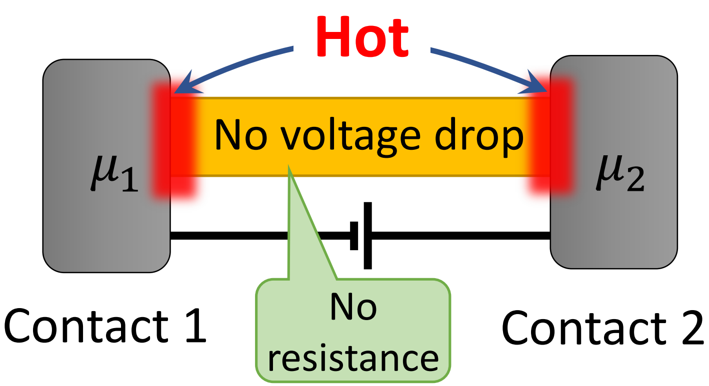
$$G = \frac{2e^2}{h} M \rightarrow$$

Contact resistance

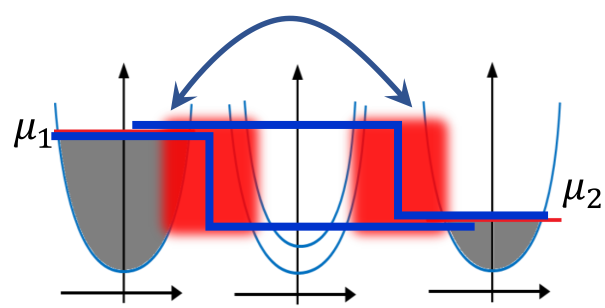
$$R_c = \frac{h}{2e^2 M} = \frac{12.9}{M}\ \mathrm{k}\Omega$$

- **Where is the voltage drop?**

  Ans. at the contacts



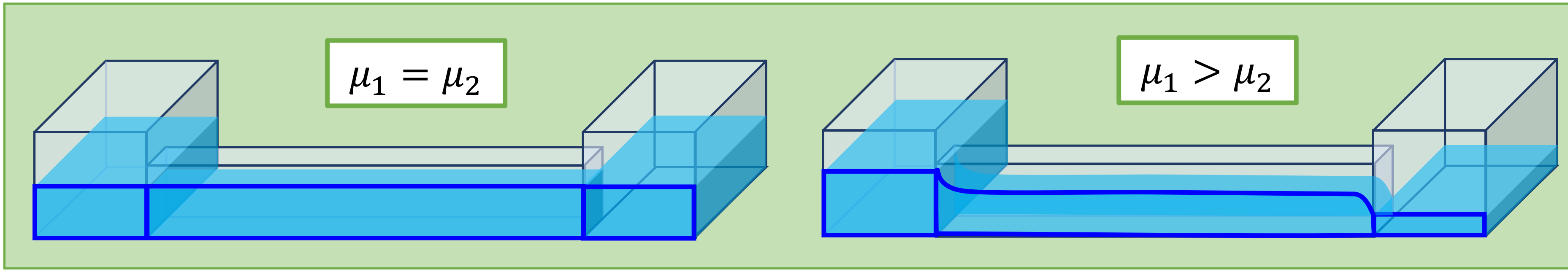
Energy dissipation should occur to fit into B.C. at infinity



i) Translational symmetry is broken at contacts
ii) Contacts are irremovable

No matter how we define the voltage drop, it occurs **at the contacts**

Physics of MQT: perfect conductor



- **Quantized conductance**

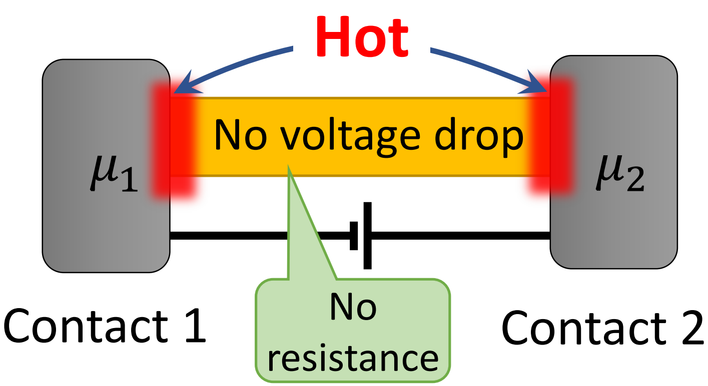
$$G = \frac{2e^2}{h} M$$

Contact resistance

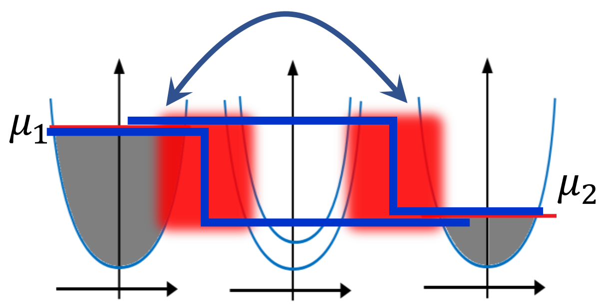
$$R_c = \frac{h}{2e^2 M} = \frac{12.9}{M}\ \mathrm{k\Omega}$$

- **Where is the voltage drop?**

  Ans. at the contacts



Energy dissipation should occur to fit into B.C. at infinity

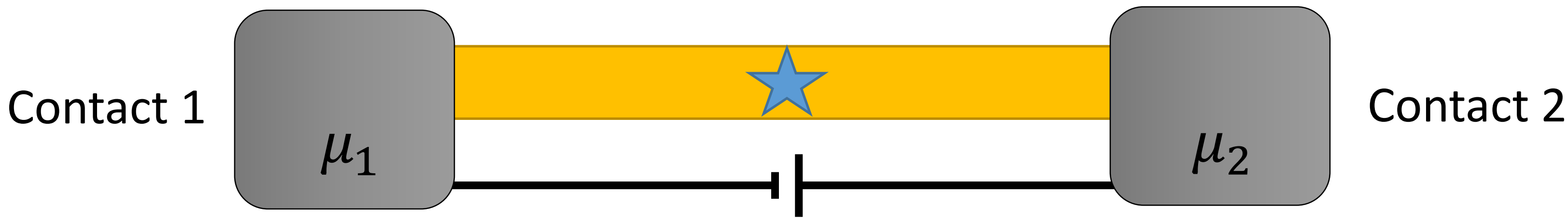


i) Translational symmetry is broken at contacts
ii) Contacts are irremovable

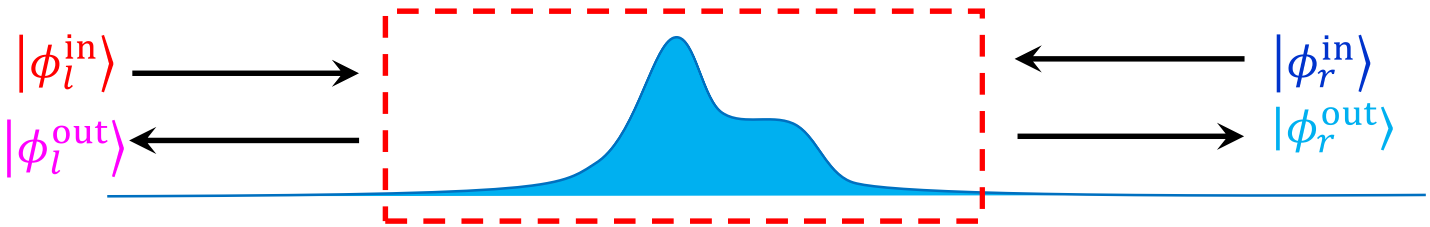
No matter how we define the voltage drop, it occurs **at the contacts**

Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_{\mathrm{m}}$



- **Scattering Matrix**



$|\phi_l\rangle \equiv \lim_{x\to-\infty} |\psi\rangle$

$|\phi_r\rangle \equiv \lim_{x\to\infty} |\psi\rangle$

General solution $\hat{H}|\psi\rangle = E|\psi\rangle$: $|\phi_l\rangle = A|\phi_l^{\mathrm{i}}\rangle + B|\phi_l^{\mathrm{o}}\rangle$ & $|\phi_r\rangle = C|\phi_r^{\mathrm{o}}\rangle + D|\phi_r^{\mathrm{i}}\rangle$.

Undergraduate courses, we deal with two cases: (i) left & (ii) right incidence. We know

(i) $B = rA$ & $C = tA$ & $D = 0$: $|\phi_l\rangle = A|\phi_l^{\mathrm{i}}\rangle + rA|\phi_l^{\mathrm{o}}\rangle$ & $|\phi_r\rangle = tA|\phi_l^{\mathrm{o}}\rangle$

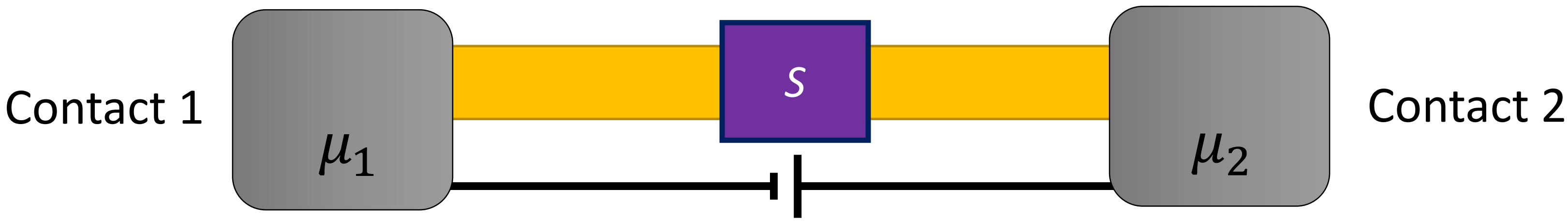
(ii) $B = t'D$ & $C = r'D$ & $A = 0$: $+$ $|\phi_l\rangle = t'D|\phi_l^{\mathrm{o}}\rangle$ & $|\phi_r\rangle = r'D|\phi_r^{\mathrm{o}}\rangle + D|\phi_r^{\mathrm{i}}\rangle$.

General solution is

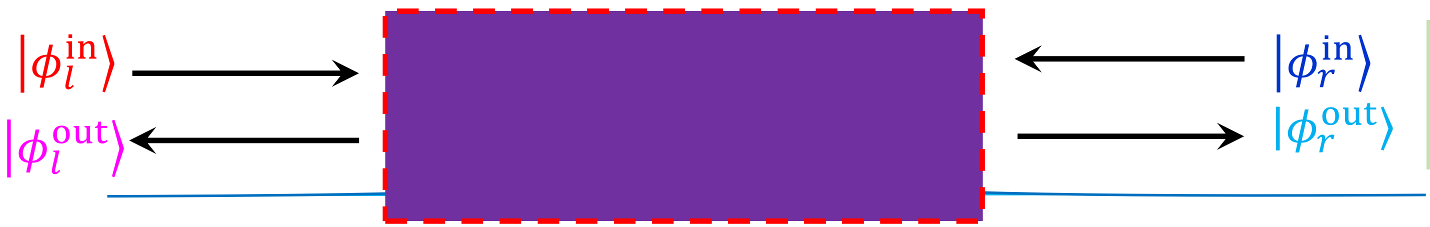
$$|\phi_l\rangle = A|\phi_l^{\mathrm{i}}\rangle + (rA + t'D)|\phi_l^{\mathrm{o}}\rangle \;\&\; |\phi_r\rangle = (tA + r'D)|\phi_r^{\mathrm{o}}\rangle + D|\phi_r^{\mathrm{i}}\rangle.$$

Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_\mathrm{m}$



- **Scattering Matrix**



$$|\phi_l^{\mathrm{i,o}}\rangle \equiv \lim_{x\to-\infty} |\psi^{\mathrm{i,o}}\rangle$$
$$|\phi_r^{\mathrm{i,o}}\rangle \equiv \lim_{x\to\infty} |\psi^{\mathrm{i,o}}\rangle$$

General solution: $|\phi_l\rangle = A|\phi_l^{\mathrm{i}}\rangle + (rA + t'D)|\phi_l^{\mathrm{o}}\rangle$ & $|\phi_r\rangle = (tA + r'D)|\phi_r^{\mathrm{o}}\rangle + D|\phi_r^{\mathrm{i}}\rangle$.

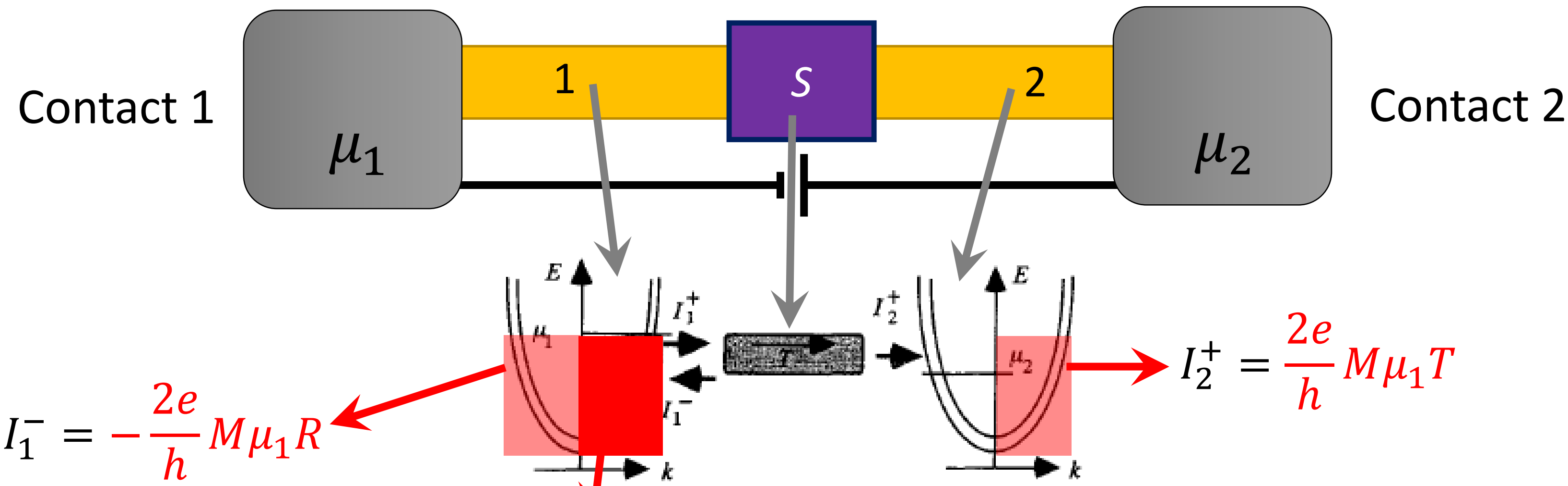
$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}$$

If interested only in amplitudes of scattering states at infinity, only thing we need to know is

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$



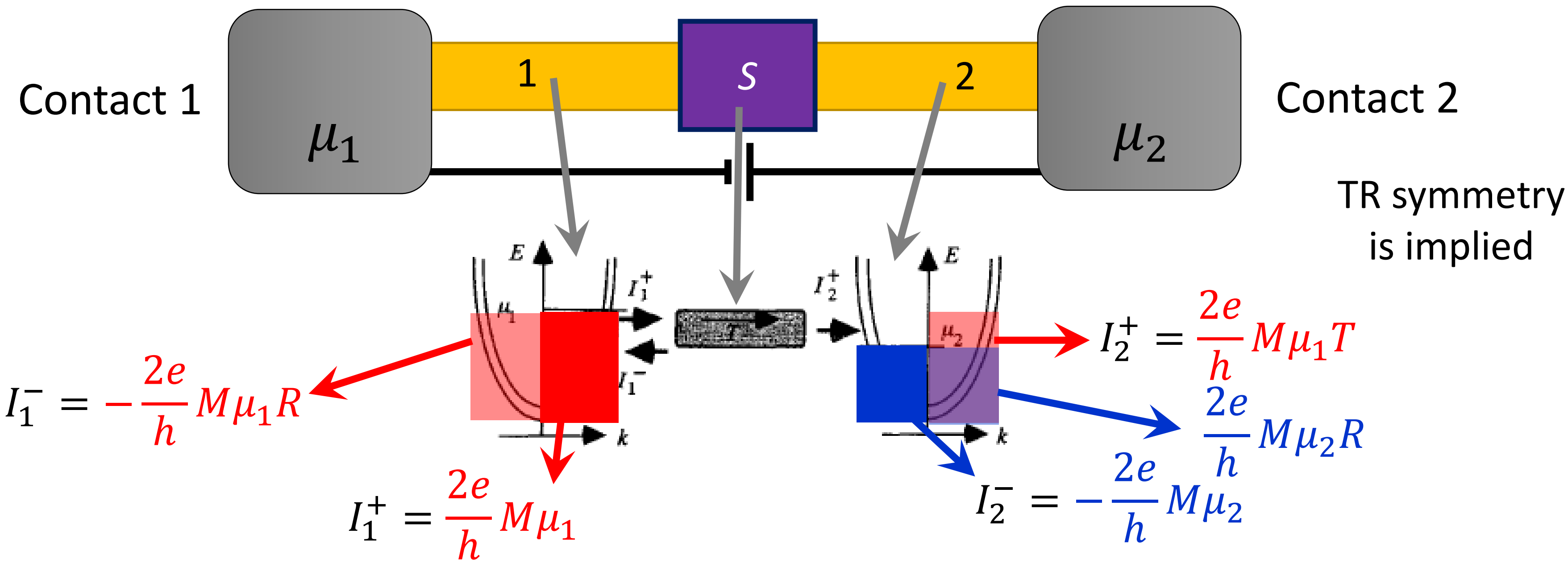
$I_1^- = -\frac{2e}{h} M\mu_1 R$

$I_1^+ = \frac{2e}{h} M\mu_1$

$I_2^+ = \frac{2e}{h} M\mu_1 T$

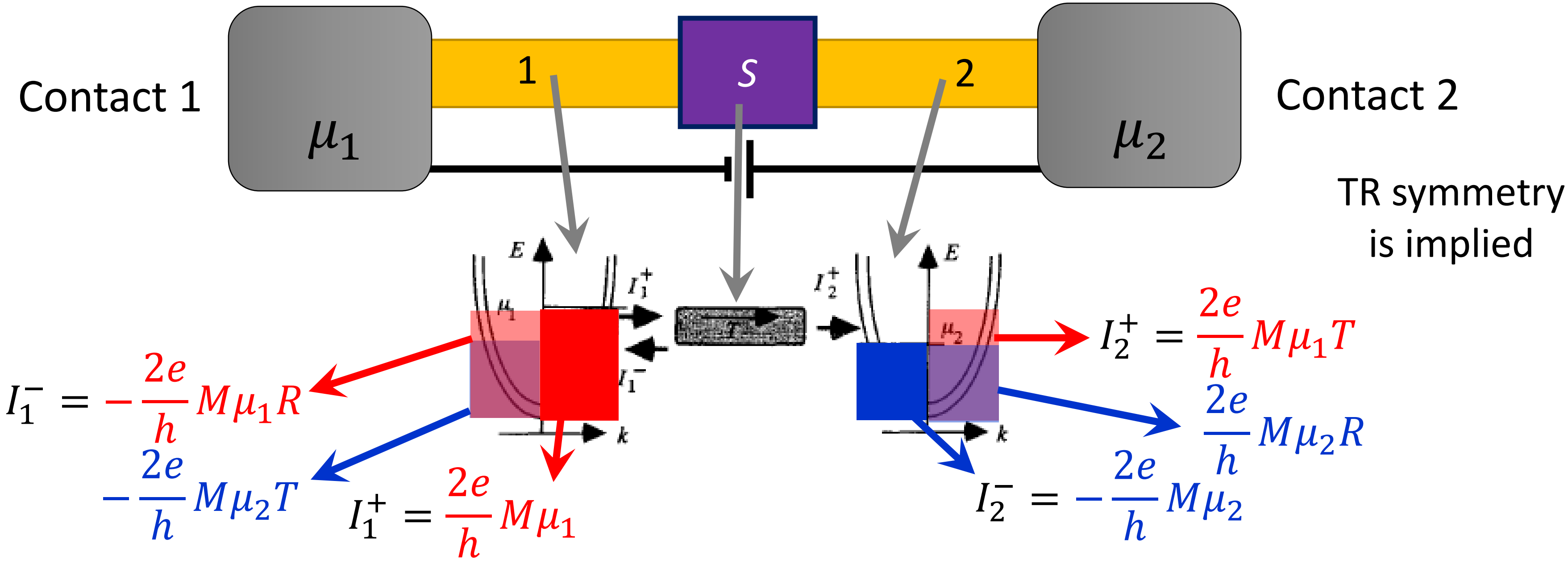
Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$



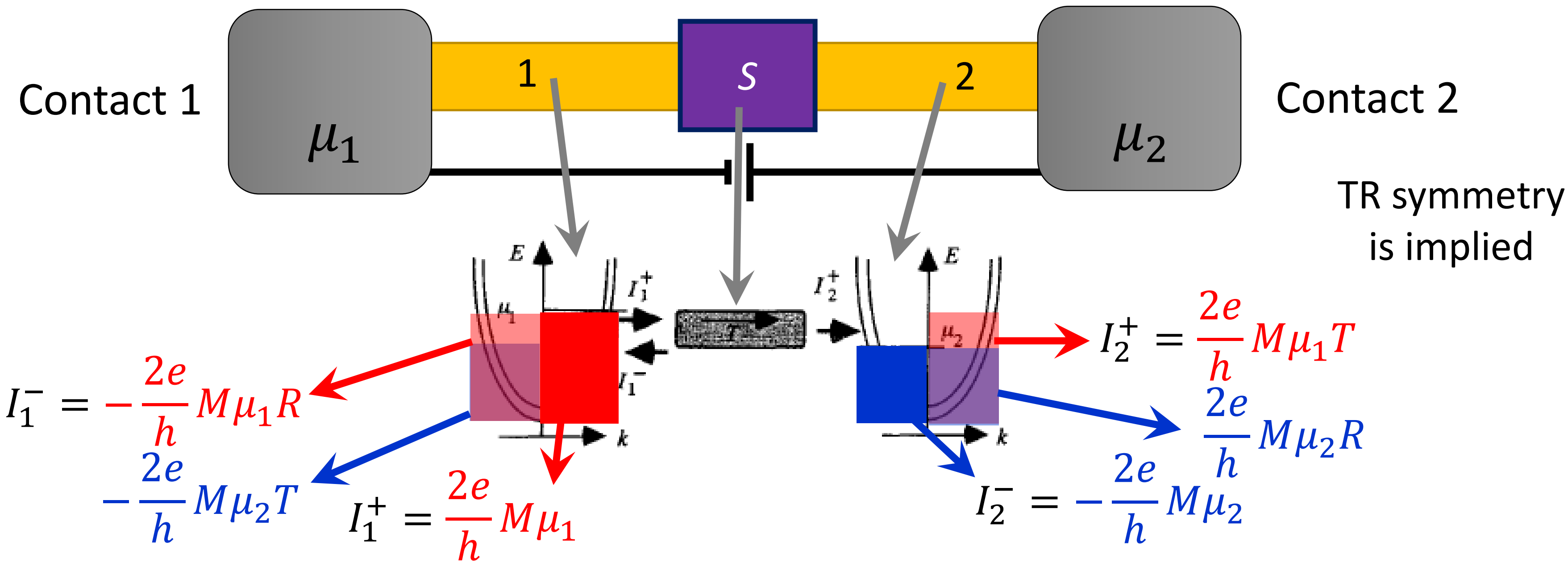
Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$



Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$

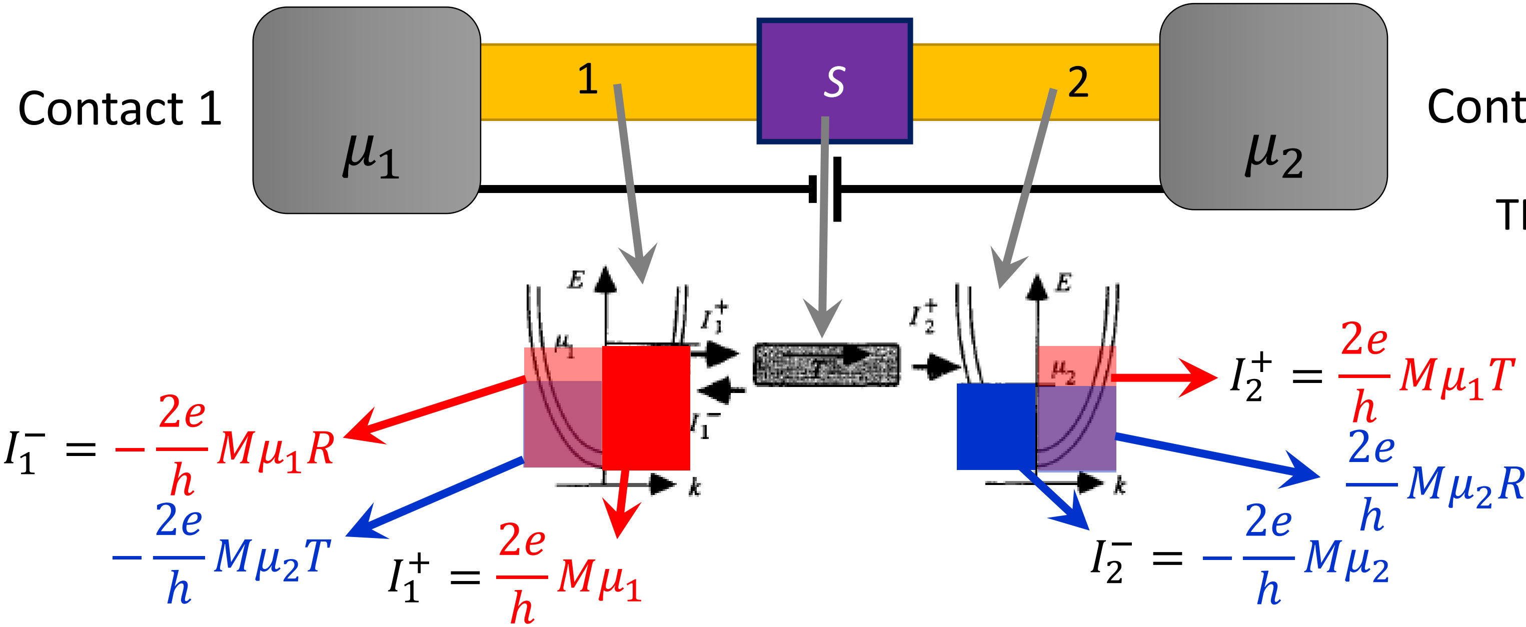


Total current at lead 1:

$$I_1 = I_1^+ + I_1^- = \frac{2e}{h}M\mu_1 - \frac{2e}{h}M\mu_1(1-T) - \frac{2e}{h}M\mu_2 T = \frac{2e}{h}M(\mu_1 - \mu_2)T$$

Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$



TR symmetry is implied

Total current at lead 1:

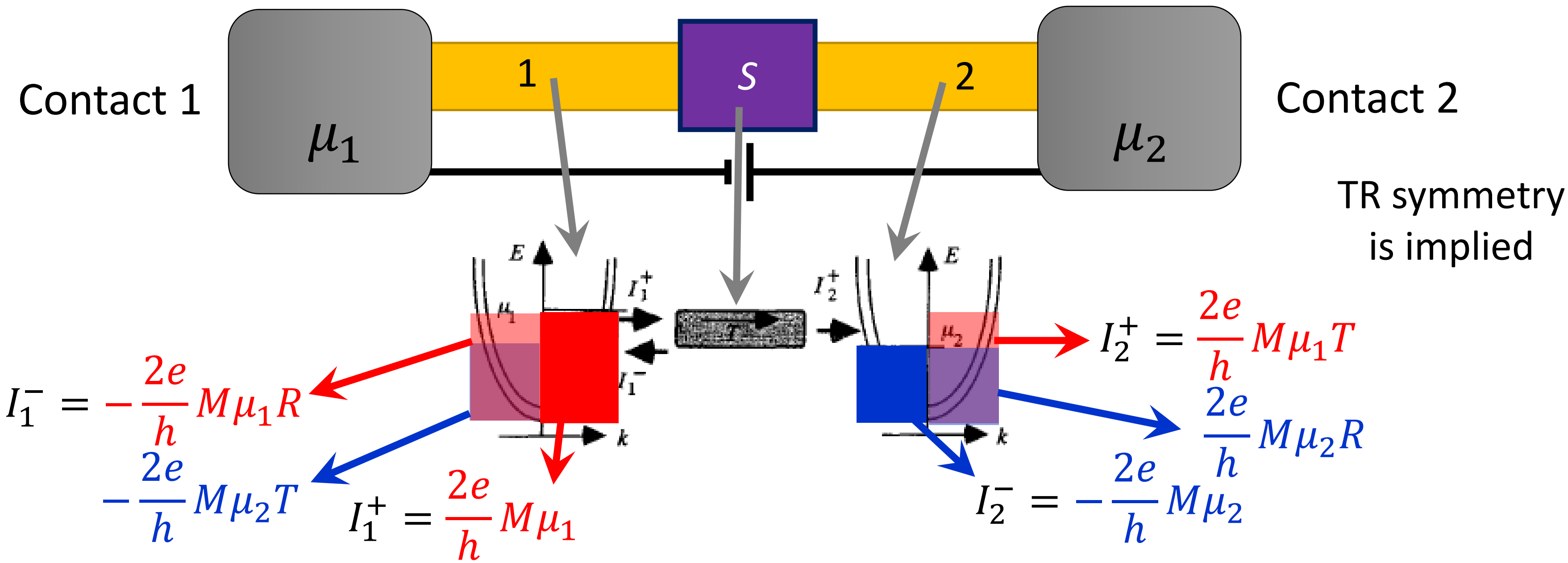
$$I_1 = I_1^+ + I_1^- = \frac{2e}{h} M\mu_1 - \frac{2e}{h} M\mu_1 (1 - T) - \frac{2e}{h} M\mu_2 T = \frac{2e}{h} M(\mu_1 - \mu_2) T$$

Total current at lead 2:

$$I_2 = I_2^+ + I_2^- = \frac{2e}{h} M\mu_1 T + \frac{2e}{h} M\mu_2 (1 - T) - \frac{2e}{h} M\mu_2 = \frac{2e}{h} M(\mu_1 - \mu_2) T$$

Physics of MQT: Not perfect but ballistic conductor

- **Ballistic conductor w/ a single impurity:** size of conductor, $L < L_m$



Total current at lead 1&2:

$$I = I_1 = I_2 = \frac{2e}{h}M(\mu_1 - \mu_2)T = \frac{2e^2}{h}MT\left(\frac{\mu_1 - \mu_2}{e}\right) = \frac{2e^2}{h}MTV$$

$$G = \frac{2e^2}{h}MT$$

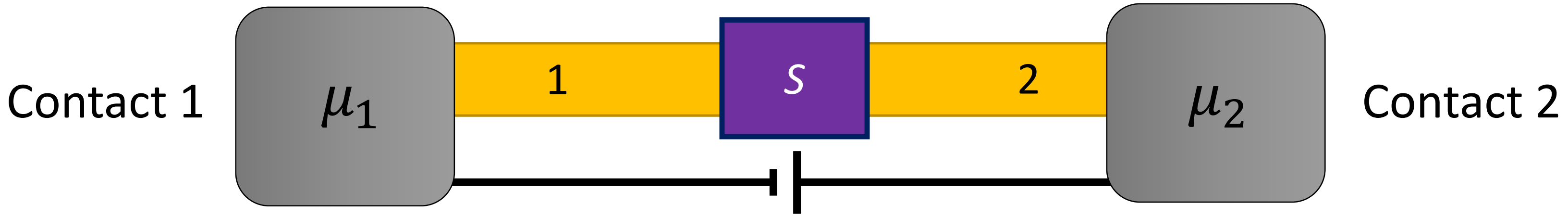
Perfect conductor $T = 1$

Physics of MQT: Not perfect but ballistic conductor

- **Landauer formula for a ballistic conductor w/ a single impurity**

$$G = \frac{2e^2}{h} M \mapsto G = \frac{2e^2}{h} MT$$

$G_Q = \frac{2e^2}{h}$ & $R_Q = G_Q^{-1} = \frac{h}{2e^2}$



Physics of MQT: Not perfect but ballistic conductor

- **Landauer formula for a ballistic conductor w/ a single impurity**

$$G = \frac{2e^2}{h} M \mapsto G = \frac{2e^2}{h} MT$$

$G_Q = \frac{2e^2}{h}$ & $R_Q = G_Q^{-1} = \frac{h}{2e^2}$

- **Where is the resistance?**

Actual resistance

Series connection of resistances

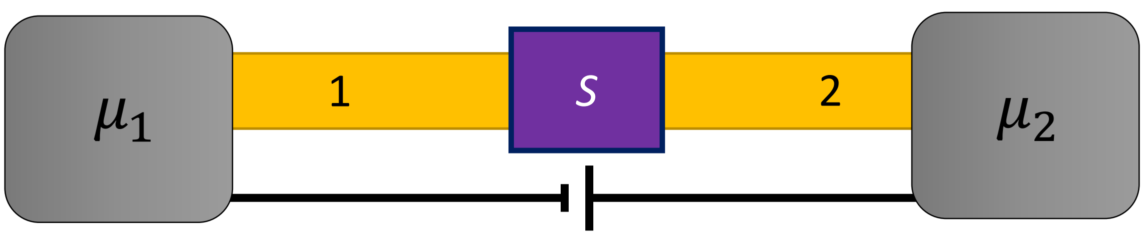
$$R = \frac{h}{2e^2 MT} = \frac{R_Q}{MT} - \frac{R_Q}{M} + \frac{R_Q}{M} = \frac{R_Q}{M}\frac{1-T}{T} + R_c$$

→ Voltage drop at contacts: $V_c = I \times R_c = G_Q MTV \times \frac{R_Q}{M} = TV$

→ Voltage drop at impurity: $V_a = I \times R_a = G_Q MTV \times \frac{R_Q}{M}\frac{1-T}{T} = (1-T)V$

→ Total voltage drop: $V_c + V_a = TV + (1-T)V = V$

Contact 1



Contact 2

Physics of MQT: Not perfect but ballistic conductor

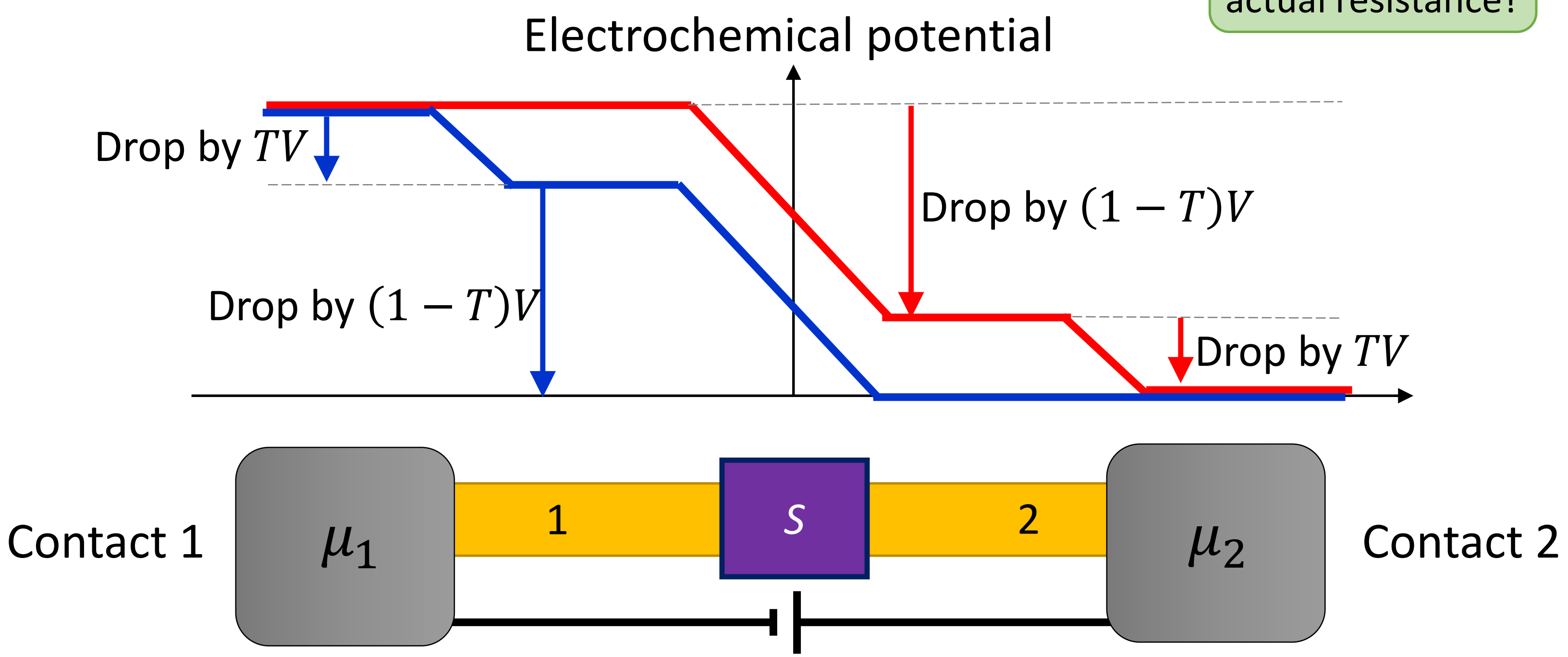
- **Where is the resistance?**

→ Voltage drop at contacts: $V_c = I \times R_c = G_Q MTV \times \frac{R_Q}{M} = TV$

→ Voltage drop at impurity: $V_a = I \times R_a = G_Q MTV \times \frac{R_Q}{M}\frac{1-T}{T} = (1-T)V$

→ Total voltage drop: $V_c + V_a = TV + (1-T)V = V$

How to measure actual resistance?



Physics of MQT: Not perfect but ballistic conductor

- **Where is the resistance?**

→ Voltage drop at contacts: $V_c = I \times R_c = G_Q MTV \times \frac{R_Q}{M} = TV$

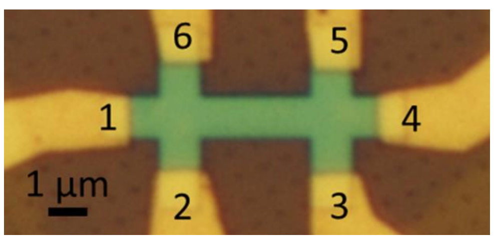
→ Voltage drop at impurity: $V_a = I \times R_a = G_Q MTV \times \frac{R_Q}{M}\frac{1-T}{T} = (1-T)V$

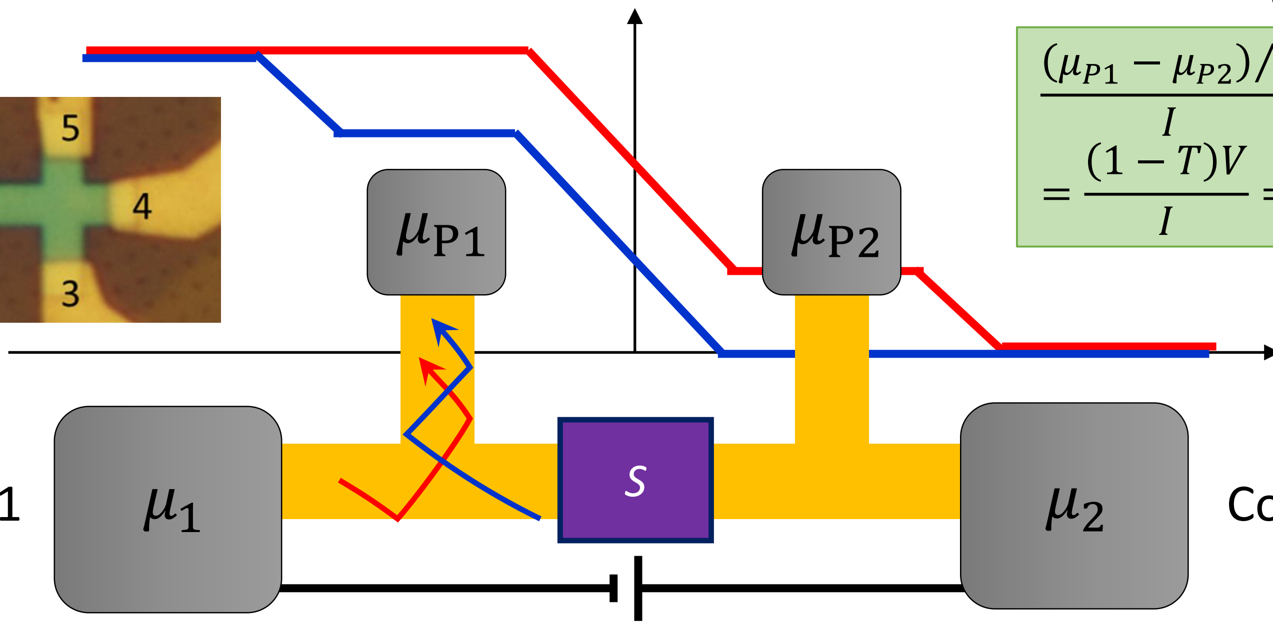
→ Total voltage drop: $V_c + V_a = TV + (1-T)V = V$

R_a

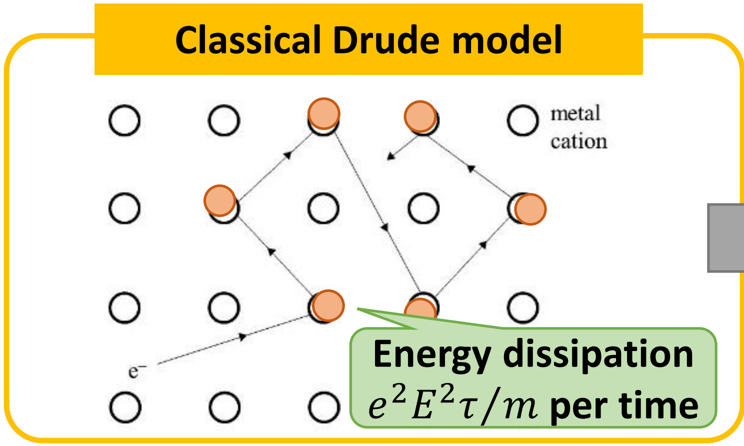
$$\frac{(\mu_{P1} - \mu_{P2})/e}{I} = \frac{(1-T)V}{I} = \frac{h}{2e^2M}\frac{1-T}{T}$$

- **Measure *actual* voltage drop**

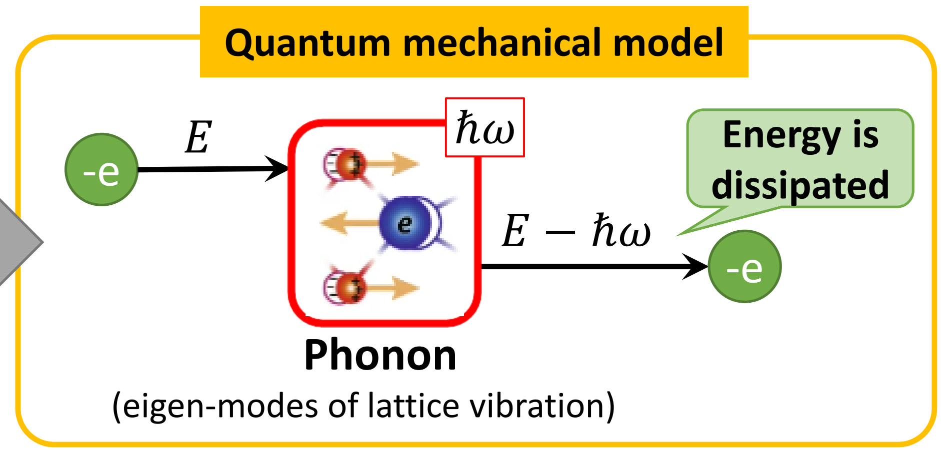


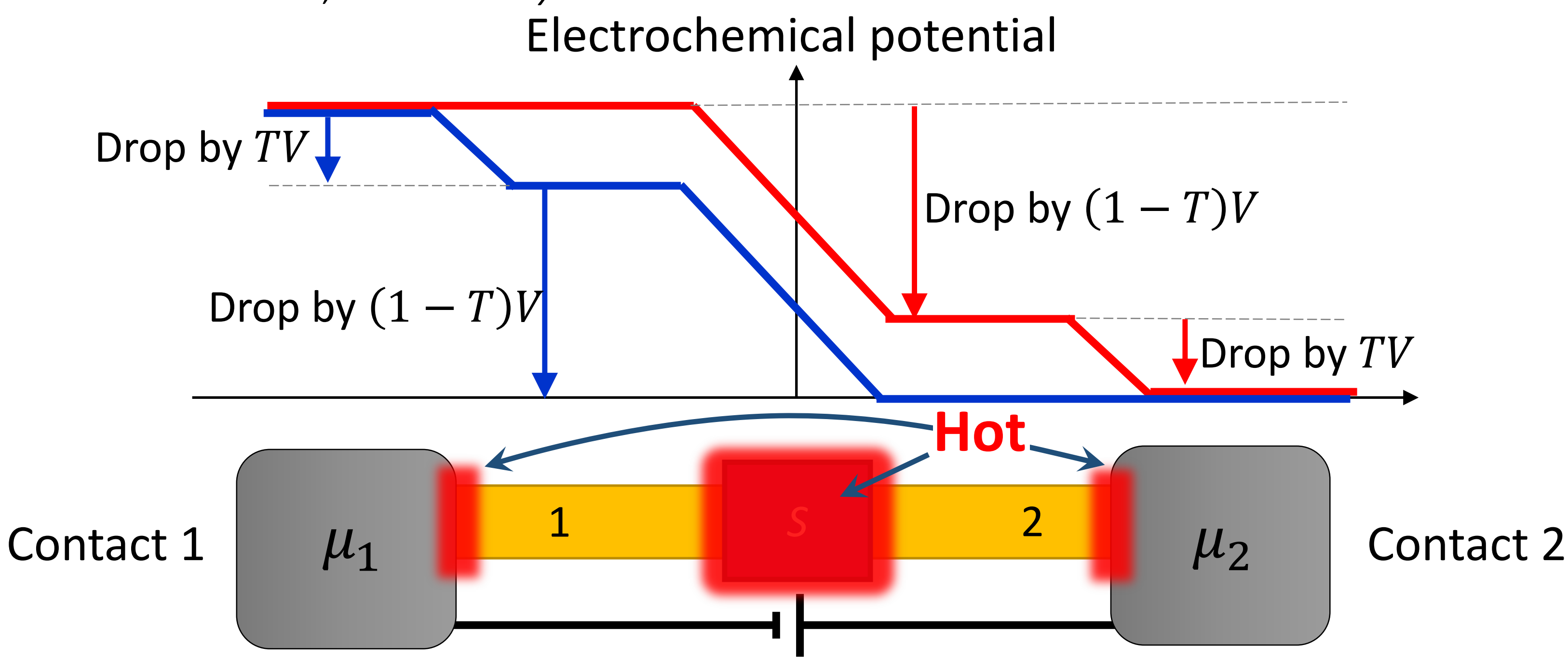


Physics of MQT: Not perfect but ballistic conductor

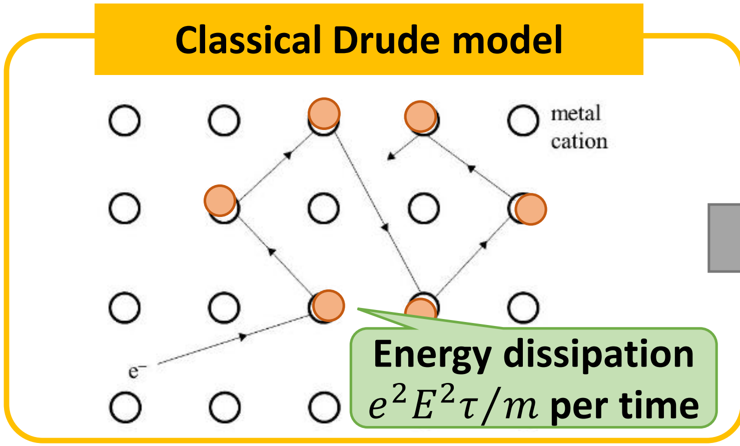


Ashcroft & Mermin, *Solid State Physics*

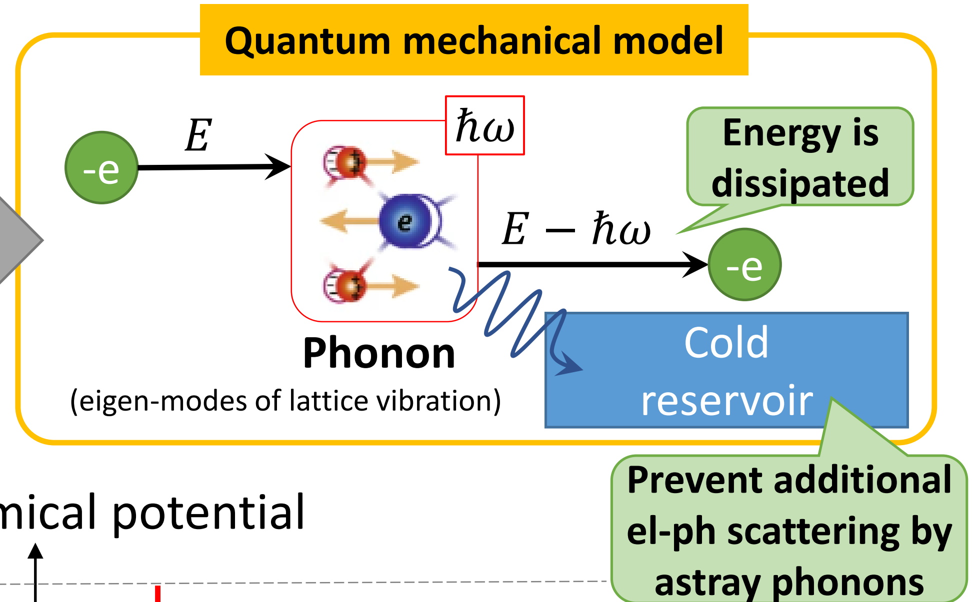


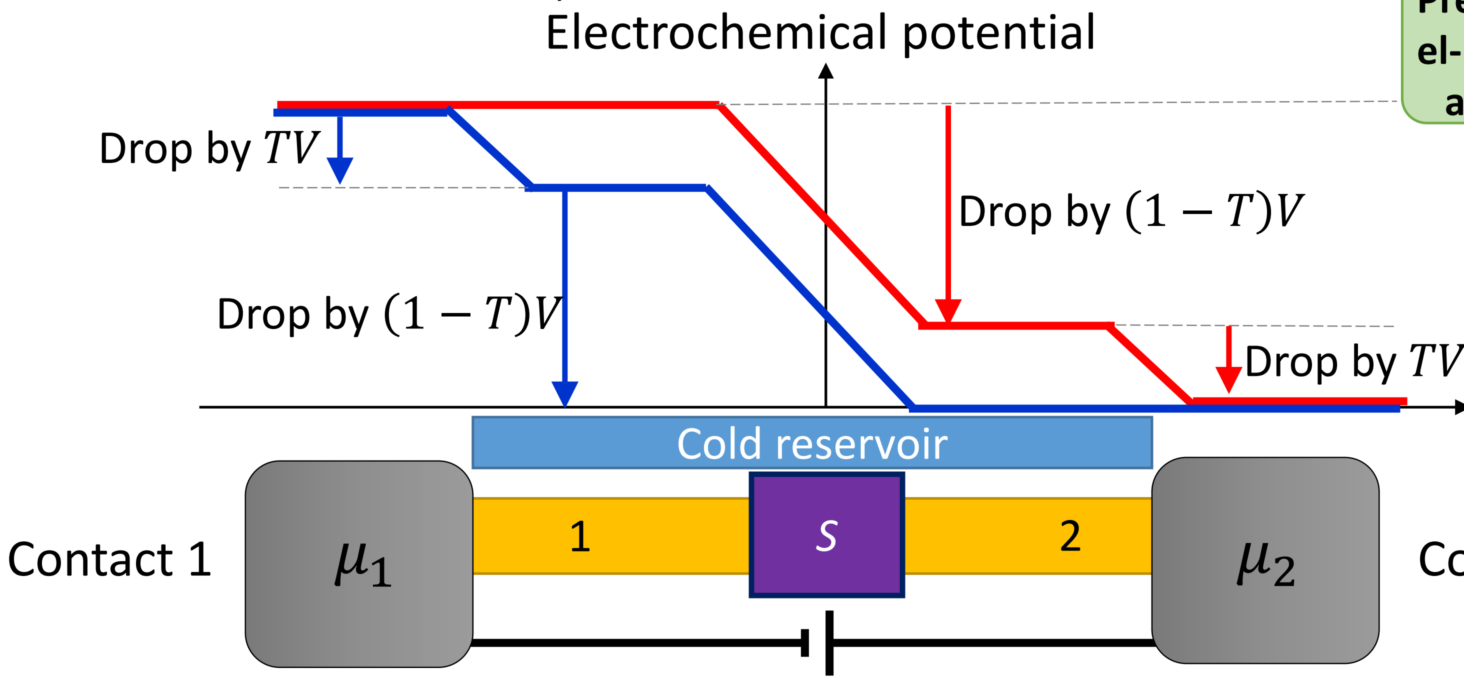


Physics of MQT: Not perfect but ballistic conductor



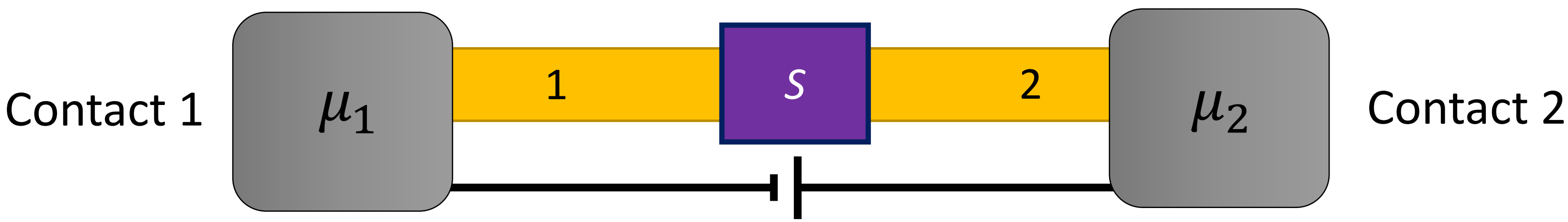
Ashcroft & Mermin, *Solid State Physics*

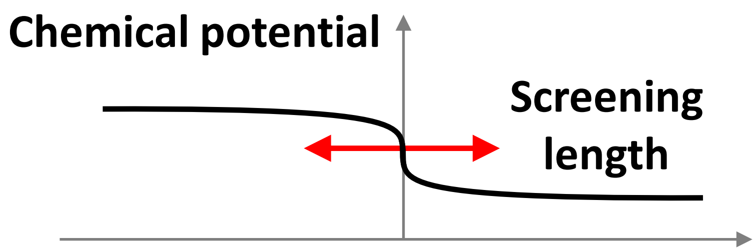




Physics of MQT: Not perfect but ballistic conductor

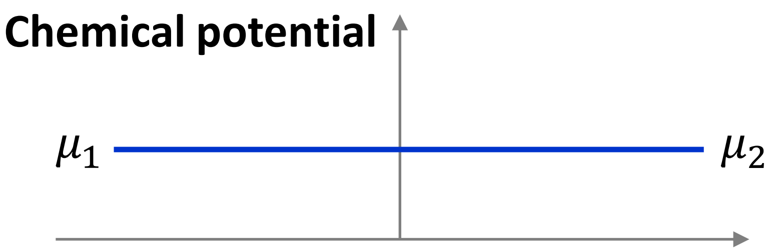
- **Are electrons transported by electric field as like Drude model?**



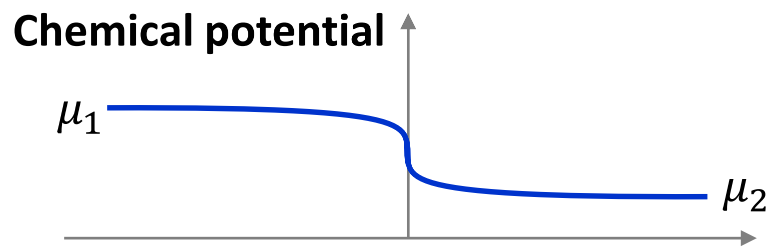


Gradient of chemical potential is generated by **Neq. Bias**

$\mu_1 = \mu_2$

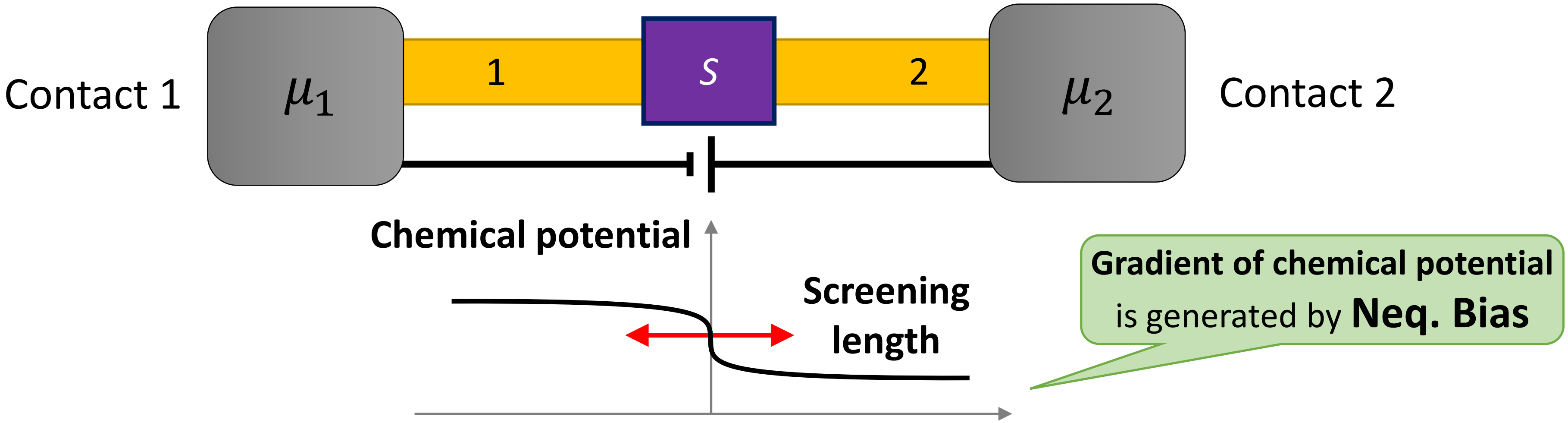


$\mu_1 > \mu_2$



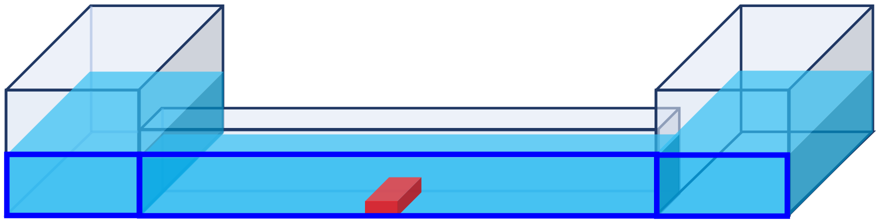
Physics of MQT: Not perfect but ballistic conductor

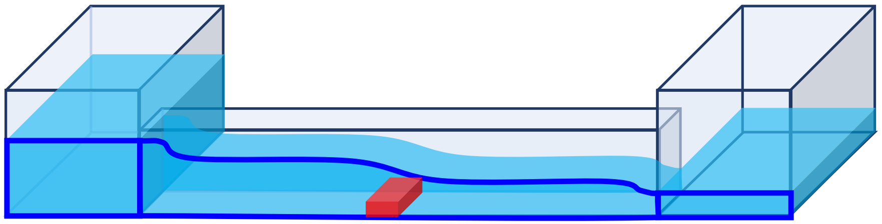
- **Are electrons transported by electric field as like Drude model?**



$\mu_1 = \mu_2$

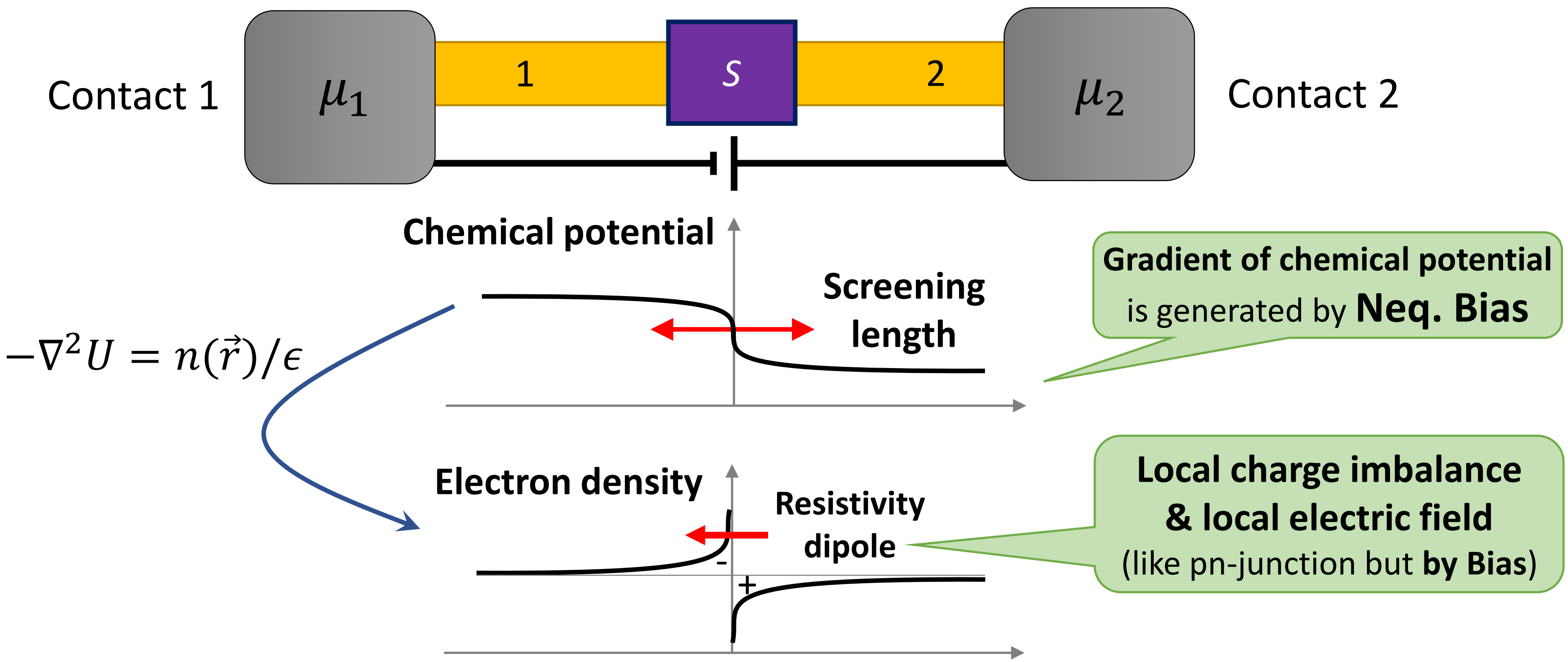
$\mu_1 > \mu_2$





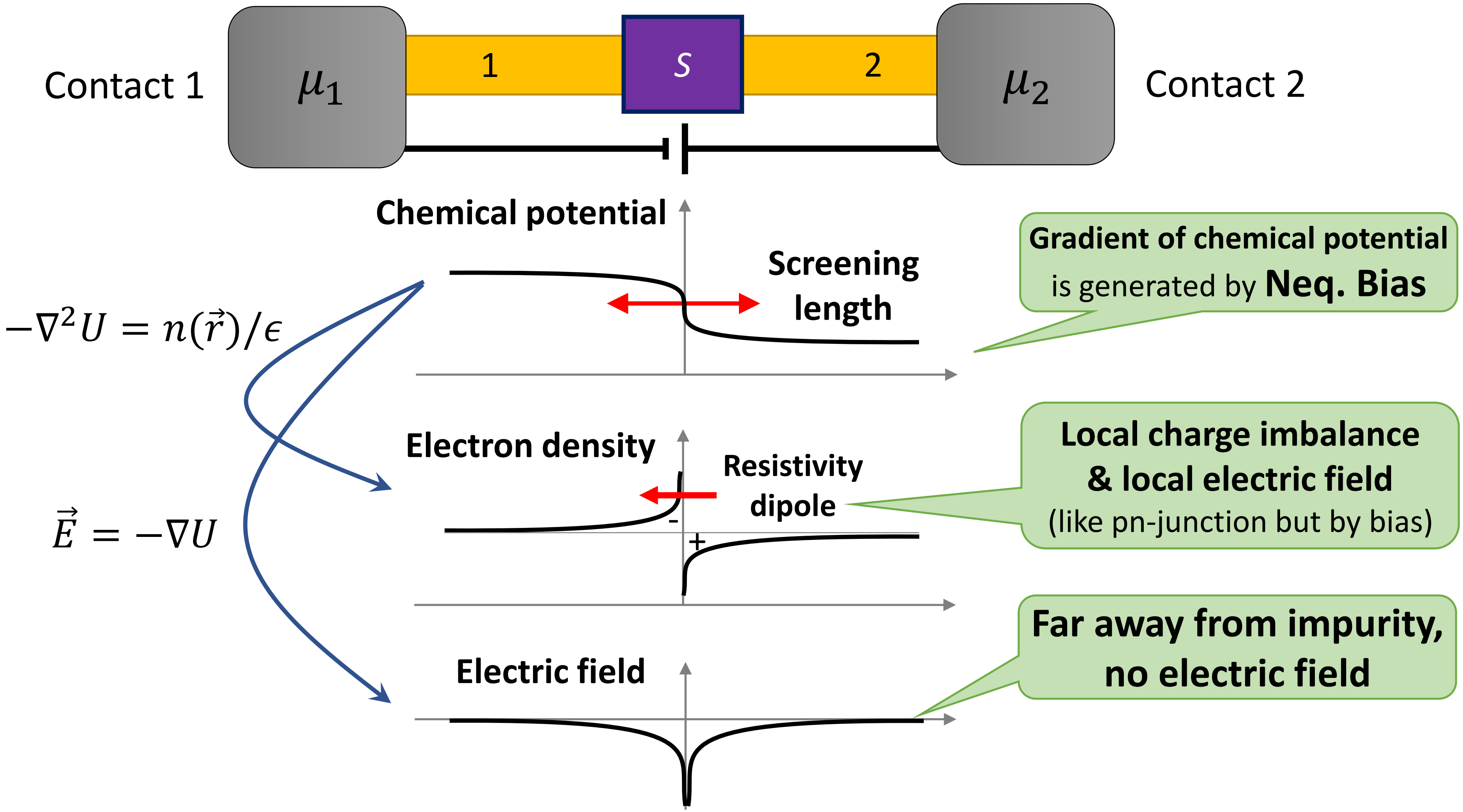
Physics of MQT: Not perfect but ballistic conductor

- **Are electrons transported by electric field as like Drude model?**



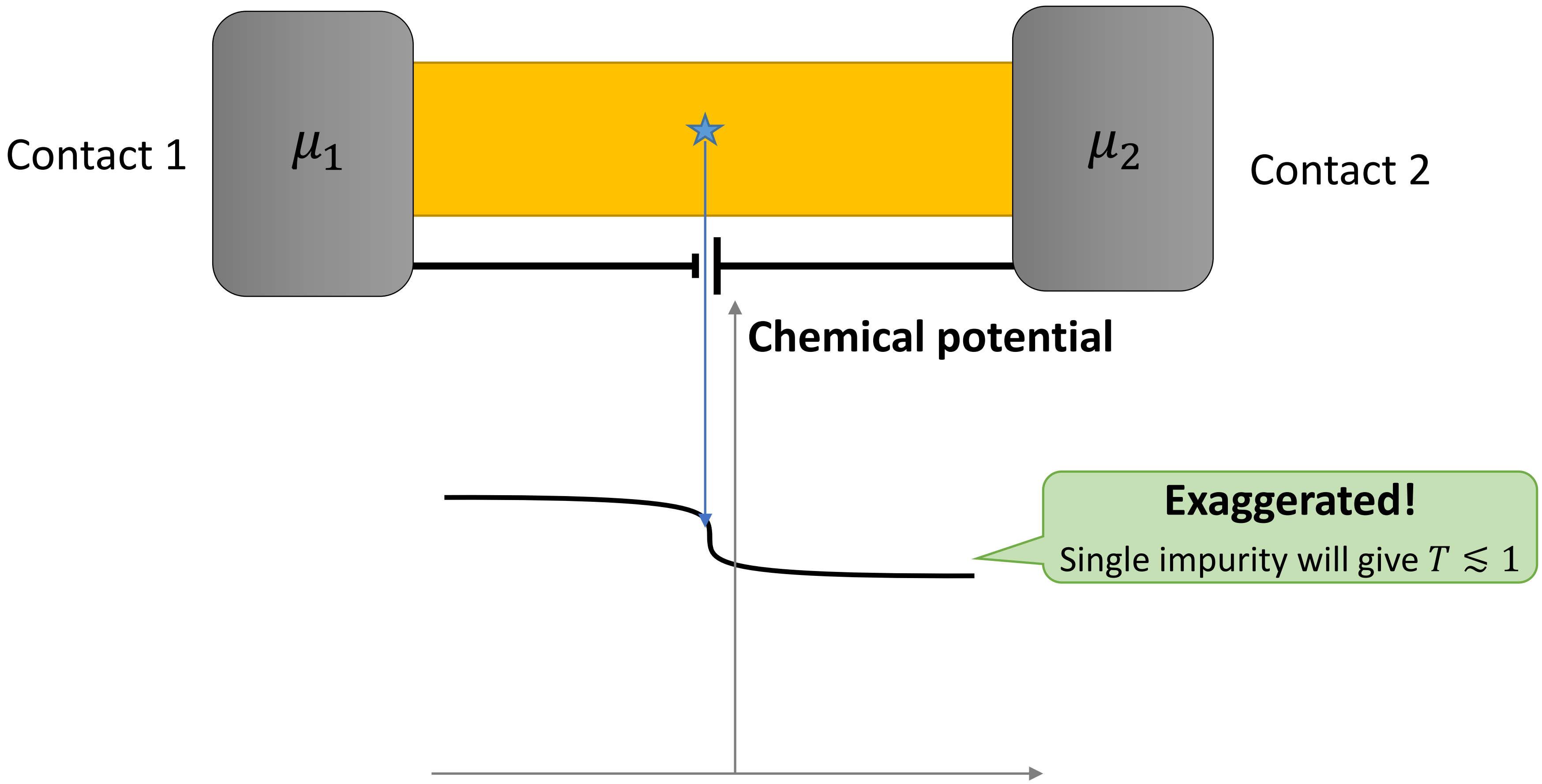
Physics of MQT: Not perfect but ballistic conductor

- **Are electrons transported by electric field as like Drude model?**



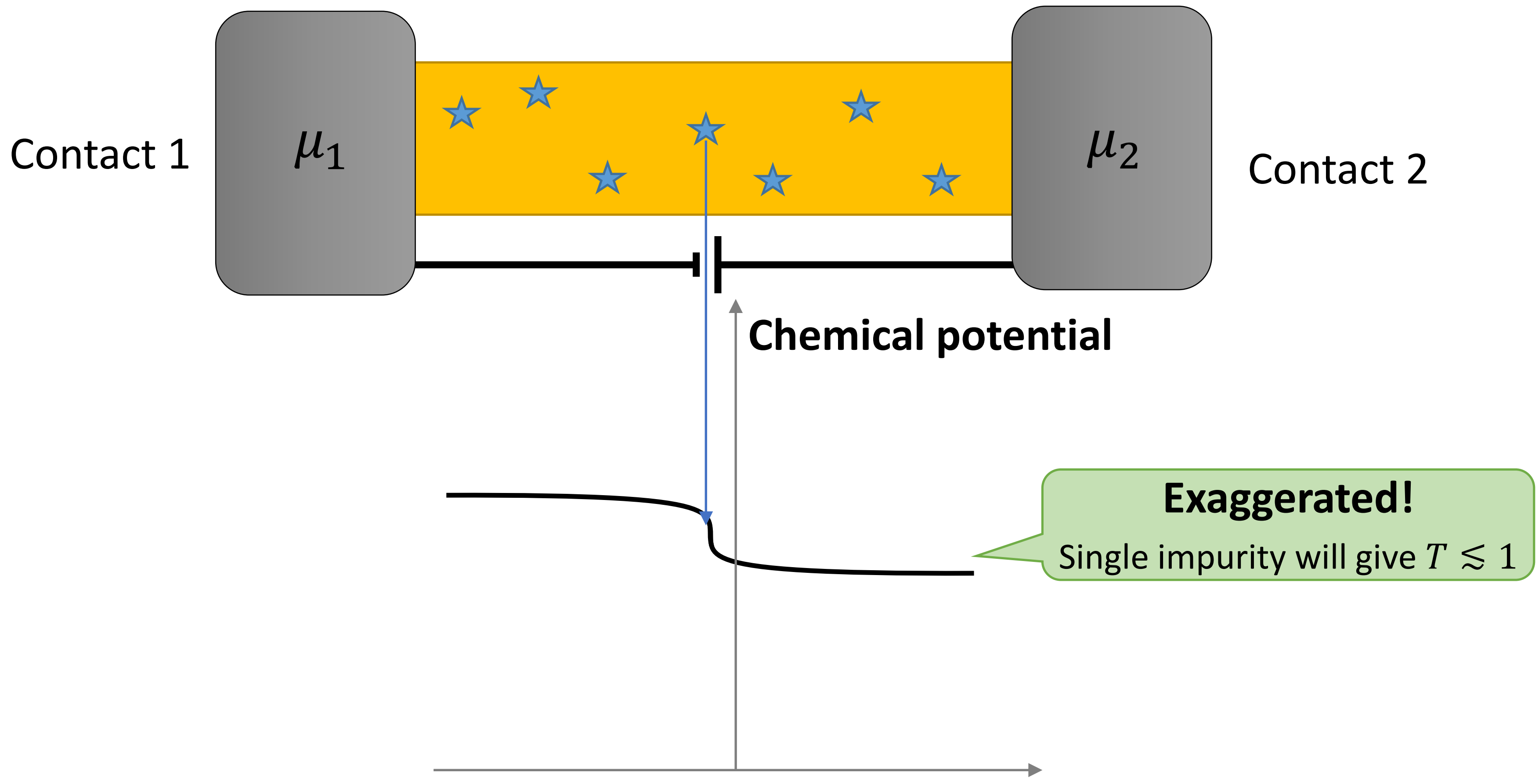
Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** L_m, $L_\varphi \ll L$, $\lambda_F \ll W$



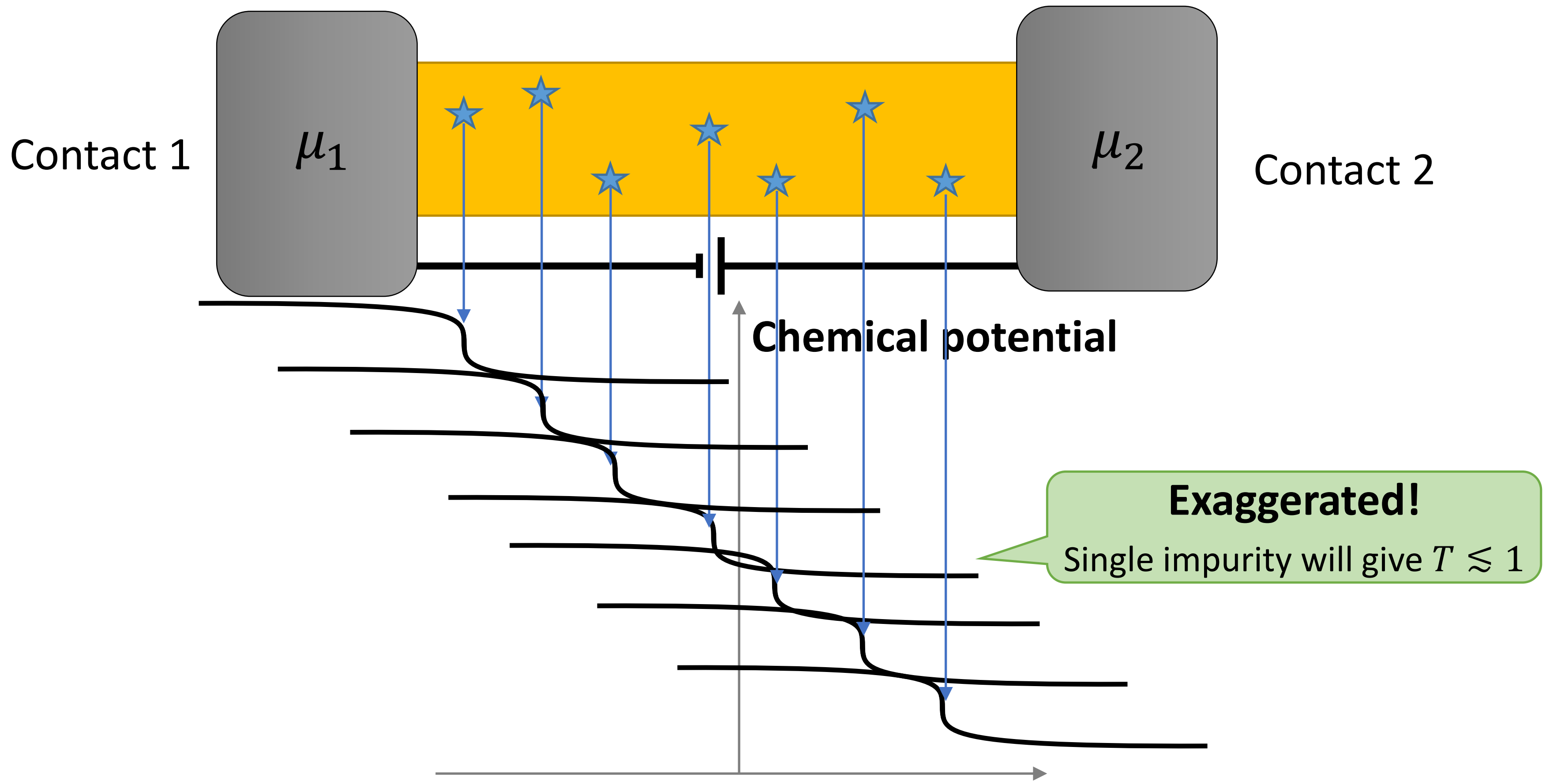
Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** L_m, $L_\varphi \ll L$, $\lambda_F \ll W$



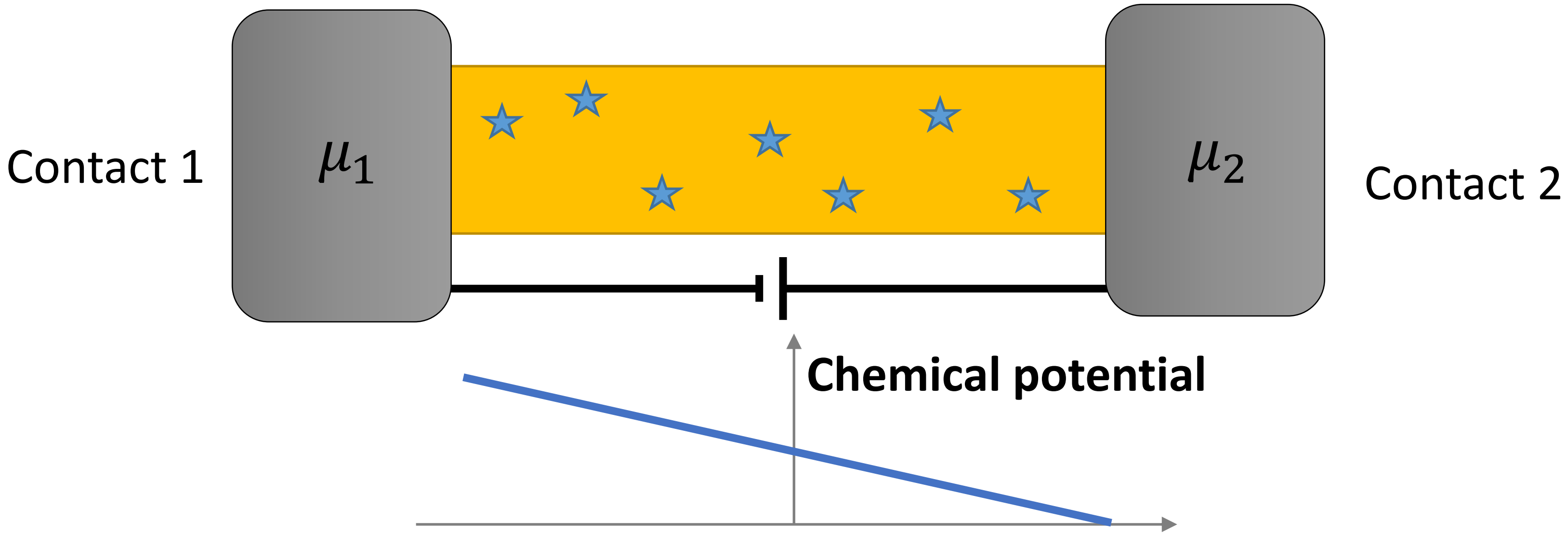
Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** L_m, $L_\varphi << L$, $\lambda_F << W$



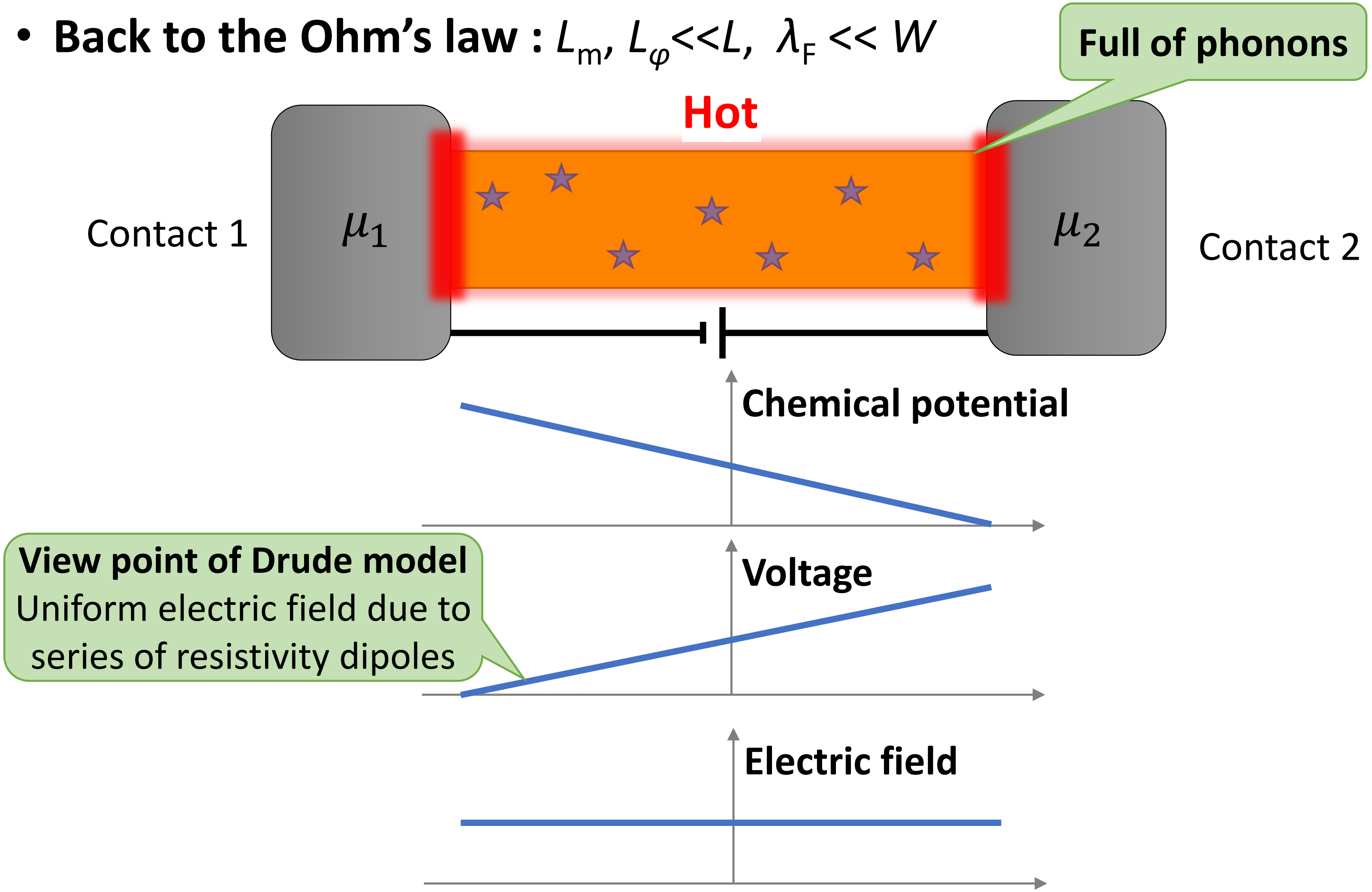
Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** L_m, $L_\varphi << L$, $\lambda_F << W$



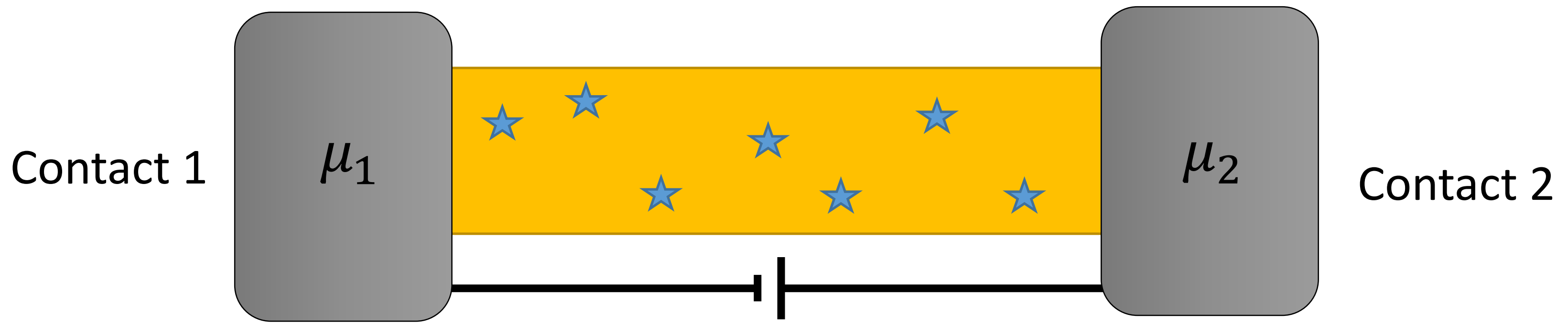
Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** $L_m, L_\varphi << L,\ \lambda_F << W$



Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** L_m, $L_\varphi \ll L$, $\lambda_F \ll W$



- **Landauer formula for Ohmic regime**

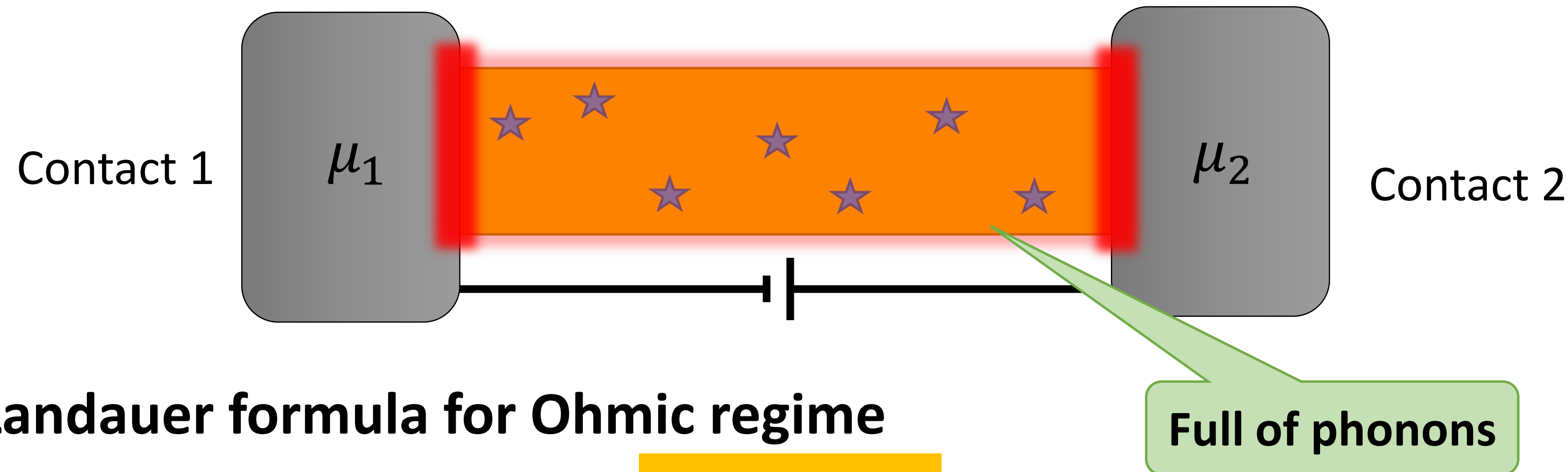
$$G = \frac{2e^2}{h} MT$$

From Landauer formula, do we recover $G = \sigma \frac{W}{L}$?

(it might be… if $M \propto W$ & $T \propto 1/L$)

Physics of MQT: No perfect & diffusive conductor

- **Back to the Ohm's law :** $L_m, L_\varphi << L,\ \lambda_F << W$



- **Landauer formula for Ohmic regime**

$$G = \frac{2e^2}{h} MT$$

$$k_n W = n\pi$$
$$k_n < k_M \sim k_F$$
$$k_F W \sim M\pi$$

$\lambda_F << W$

Hence,

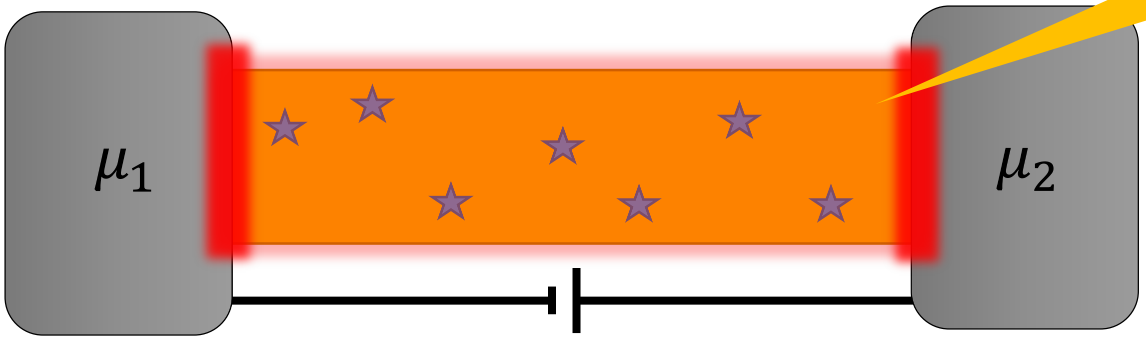
$$M \sim \frac{k_F W}{\pi}$$

Diffusive regime, $L_\varphi << L$

Otherwise, the scattering problem will be about Anderson localization

Physics of MQT: Not perfect but ballistic conductor

- **Back to the Ohm's law :** $L_m, L_\varphi << L,\ \lambda_F << W$



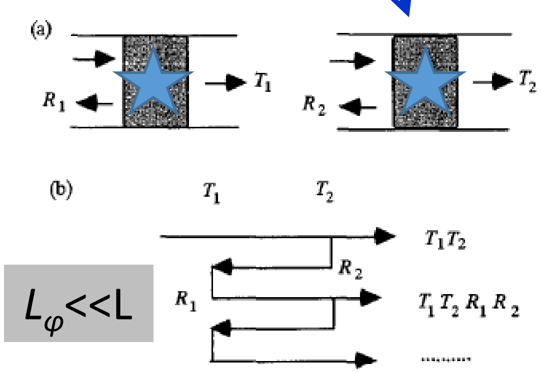
- **Landauer formula for Ohmic regime**

$$G = \frac{2e^2}{h} MT$$

$$k_n W = n\pi$$
$$k_n < k_M \sim k_F$$
$$k_F W \sim M\pi$$

Hence,

$$M \sim \frac{k_F W}{\pi}$$



$$T_{12} = T_1T_2 + T_1T_2R_1R_2 + \cdots$$
$$= \frac{T_1T_2}{1-R_1R_2} = \frac{T_1T_2}{1-(1-T_1)(1-T_2)}.$$

Observe $\frac{1-T_{12}}{T_{12}} = \frac{1-T_1}{T_1} + \frac{1-T_2}{T_2}$.

Then, $\frac{1-T_{123}}{T_{123}} = \frac{1-T_{12}}{T_{12}} + \frac{1-T_3}{T_3}$

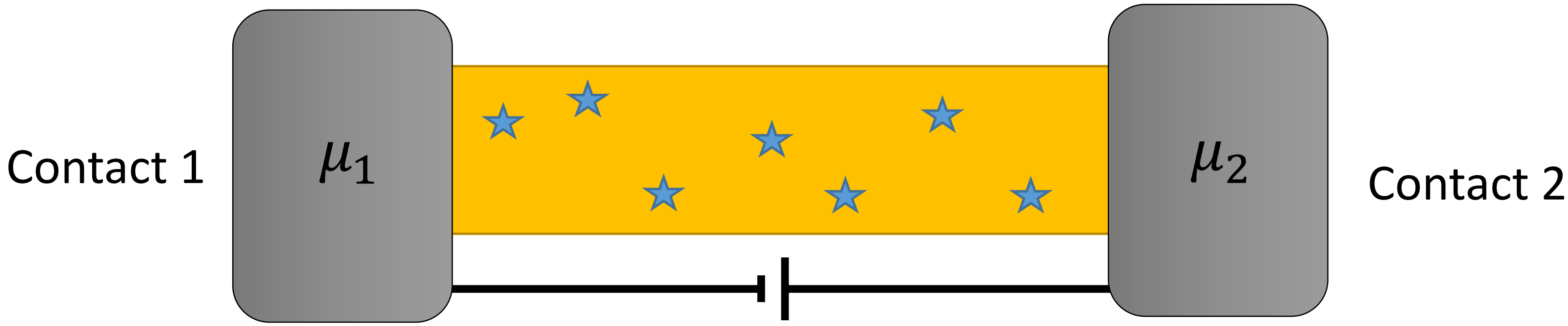
$$= \frac{1-T_1}{T_1} + \frac{1-T_2}{T_2} + \frac{1-T_3}{T_3}.$$

$\frac{1-T(N)}{T(N)} = N\frac{1-T}{T}$. Hence,

$$T(N) = \frac{T}{N(1-T)+T}$$

Physics of MQT: Not perfect but ballistic conductor

- **Back to the Ohm's law :** $L_{\mathrm{m}}, L_{\varphi} \ll L,\ \lambda_{\mathrm{F}} \ll W$



- **Landauer formula for Ohmic regime**

$$G = \frac{2e^2}{h} MT$$

$$k_n W = n\pi$$
$$k_n < k_M \sim k_F$$
$$k_F W \sim M\pi$$

Hence,

$$M \sim \frac{k_F W}{\pi}$$

$$T(N) = \frac{T}{N(1-T)+T} = \frac{T}{\nu L(1-T)+T}$$

Impurity density ν, $N = \nu L$

$$L_0 \equiv \frac{T}{\nu(1-T)}$$
$$(1-T)\nu L_{\mathrm{m}} \sim 1$$

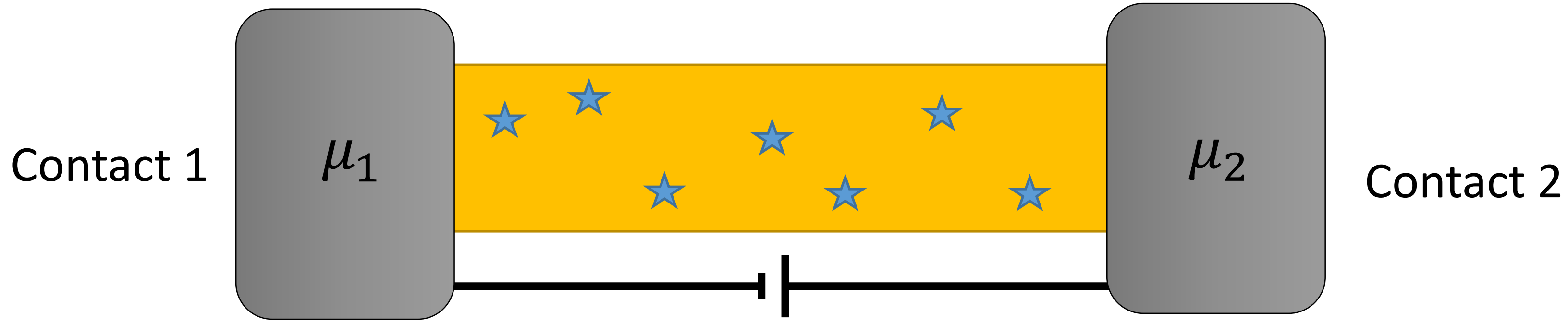
If $T \lesssim 1 \Rightarrow L_{\mathrm{m}} \sim L_0$

$$T(N) = \frac{L_0}{L+L_0} \sim \frac{L_{\mathrm{m}}}{L+L_{\mathrm{m}}} \sim \frac{L_{\mathrm{m}}}{L}$$

$$L_{\mathrm{m}} \ll L$$

Physics of MQT: Not perfect but ballistic conductor

- **Back to the Ohm's law :** L_m, $L_\varphi << L$, $\lambda_F << W$



- **Landauer formula for Ohmic regime**

$$G = \frac{2e^2}{h} MT$$

$$G = \sigma \frac{W}{L} = \frac{ne^2\tau}{m}\frac{W}{L}.$$

for L_m, $L_\varphi << L$, $\lambda_F << W$

$$M \sim \frac{k_F W}{\pi}$$

$$T(N) \sim \frac{L_m}{L}$$

$$G = \frac{2e^2}{h}\frac{k_F W}{\pi}\frac{L_m}{L} = \left(\frac{2e^2 k_F L_m}{h}\right)\frac{W}{L} = \sigma\frac{W}{L}$$

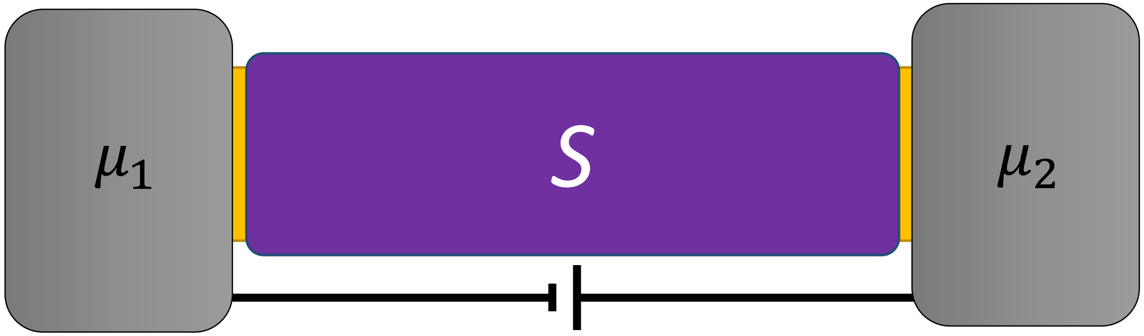
$$\sigma = \frac{2e^2 k_F}{h}\frac{h k_F \tau}{2\pi m} = \frac{k_F^2}{\pi}\frac{e^2\tau}{m} = \frac{ne^2\tau}{m}$$

$$\hbar k_F = m v_F = m L_m/\tau$$
$$\Leftrightarrow L_m = \hbar k_F \tau/m$$

$$N = \pi k_F^2/\Delta k_x \Delta k_y \Leftrightarrow n = N/LW = k_F^2/\pi$$

Physics of MQT: Not perfect but ballistic conductor

- **Back to the Ohm's law :** $L_\mathrm{m}, L_\varphi \ll L,\ \lambda_\mathrm{F} \ll W$



- **Landauer formula for Ohmic regime**

$$G = \frac{2e^2}{h} MT$$

$$M \sim \frac{k_F W}{\pi}$$

$$T(N) \sim \frac{L_\mathrm{m}}{L}$$

$$G = \frac{2e^2}{h} \frac{k_F W}{\pi} \frac{L_\mathrm{m}}{L} = \left(\frac{2e^2 k_F L_\mathrm{m}}{h}\right) \frac{W}{L}$$

$$\sigma = \frac{2e^2 k_F}{h} \frac{h k_F \tau}{2\pi m} = \frac{k_F^2}{\pi} \frac{e^2 \tau}{m} = \frac{n e^2 \tau}{m}$$

Ohm's Law is derived

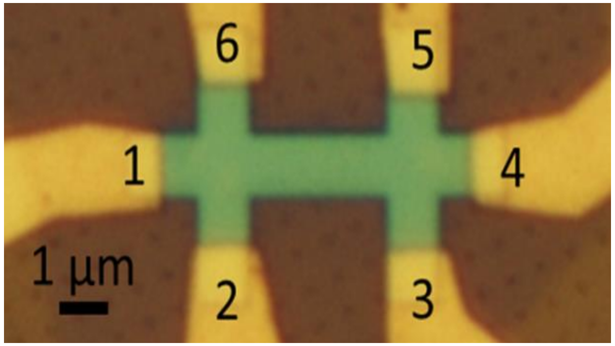
(Lesson) Now we know when MQT becomes classical from a microscopic view point & How limited Drude model is.

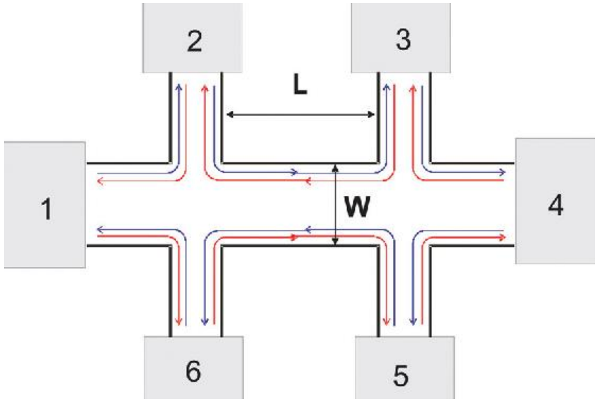
Landauer formalism gives another lesson:

all you need to know for transport is the S-matrix.

(as long as it is a single particle physics)

Physics of MQT: multi-terminal transport





- **Büttiker formula: multi-terminal transport**

$$I_p = \frac{2e}{h}\sum_q\left[T_{q\leftarrow p}\mu_p - T_{p\leftarrow q}\mu_q\right] = \sum_q\left[G_{qp}V_p - G_{pq}V_q\right]$$

$$G_{qp} = \frac{2e^2}{h}T_{q\leftarrow p}$$

c.f. two-terminal case

$T_{21} = T_{12}$ to have $I_1 = 0$ for $\mu_1 - \mu_2$

$$I_1 = \frac{2e}{h}(T_{21}\mu_1 - T_{12}\mu_2) = \frac{2e}{h}T_{12}(\mu_1 - \mu_2) = GV$$

- **Sum rule:** $\sum_q G_{qp} = \sum_q G_{pq}$ to have $I_p = 0$ for $V_p = V_q = V_0$

Physics of MQT: finite voltage bias and temperature

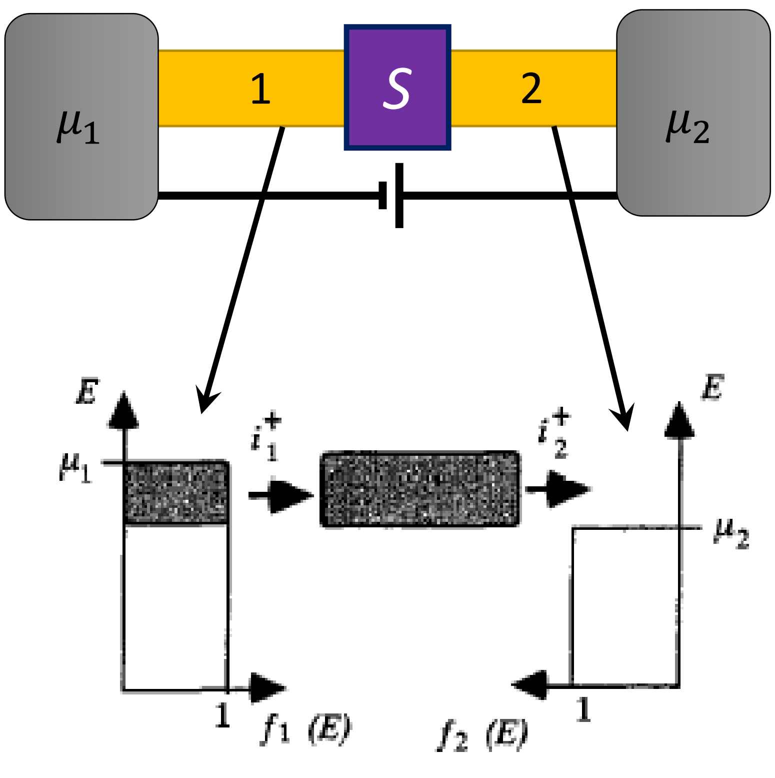
- **Beyond the linear response regime: Kubo's formula is not enough**

  → *S*-matrix, energy-dependent

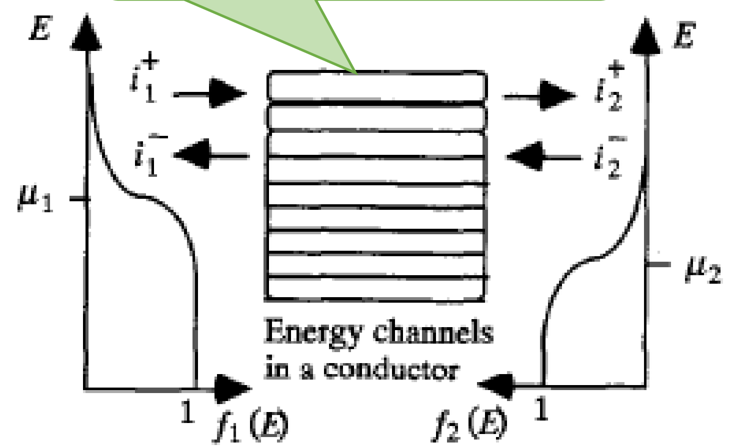
  → Non-zero temperature

$$I = \frac{2e}{h} MT(\mu_1 - \mu_2) = \frac{2e}{h} MT \int [f_1(E) - f_2(E)] dE$$

$$\mapsto \frac{2e}{h} \sum_n \int T_n(E)[f_1(E) - f_2(E)] dE$$



Thermoelectric transport can be dealt



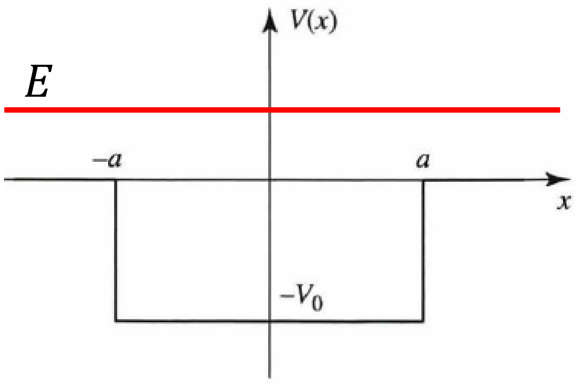
Application of Landauer-Büttiker formalism

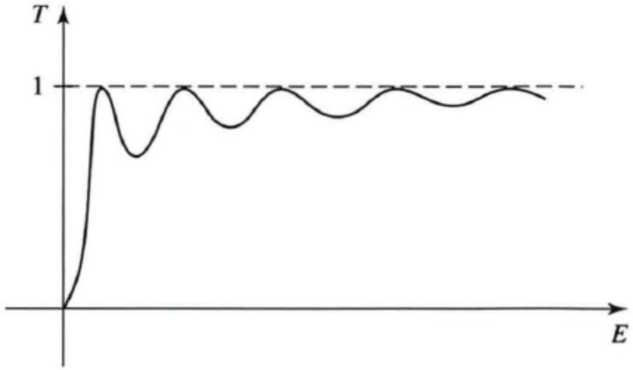
- **Usages of Landauer-Büttiker formalism in research (analytical)**

  → **Universal physics**: precise S-matrix may not be required much

  → **Symmetry**: S-matrix can be known solely from symmetry

Ramsauer-Townsend Effect: Ballistic and coherent





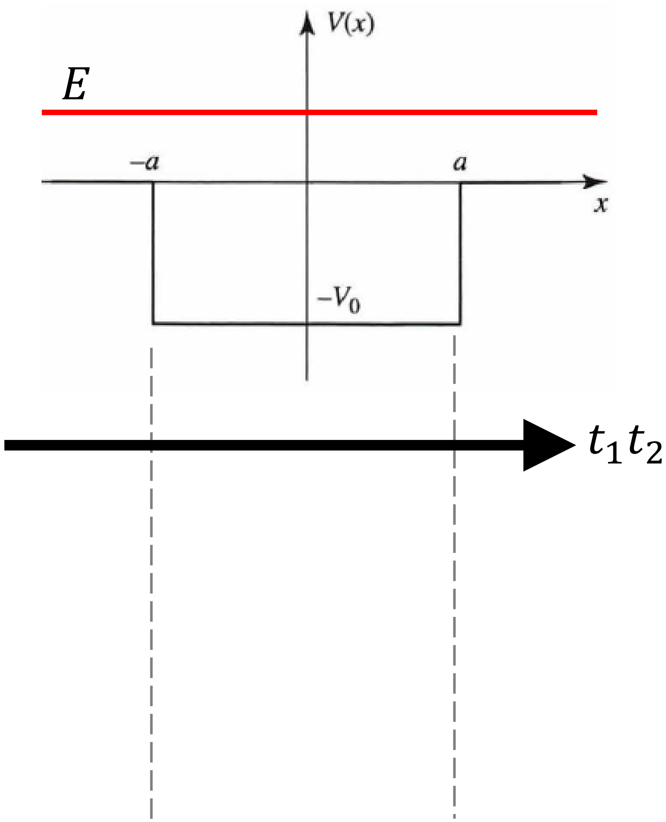
$$T(E) = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}$$

Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**

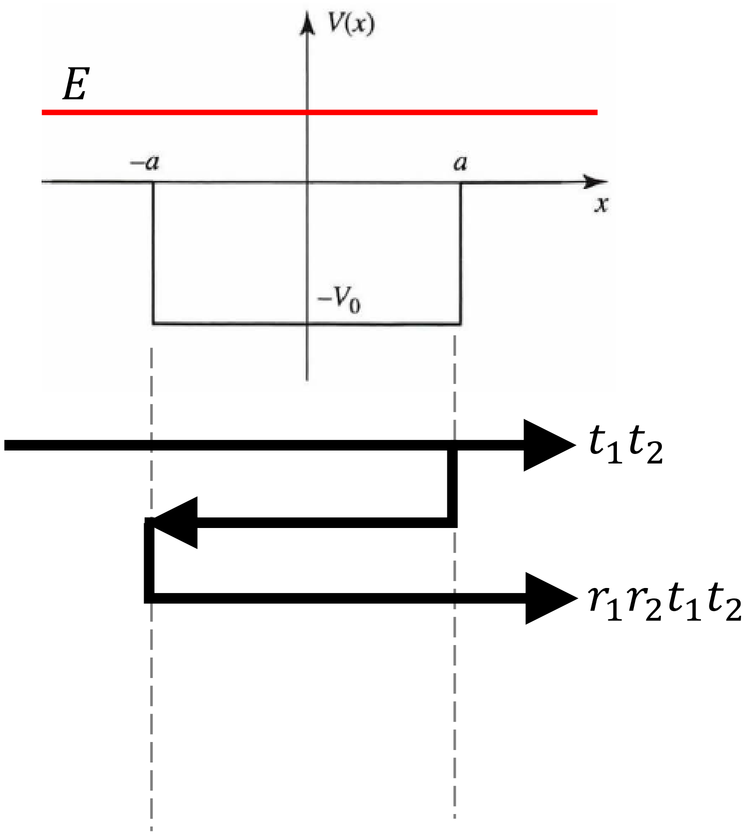
  → **Universal physics**: precise S-matrix may not be required much

  → **Symmetry**: S-matrix can be known solely from symmetry



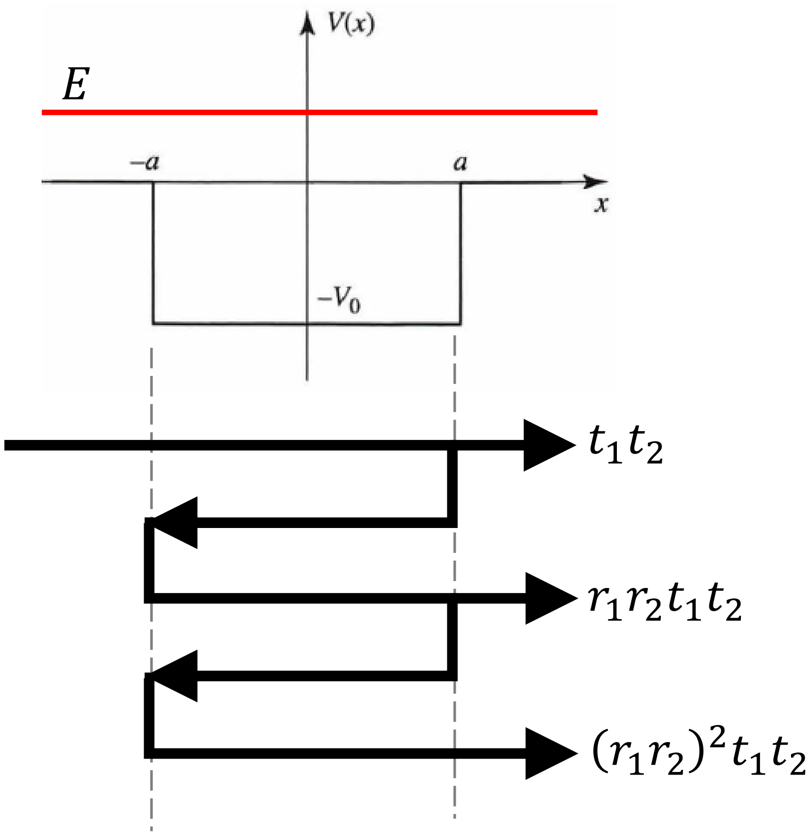
Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**
  - → **Universal physics**: precise S-matrix may not be required much
  - → **Symmetry**: S-matrix can be known solely from symmetry



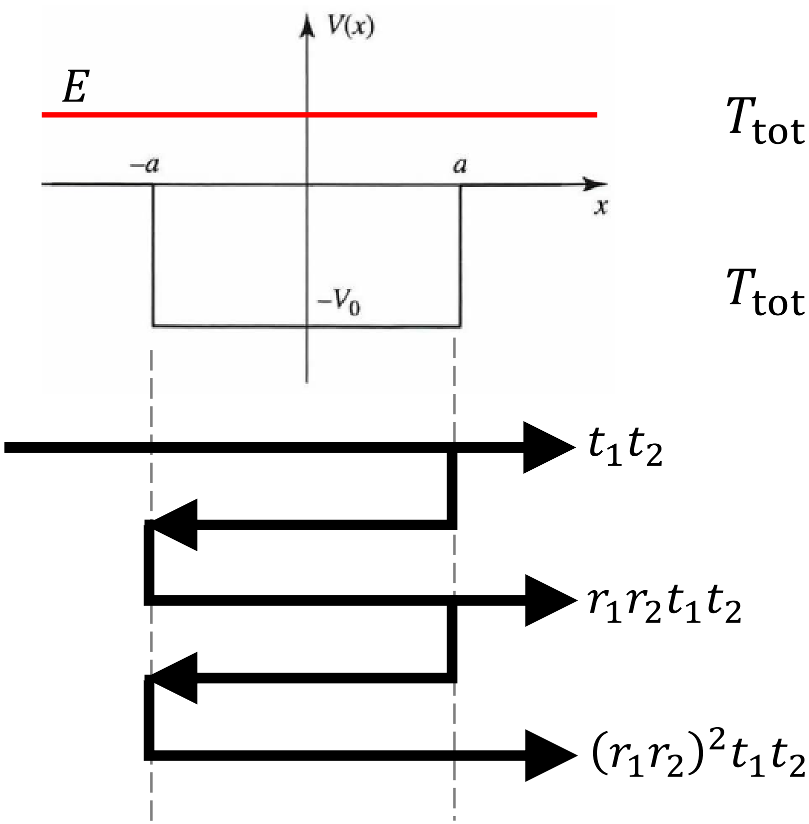
Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**
  → **Universal physics**: precise S-matrix may not be required much
  → **Symmetry**: S-matrix can be known solely from symmetry



Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**
  - → **Universal physics**: precise S-matrix may not be required much
  - → **Symmetry**: S-matrix can be known solely from symmetry



$e^{i\theta} = \arg(r_1 r_2)$

$$T_{\mathrm{tot}} = \left|\frac{t_1 t_2}{1 - r_1 r_2}\right|^2 = \frac{|t_1|^2 |t_2|^2}{1 + |r_1|^2 |r_2|^2 - 2|r_1||r_2| \cos\theta}$$

$T = |t_1|^2 = |t_2|^2$

$R + T = 1$

$$T_{\mathrm{tot}} = |\tau|^2 = \frac{T^2}{T^2 + 4(1-T)\sin^2\left(\frac{\theta}{2}\right)}$$

$\theta = 2n\pi$

$$T_{\mathrm{tot}} = 1$$

Resonant tunneling!
Every back&forth scattering adds $\theta = 2n\pi$ phase
⇒ constructive interference
(T=1 despite broken translational symmetry)

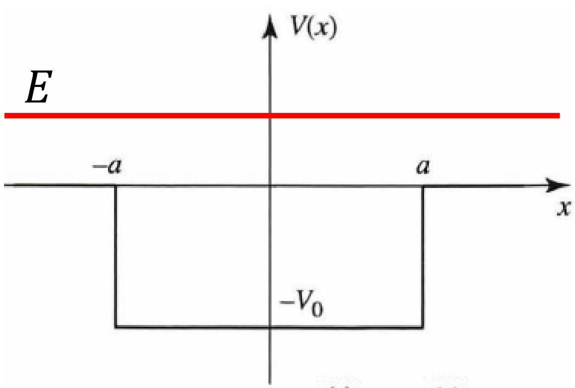
Application of Landauer-Büttiker formalism

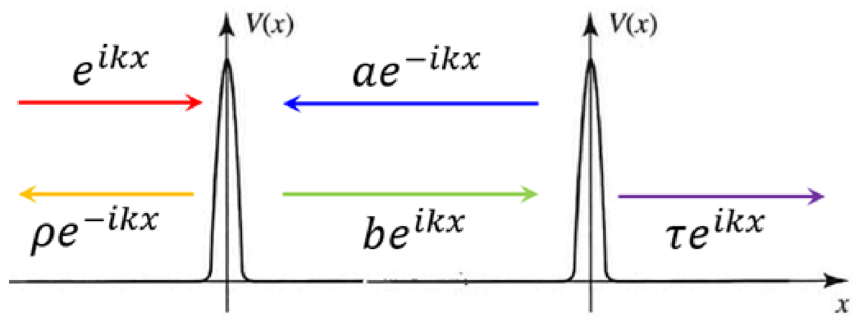
- **Usages of Landauer-Büttiker formalism in research (analytical)**

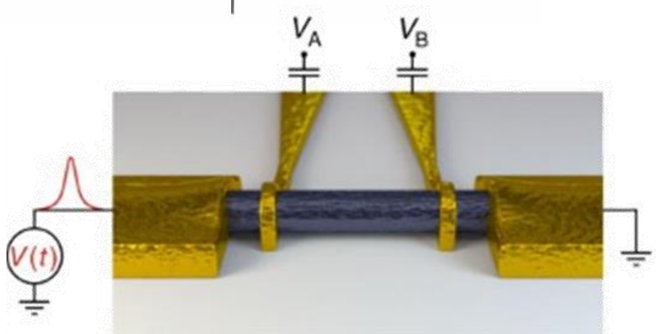
  → **Universal physics**: precise S-matrix may not be required much

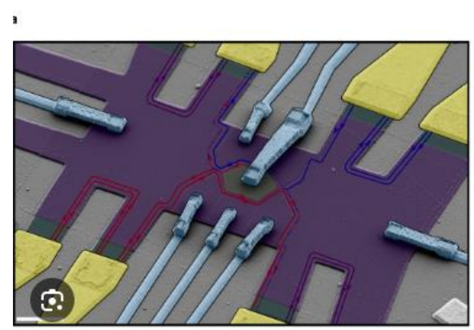
  → **Symmetry**: S-matrix can be known solely from symmetry

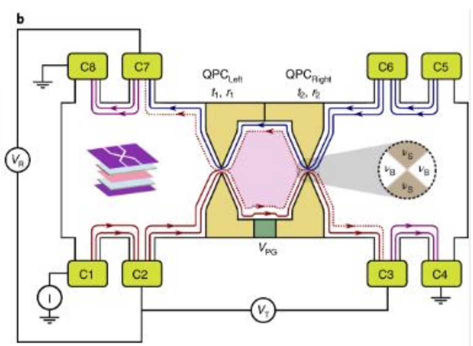
Resonant tunneling in MQT is universal in that particular shapes $V(x)$ or materials do not matter





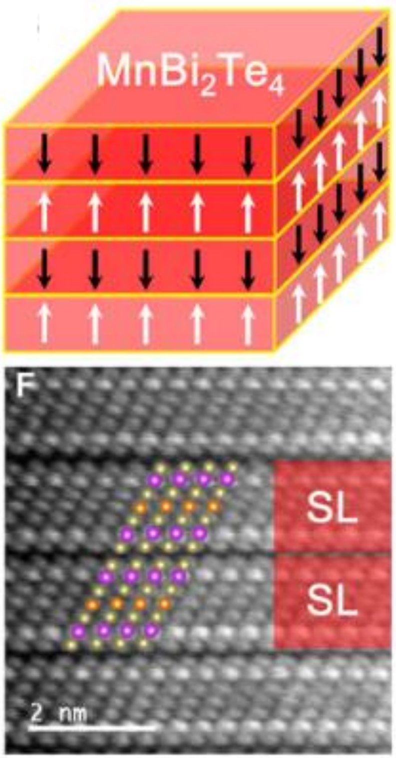


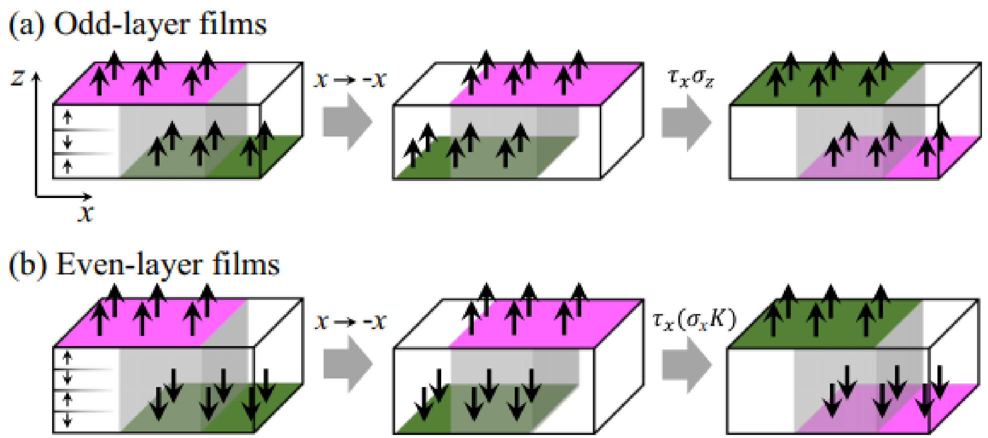


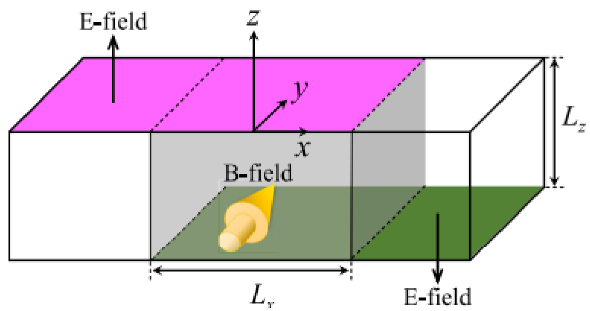


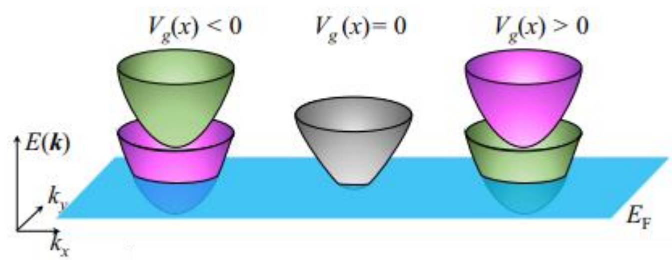
Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**
  - → **Universal physics**: precise S-matrix may not be required much
  - → **Symmetry**: S-matrix can be known solely from symmetry





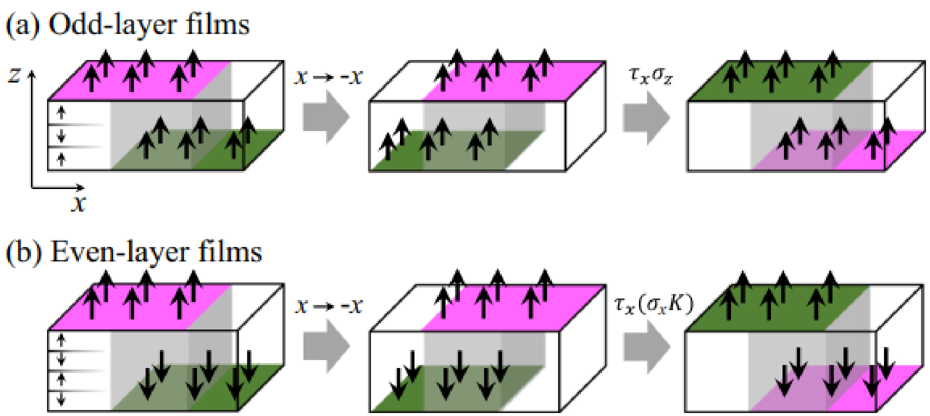




Sang-Jun Choi, Hai-Peng Sun, and Björn Trauzettel, *PRB* **107**, 235415 (2023)

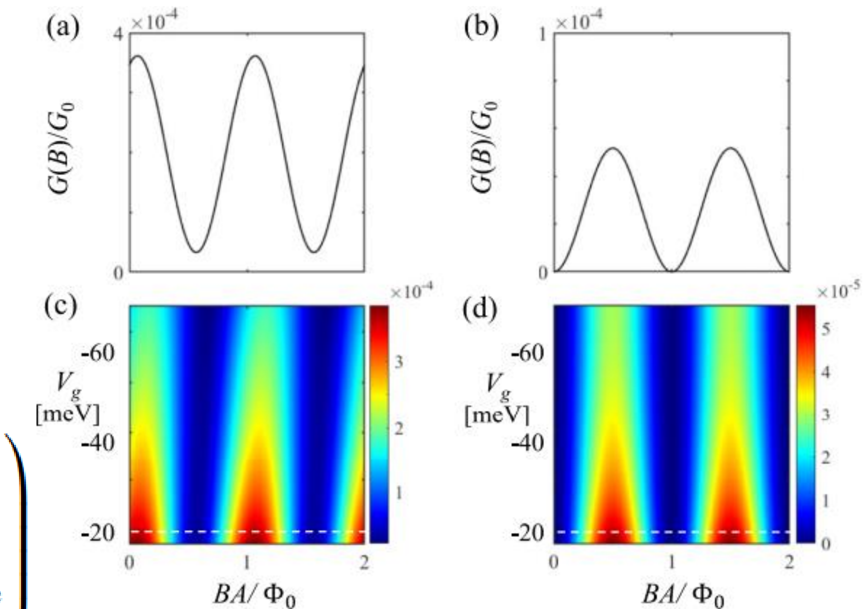
Application of Landauer-Büttiker formalism

- **Usages of Landauer-Büttiker formalism in research (analytical)**
  - → **Universal physics**: precise S-matrix may not be required much
  - → **Symmetry**: S-matrix can be known solely from symmetry



Odd layers

Even layers



$$S_{tb}^{\text{odd}} = \begin{pmatrix} t'_{\text{o}} & r'_{\text{o}} & t''_{\text{o}} & r''_{\text{o}} \\ r'_{\text{o}} & t'_{\text{o}} & r''_{\text{o}} & t''_{\text{o}} \\ t''_{\text{o}} & r''_{\text{o}} & t'_{\text{o}} & r'_{\text{o}} \\ r''_{\text{o}} & t''_{\text{o}} & r'_{\text{o}} & t'_{\text{o}} \end{pmatrix} \qquad S_{tb}^{\text{even}} = \begin{pmatrix} t'_{\text{e}} & r'_{\text{e}} & 0 & r''_{\text{e}} \\ r'_{\text{e}} & t'_{\text{e}} & r''_{\text{e}} & 0 \\ 0 & r''_{\text{e}} & t'_{\text{e}} & -r'_{\text{e}} \\ r''_{\text{e}} & 0 & -r'_{\text{e}} & t'_{\text{e}} \end{pmatrix}$$

π phase shift of $G(B)$

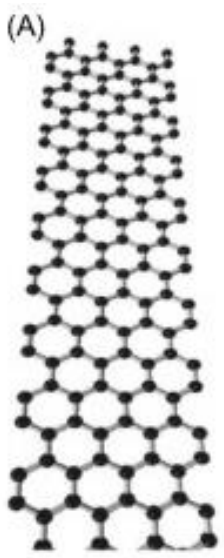
Sang-Jun Choi, Hai-Peng Sun, and Björn Trauzettel, *PRB* **107**, 235415 (2023)

Application of Landauer-Büttiker formalism

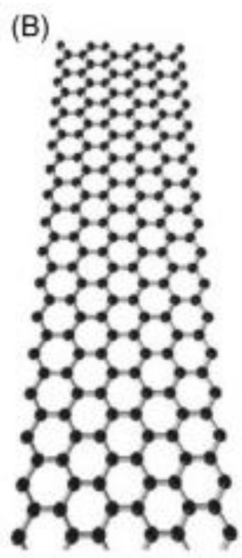
- **Usages of Landauer-Büttiker formalism in research (numerical)**

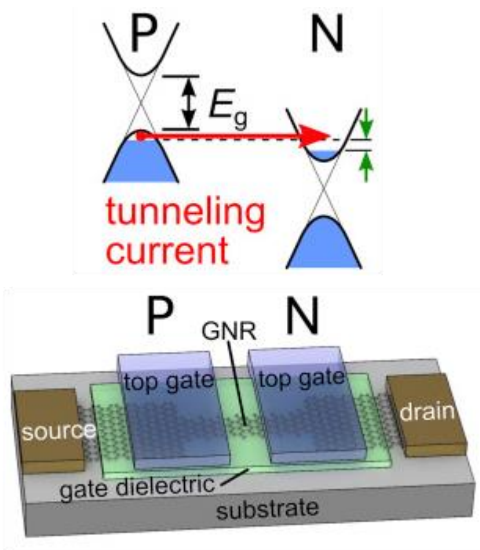
  → Various geometries and situations can be calculated

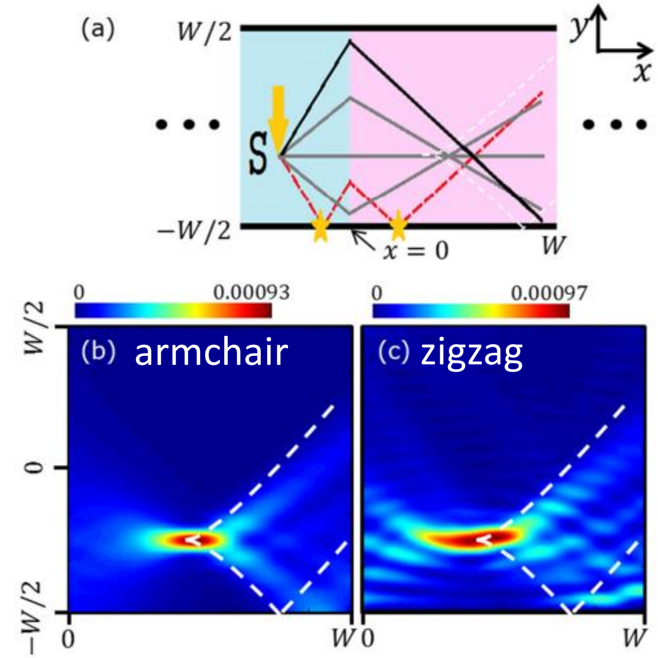
GNR w/ armchair edge



GNR w/ zigzag edge





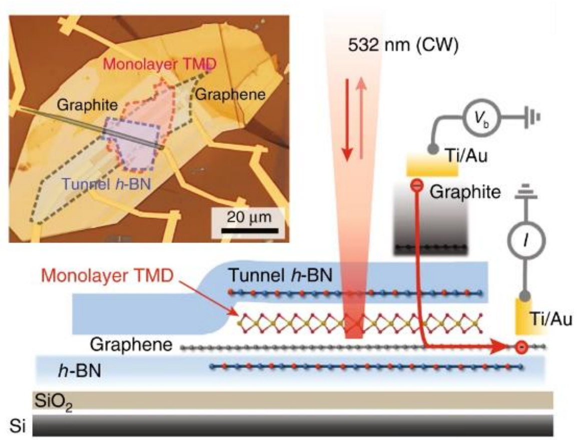


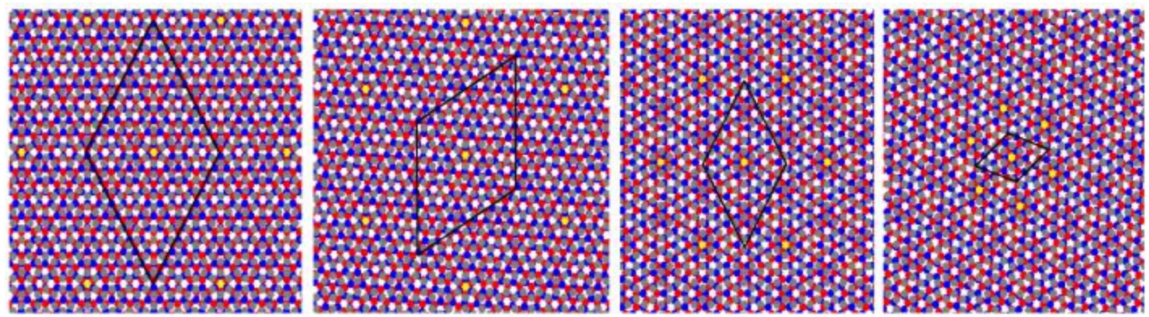
Sang-Jun Choi, Sunghun Park, and H.-S. Sim, PRB **89**, 155412 (2014)

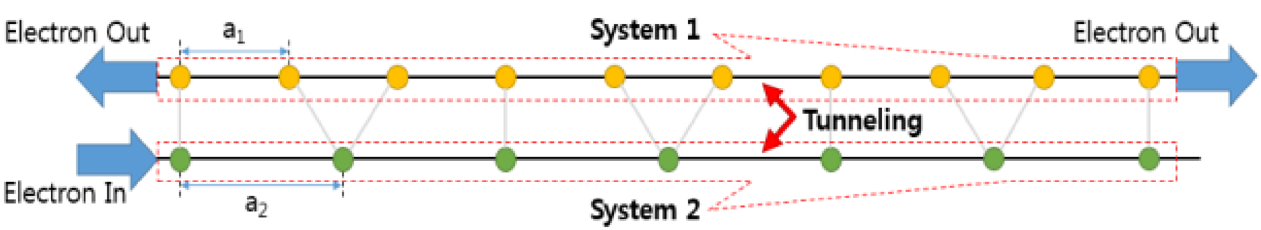
Application of Landauer-Büttiker formalism

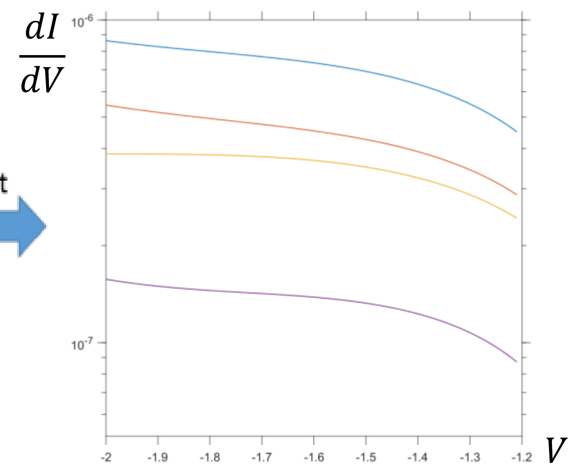
- **Usages of Landauer-Büttiker formalism in research (numerical)**

  → Various geometries and situations can be calculated









Tae Young Jeong, Hakseong Kim, **Sang-Jun Choi**, et al., *Nature Communications* **10**, 3825 (2019)

How to obtain S-matrix using Green functions

- **Nonequilibrium Green Function (NEGF) formalism** (Keldysh formalism)

Green function → Scattering matrix

- **Single-particle Green function:**

→ Probability amplitude of a propagating particle for an impulse

$$\left[E + i0^+ + \frac{\hbar^2}{2m}\nabla^2 - U(\vec{r})\right] G^r(\vec{r},\vec{r}') = \delta(\vec{r},\vec{r}')$$

$$\left[E - i0^+ + \frac{\hbar^2}{2m}\nabla^2 - U(\vec{r})\right] G^a(\vec{r},\vec{r}') = \delta(\vec{r},\vec{r}')$$

- **Fisher-Lee relation** for single-mode lead

(for a single mode) $s_{qp} = -\delta_{qp} + i\hbar\sqrt{v_q v_p}\, G^r_{qp}$

Scattering of a particle

Propagation of a particle

D. S. Fisher and P. A. Lee, *PRB* **23**, 6851 (1981)

How to obtain S-matrix using Green functions

- **Fisher-Lee relation** for multimode leads

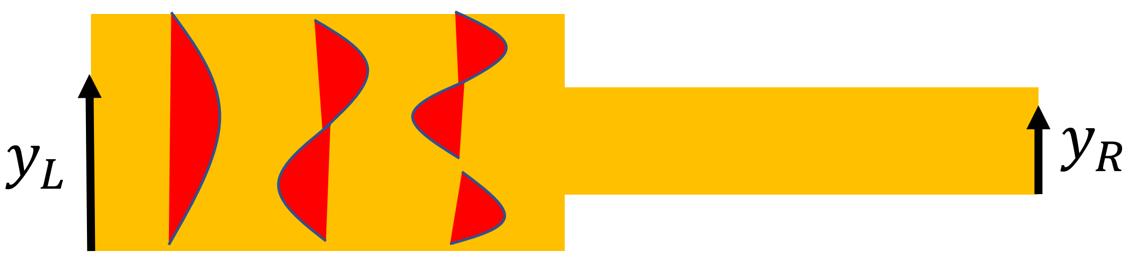
$$s_{nm}^{qp} = -\delta_{nm}^{qp} + i\hbar\sqrt{v_n v_m} \iint \chi_n(y_q)\left[G_{qp}^r(y_q, y_p)\right]\chi_m(y_p)\,dy_q\,dy_p$$

n-th mode in lead q

m-th mode in lead p

Indices for leads

e.g., $s_{12}^{RL} = i\hbar\sqrt{v_{1R} v_{2L}} \iint \chi_{1R}(y_R)\left[G_{RL}^r(y_R, y_L)\right]\chi_{2L}(y_L)\,dy_R\,dy_L$



How to obtain S-matrix using Green functions

- **Fisher-Lee relation** for multimode leads

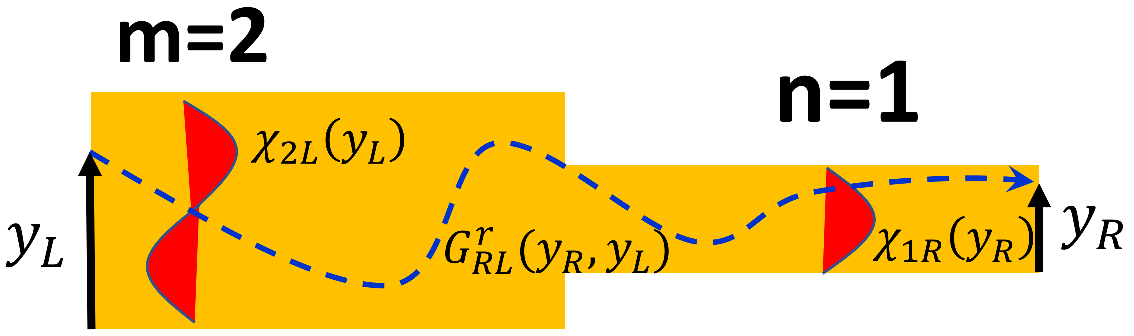
$$s_{nm}^{qp} = -\delta_{nm}^{qp} + i\hbar\sqrt{v_n v_m} \iint \chi_n(y_q)[G_{qp}^r(y_q, y_p)]\chi_m(y_p)dy_q dy_p$$

n-th mode in lead q

m-th mode in lead p

Indices for leads

e.g., $s_{12}^{RL} = i\hbar\sqrt{v_{1R}v_{2L}} \iint \chi_{1R}(y_R)[G_{RL}^r(y_R, y_L)]\chi_{2L}(y_L)dy_R dy_L$



How to obtain S-matrix using Green functions

- **Fisher-Lee relation** for multimode leads

$$s_{nm}^{qp} = -\delta_{nm}^{qp} + i\hbar\sqrt{v_n v_m} \iint \chi_n(y_q)[G_{qp}^r(y_q, y_p)]\chi_m(y_p)dy_q dy_p$$

For numerical calculations

If we put the system on a lattice with discretization of y_q, y_p

$$s_{nm}^{qp} = i\hbar\sqrt{v_n}[\chi_n(\Delta y_q) \quad \cdots \quad \chi_n(N_q\Delta y_q)]G_{qp}^r \begin{bmatrix} \chi_m(\Delta y_p) \\ \vdots \\ \chi_m(N_p\Delta y_p) \end{bmatrix} \sqrt{v_m}$$

$p \neq q$

$$S^{qp} = \begin{bmatrix} s_{11}^{qp} & \cdots & s_{1M}^{qp} \\ \vdots & \ddots & \vdots \\ s_{N1}^{qp} & \cdots & s_{NM}^{qp} \end{bmatrix}$$

$$= i\hbar \begin{bmatrix} \sqrt{v_1}\chi_1(\Delta y_q) & \cdots & \sqrt{v_1}\chi_1(N_q\Delta y_q) \\ \vdots & \ddots & \vdots \\ \sqrt{v_N}\chi_N(\Delta y_q) & \cdots & \sqrt{v_N}\chi_N(N_q\Delta y_q) \end{bmatrix} G_{qp}^r \begin{bmatrix} \sqrt{v_1}\chi_1(\Delta y_q) & \cdots & \sqrt{v_M}\chi_M(\Delta y_q) \\ \vdots & \ddots & \vdots \\ \sqrt{v_1}\chi_1(N_p\Delta y_q) & \cdots & \sqrt{v_M}\chi_M(N_p\Delta y_q) \end{bmatrix}$$

How to obtain S-matrix using Green functions

Discretizing 1D electron gas: $H\psi(x) = -\frac{\hbar^2}{2m}\psi''(x)$

$\psi_n \equiv \psi(na)$

Tridiagonal matrix

$$H\psi(x) \mapsto \begin{pmatrix} \ddots & \vdots & & \vdots & \vdots & ⋰ \\ \cdots & -2t & & -t & 0 & \cdots \\ \cdots & -t & -2t & & -t & \cdots \\ \cdots & 0 & -t & & -2t & \cdots \\ ⋰ & \vdots & \vdots & & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix}$$

Energy eigenvalues

$E(k) = -2t - 2t\cos(ka)$

$\sim \hbar^2 k^2/2m$

(for $ka \ll 1$ and $t = \hbar^2/2ma^2$)

(see J.J. Sakurai *Modern Quantum Mechanics* for diagonalization)

Atomic chain with hopping energy $-2t$ & on-site energy $-t$

How to obtain S-matrix using Green functions

Discretizing 1D electron gas: $H\psi(x) = -\frac{\hbar^2}{2m}\psi''(x)$

$\psi_n \equiv \psi(na)$

Tridiagonal matrix

$$H\psi(x) \mapsto \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & ⋰ \\ \cdots & -2t & -t & 0 & \cdots \\ \cdots & -t & -2t & -t & \cdots \\ \cdots & 0 & -t & -2t & \cdots \\ ⋰ & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix}$$

Energy eigenvalues

$E(k) = -2t - 2t\cos(ka)$

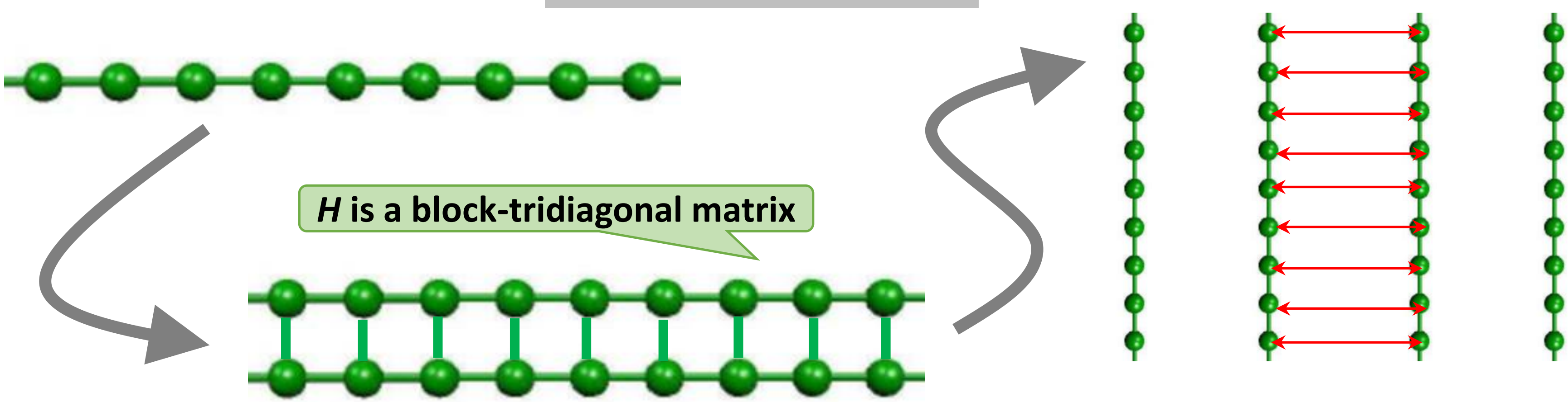
$\sim \hbar^2 k^2/2m$

(for $ka \ll 1$ and $t = \hbar^2/2ma^2$)

(see J.J. Sakurai *Modern Quantum Mechanics* for diagonalization)

Atomic chain with hopping energy $-2t$ & on-site energy $-t$

Discretizing 2D electron gas $\psi_{n,m} \equiv \psi(na_x, ma_y)$



How to obtain S-matrix using Green functions

- $s_{nm}^{qp} = i\hbar\sqrt{v_n}\begin{bmatrix}\chi_n(\Delta y_q) & \cdots & \chi_n(N_q\Delta y_q)\end{bmatrix} G_{qp}^r \begin{bmatrix}\chi_m(\Delta y_p) \\ \vdots \\ \chi_m(N_p\Delta y_p)\end{bmatrix}\sqrt{v_m}$

$$S^{qp} = \begin{bmatrix} s_{11}^{qp} & \cdots & s_{1M}^{qp} \\ \vdots & \ddots & \vdots \\ s_{N1}^{qp} & \cdots & s_{NM}^{qp} \end{bmatrix}$$

$$= i\hbar \begin{bmatrix} \sqrt{v_1}\chi_1(\Delta y_q) & \cdots & \sqrt{v_1}\chi_1(N_q\Delta y_q) \\ \vdots & \ddots & \vdots \\ \sqrt{v_N}\chi_N(\Delta y_q) & \cdots & \sqrt{v_N}\chi_N(N_q\Delta y_q) \end{bmatrix} G_{qp}^r \begin{bmatrix} \sqrt{v_1}\chi_1(\Delta y_q) & \cdots & \sqrt{v_M}\chi_M(\Delta y_q) \\ \vdots & \ddots & \vdots \\ \sqrt{v_1}\chi_1(N_p\Delta y_q) & \cdots & \sqrt{v_M}\chi_M(N_p\Delta y_q) \end{bmatrix}$$

- **Transmission from S-matrix ($p \neq q$)**

$$\Gamma_p = \hbar \sum_{m\in p} \begin{bmatrix} \sqrt{v_m}\chi_m(p_1)\chi_m(p_1) & \cdots & \sqrt{v_m}\chi_m(p_1)\chi_m\left(p_{N_p}\right) \\ \vdots & \ddots & \vdots \\ \sqrt{v_m}\chi_m\left(p_{N_p}\right)\chi_m(p_1) & \cdots & \sqrt{v_m}\chi_m\left(p_{N_p}\right)\chi_m\left(p_{N_p}\right) \end{bmatrix}$$

$$T_{qp} = \sum_{n,m} \left|s_{nm}^{qp}\right|^2 = \mathrm{Tr}\left[\Gamma_q G_{qp}^r \Gamma_p G_{qp}^a\right]$$

How do we get $\Gamma_q, G^r, \Gamma_p, G^a$?

How to obtain S-matrix using Green functions

- **Steps to obtain $\Gamma_q, G^r, \Gamma_p, G^a$ numerically**

1) Calculate surface retarded Green function of semi-infinite leads

$$g^r_{L,R}(E) = \left[(E + i\eta)I - H_{L,R}\right]^{-1}$$

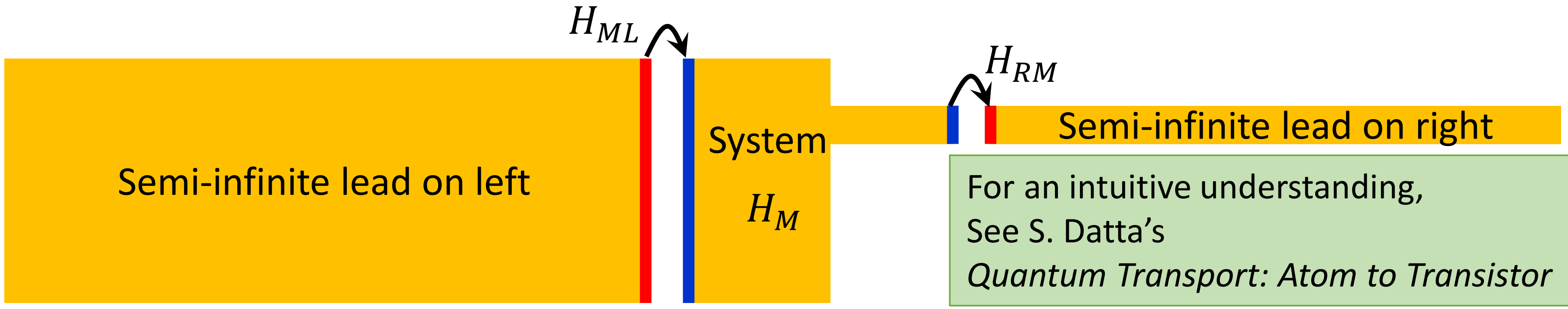
2) Obtain self-energy: additional matrix elements to $\boldsymbol{H_M}$ from leads

$$\Sigma_L(E) = H_{ML} g^r_L(E)[H_{ML}]^+ \text{ \& } \Sigma_R(E) = [H_{RM}]^+ g^r_R(E) H_{RM}$$

3) Obtain Gamma's: $\Gamma_{L,R} = i\left[\Sigma_{L,R} - \Sigma^+_{L,R}\right]$

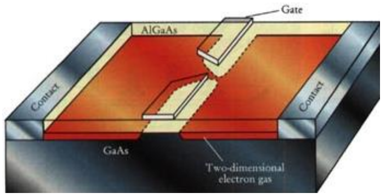
4) Obtain Green functions of middle region, $G^a = [G^r]^+$

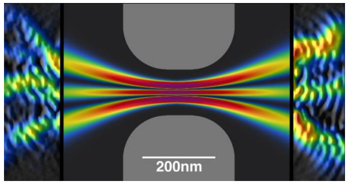
$$G^r(E) = [(E + i\eta)I - H_M - \Sigma_L - \Sigma_R]^{-1}$$



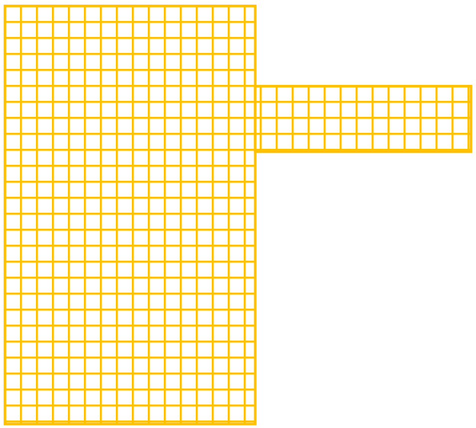
For an intuitive understanding,
See S. Datta's
Quantum Transport: Atom to Transistor

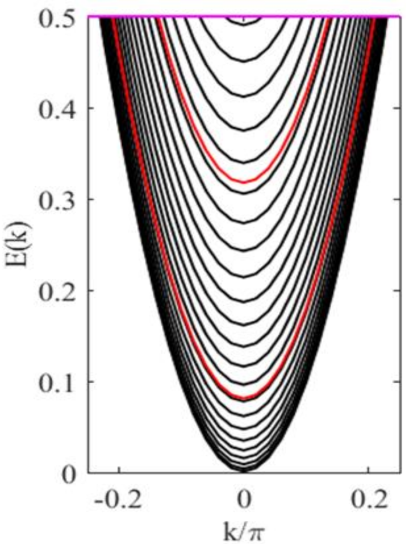
How to obtain S-matrix using Green functions

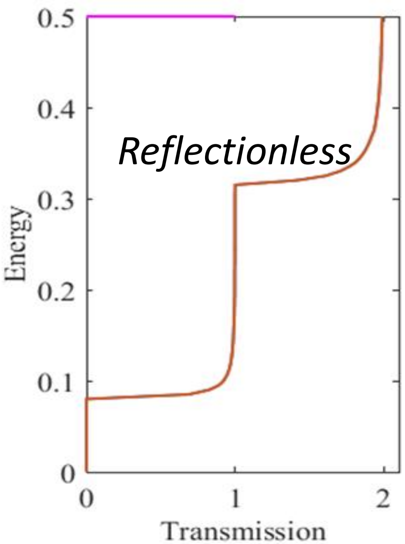


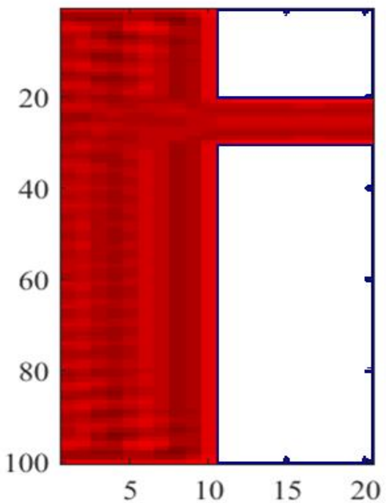


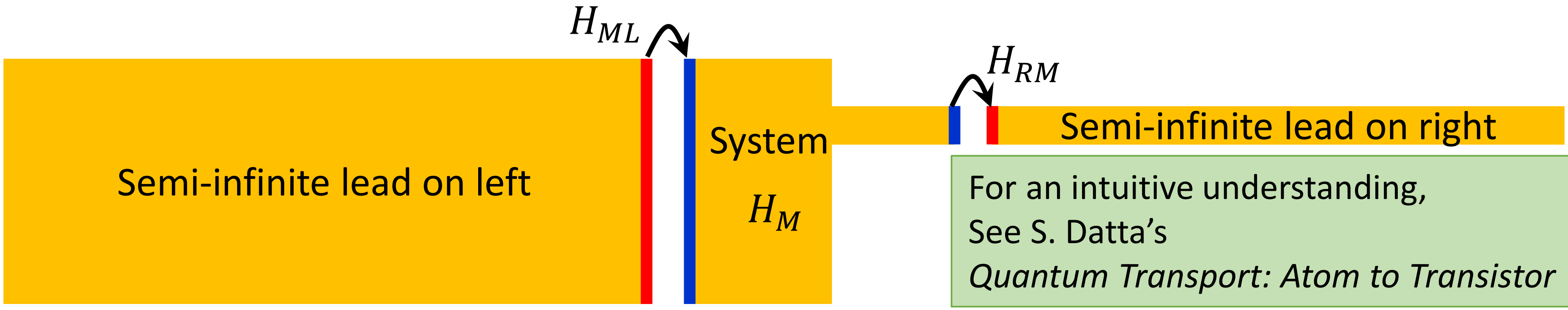
$$G = \frac{2e^2}{h} M$$









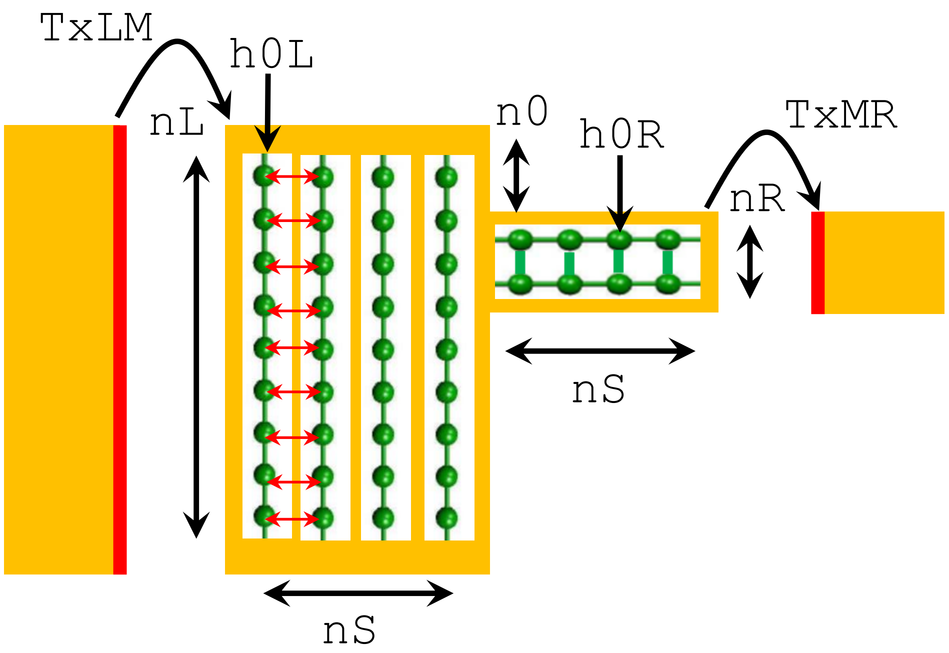


For an intuitive understanding,
See S. Datta's
Quantum Transport: Atom to Transistor

How to obtain S-matrix using Green functions

- **Matlab code** (subroutines available upon request)

```
tl = -1.0; % hopping energy of left region
tr = -1.0; % hopping energy of right region

nL = 100; % # of lateral sites of left region
nR = 10; % # of lateral sites of right region
n0 = 20; % position of junction
nS = 10; % # of longitudinal lattice sites

% Energy window to calculate
En = 0 : 0.0025*2 : 0.5;

% Hamiltonian generation
h0L = The_make_tridiagonal(-4*tl,tl,nL,1);
txL = tl*eye(nL);
h0R = The_make_tridiagonal(-4*tr,tr,nR,1);
txR = tr*eye(nR);
txLR = zeros(nL,nR);
txLR(n0+1:n0+nR,1:nR) = tr*eye(nR);
txRL = txLR';
H0L = The_make_tridiagonal(h0L,txL,nS,nL);
H0R = The_make_tridiagonal(h0R,txR,nS,nR);
H0 = The_Connect(H0R,H0L,txLR,txRL,0);
nM = length(H0);
TxLM = zeros(nL,nM);
TxLM(1:nL,nM-nL+1:nM) = txL;
TxML = TxLM';
TxRM = zeros(nR,nM);
TxRM(1:nR,1:nR) = txR;
TxMR = TxRM';
```



How to obtain S-matrix using Green functions

- **Matlab code** (subroutines available upon request)

- **Steps to obtain $\Gamma_q, G^r, \Gamma_p, G^a$ numerically**

  1) Calculate surface retarded Green function of semi-infinite leads

$$g^r_{L,R}(E) = \left[(E + i\eta)I - H_{L,R}\right]^{-1}$$

  2) Obtain self-energy: additional matrix elements to $\boldsymbol{H_M}$ from leads

$$\Sigma_L(E) = H_{ML} g^r_L(E)[H_{ML}]^+$$

$$\Sigma_R(E) = [H_{RM}]^+ g^r_R(E) H_{RM}$$

  3) Obtain Gamma's: $\Gamma_{L,R} = i\left[\Sigma_{L,R} - \Sigma^+_{L,R}\right]$

  4) Obtain Green functions of middle region,

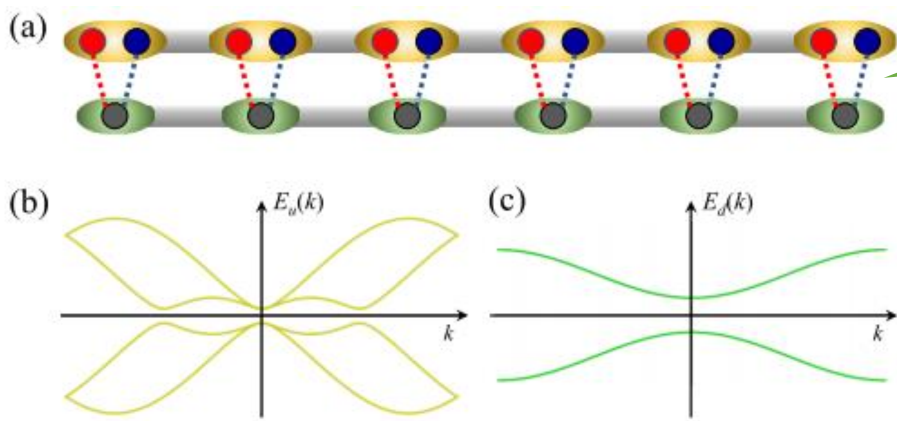
$$G^a = [G^r]^+$$

$$G^r(E) = [(E + i\eta)I - H_M - \Sigma_L - \Sigma_R]^{-1}$$

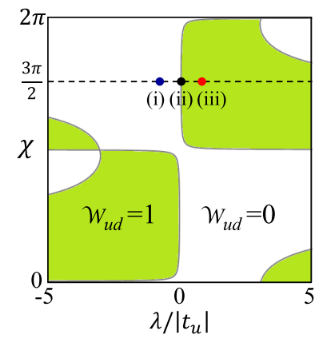
```
% Calculating transmission from Green functions
Tmp = zeros(nM,length(En));
for n=1:length(En)
    en = En(n);
    gL = leftL(en,h0L,txL,nL);
    gR = leftL(en,h0R,txR,nR);

    selfL = TxML*gL*TxLM;
    selfR = TxMR*gR*TxRM;
    gamL = 1i*(selfL-selfL');
    gamR = 1i*(selfR-selfR');
    gM = inv(en*eye(nM) - H0 - selfL - selfR);

    T(n,1) = trace(gamL*gM*gamR*gM'); % Transmission
    T(n,2) = trace(gamR*gM*gamL*gM');
    Tmp(:,n) = -imag(diag(gM))/pi; % for Ldos
end
% Generating Ldos
for n=1:length(En)
    Ldos_{n} = zeros(nL,2*nS) -1;
    for m=1:nS
        tmp = (m-1)*nR;
        Ldos_{n}(n0+1:n0+nR,m) = Tmp(tmp+1:tmp+nR,n);
    end
    for m=nS+1:2*nS
        tmp = 10*nR + (m-nS-1)*nL;
        Ldos_{n}(1:nL,m) = Tmp(tmp+1:tmp+nL,n);
    end
    Ldos_{n} = fliplr(Ldos_{n});
end
```

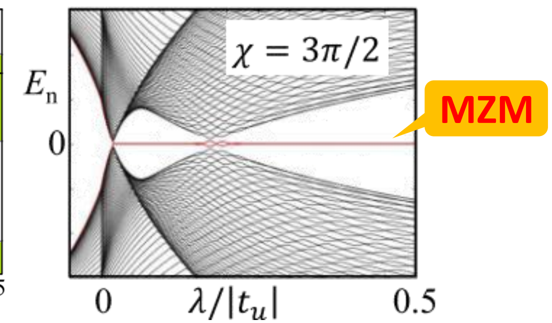
How to obtain S-matrix using Green functions

- **Application to more complex systems**
  → spinful systems (including SO-coupling)
  → superconducting systems (s/p-wave superconductivity)



Stacking an atomic chain to a nanowire with SO-coupling & s-wave SC leads to topological SC





$$\mathcal{H}_{\mathrm{BdG}} = \begin{pmatrix} t_u\cos k - \mu_u & -il_{\mathrm{so}}\sin k & \Delta & 0 & \frac{-v_2-w_2}{2} & \frac{-v_2+w_2}{2} \\ il_{\mathrm{so}}\sin k & t_u\cos k - \mu_u & 0 & \Delta & \frac{v_1+w_1}{2} & \frac{v_1-w_1}{2} \\ \Delta & 0 & -t_u\cos k + \mu_u & il_{\mathrm{so}}\sin k & \frac{-v_1+w_1}{2} & \frac{-v_1-w_1}{2} \\ 0 & \Delta & -il_{\mathrm{so}}\sin k & -t_u\cos k + \mu_u & \frac{-v_2+w_2}{2} & \frac{-v_2-w_2}{2} \\ \frac{-v_2-w_2}{2} & \frac{v_1+w_1}{2} & \frac{-v_1+w_1}{2} & \frac{-v_2+w_2}{2} & t_d\cos k - \mu_d & 0 \\ \frac{-v_2+w_2}{2} & \frac{v_1-w_1}{2} & \frac{-v_1-w_1}{2} & \frac{-v_2-w_2}{2} & 0 & -t_d\cos k + \mu_d \end{pmatrix}$$

Hamiltonian in k-space

Sang-Jun Choi and Björn Trauzettel, *PRB* **107**, 245409 (2023)

Beyond coherent & metallic conductions

- **More about Landauer-Büttiker formalism**

→ MQT is quantal: DC current = $\langle \hat{I} \rangle$, i.e., long-time average of current

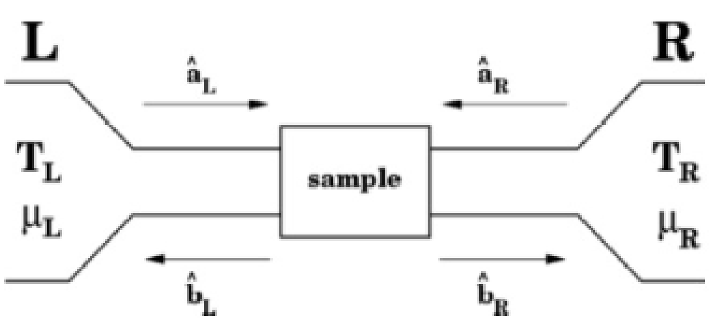
→ Shot noise is also available [M. Büttiker, (1990)]

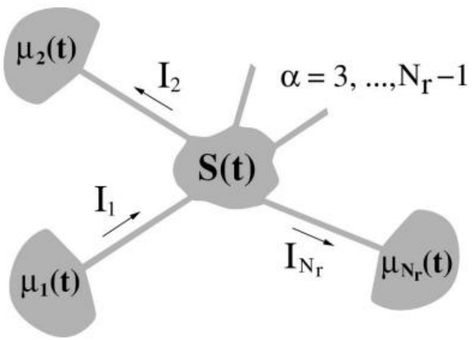
$$S = \frac{2e^2}{h}|eV|\mathrm{tr}(tt^+rr^+) = \frac{2e^2}{h}|eV|\sum_n T_n(1-T_n)$$

If all $T_n \ll 1, S = 2e|I|$.

→ Periodically driven quantum pumps can be dealt [M. Büttiker, (1990)]

$$\frac{dI}{dE} = i\frac{e}{2\pi}\left(\frac{\partial S}{\partial t}\frac{\partial S^+}{\partial E} - \frac{\partial S}{\partial E}\frac{\partial S^+}{\partial t}\right)$$

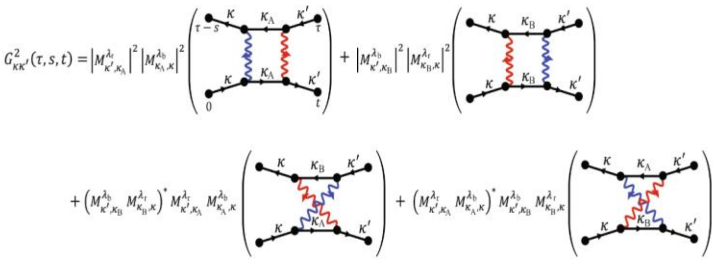


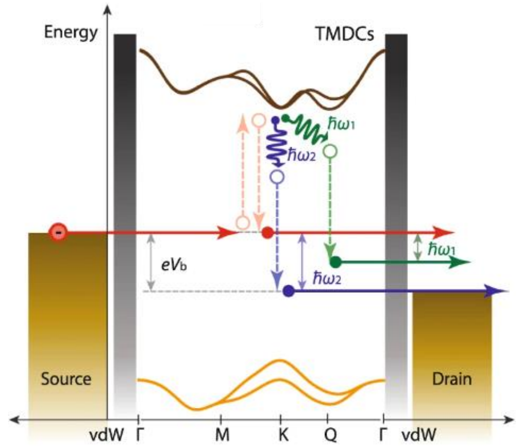


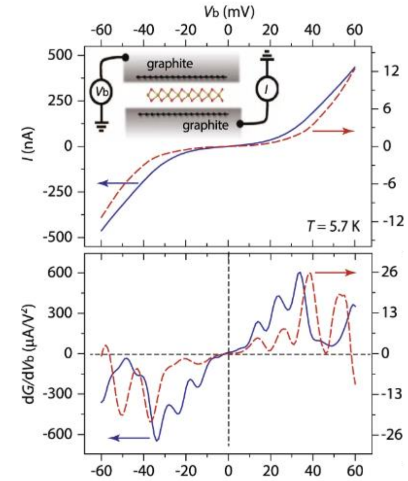
Beyond coherent & metallic conductions

- **Beyond Landauer-Büttiker formalism: other methods for MQT**

Inelastic electron tunneling via el-ph interaction

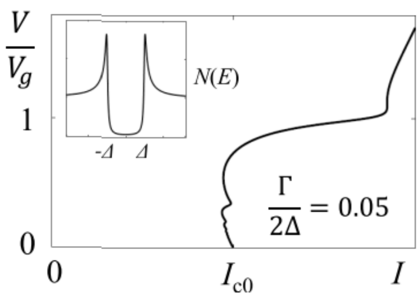


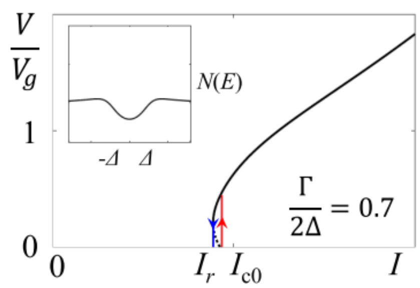


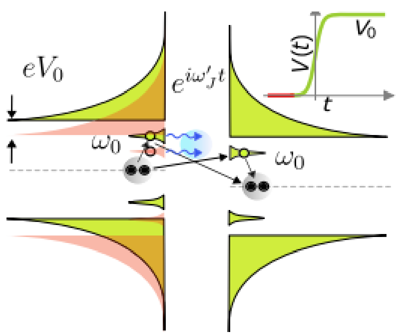


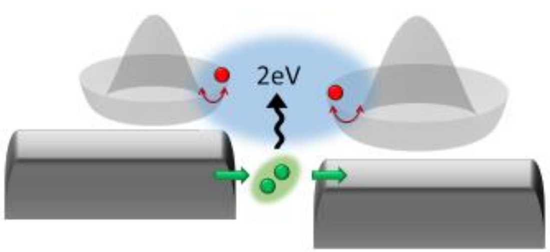
DH Lee, **Sang-Jun Choi** (equal), *et al.*, *Nat. Commun.* **12**, 4520 (2021)

Nonequilibrium Josephson effects









Sang-Jun Choi and Björn Trauzettel, *PRL* **128**, 126801 (2022)
Aritra Lahiri, **Sang-Jun Choi** (corresponding), and Björn Trauzettel, *PRL* **131**, 126301 (2023)
Aritra Lahiri, **Sang-Jun Choi**, and Björn Trauzettel, arXiv: 2402.13074 (2024)

Beyond coherent & metallic conductions

- **More about Landauer-Büttiker formalism**

  → MQT is quantal: DC current = $\langle \hat{I} \rangle$, i.e., long-time average of current

  → Current shot noise is also available [M. Büttiker, *PRB* **46**, 12485 (1992)]

  → Periodically driven quantum pumps can be dealt [M. Büttiker, (1990)]

- **Beyond Landauer-Büttiker formalism: other methods for MQT**

Formalisms	Advantages	Disadvantages
Landauer-Büttiker	Intuitive & quick calculations. Finite voltage bias & temperature	Cannot deal with many-body physics
Kubo's linear response theory	Relatively easy & quick, while allowing many-body physics	Only allows physics around equilibrium states
Master equation	Allowing many-body physics & Nonequilibrium bias & finite temp.	Particularly useful at tunneling regime
Keldysh formalism	All the above	Not so easy for everyone