Institut Matériaux Microélectronique
Nanosciences de Provence

Electron Transport

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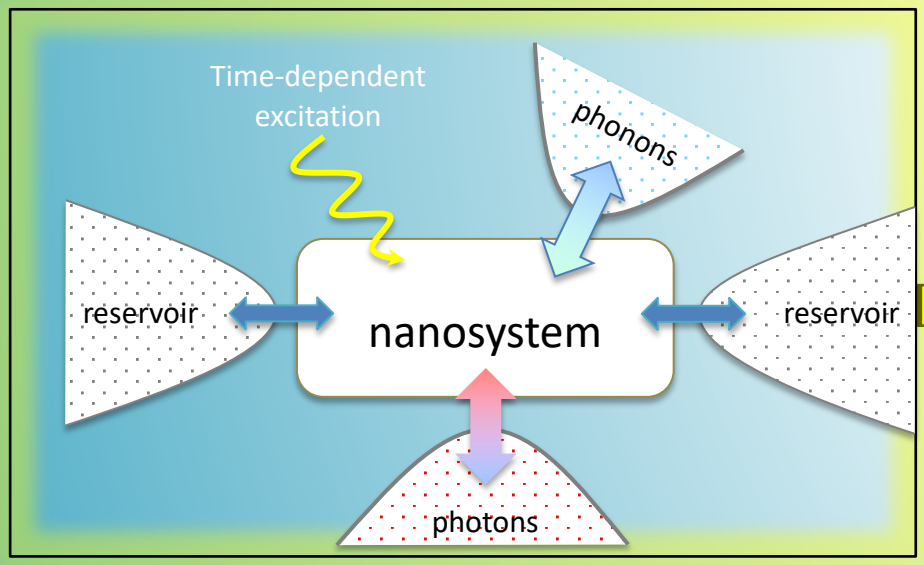
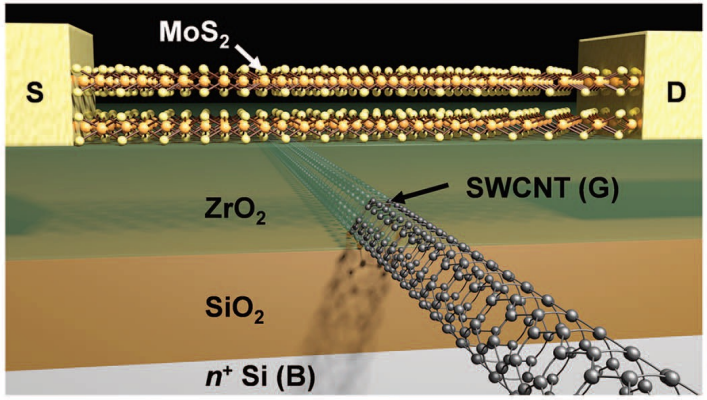
INTRODUCTION



ELECTRON QUANTUM TRANSPORT

NANO-DEVICE



From Pr. Ali Javey: Schematic of 1D2D-FET with a MoS2 channel and single-walled carbon nanotube gate (Science 354, 99).

OUTLINE

- ✓ An electron in condensed matter
- ✓ Down to nanoscale
- ✓ Transport: from classical to quantum
- ✓ Methodology for quantum transport
- ✓ Particle current *without interaction*
- ✓ Energy and Heat currents *without interaction*

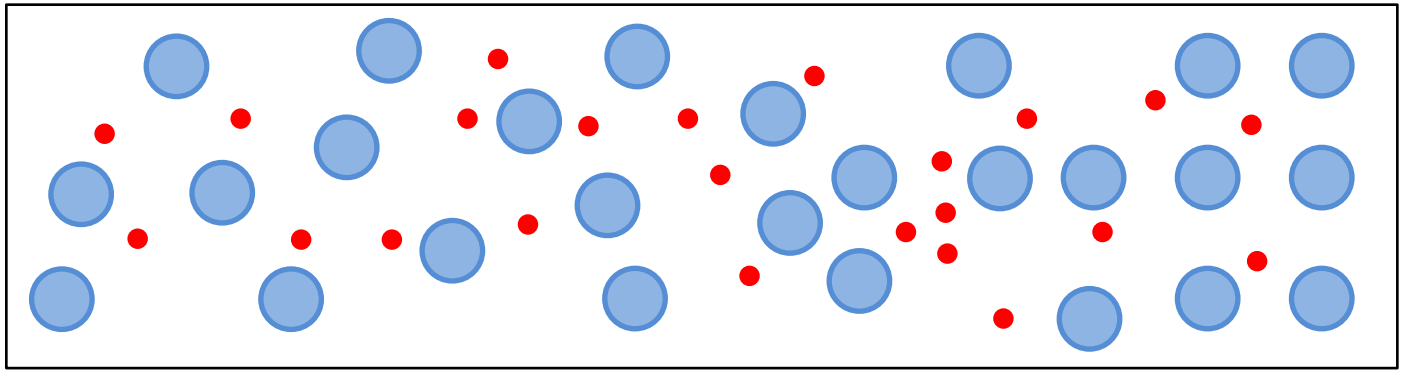
Quantum electron transport

WHERE ?

In matter condensed at nanoscale

An electron in condensed matter

A condensed matter sample

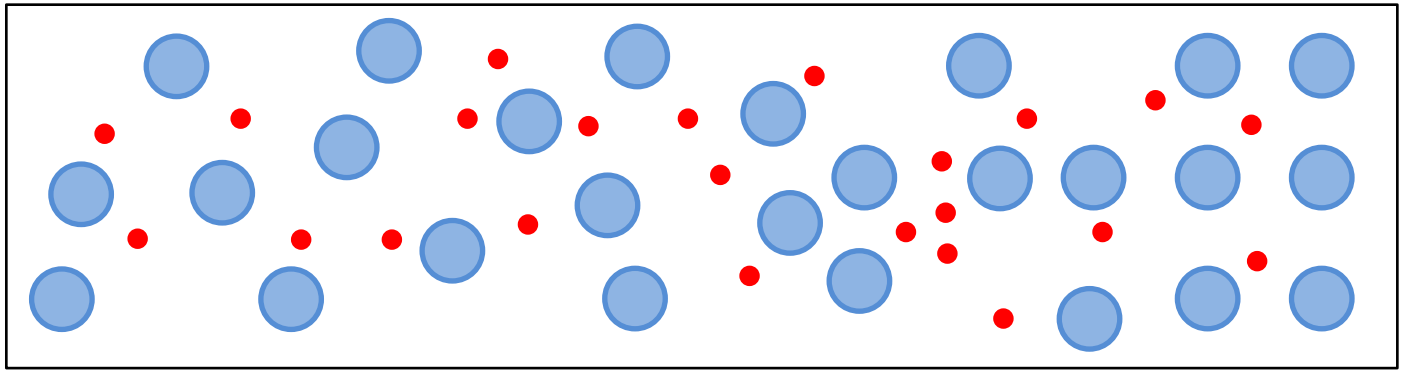


electrons

nuclei

An electron in condensed matter

A condensed matter sample



electrons

m_0 , $\mathbf{r}_i$, $\mathbf{p}_i$

nuclei

$M_\alpha, Z_\alpha, \mathbf{R}_\alpha, \mathbf{P}_\alpha$

$$H = K_e + K_n + V_{e-n} + V_{e-e} + V_{n-n}$$

Many-body problem

Kinetic energy $K_e = \sum_i \frac{p_i^2}{2m_0}$ $K_n = \sum_\alpha \frac{P_\alpha^2}{2M_\alpha}$

Potential energy $V_{e-n} = -\sum_{i,\alpha} \frac{e^2 Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}$

$V_{e-e} = +\frac{1}{2}\sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$

$V_{n-n} = +\frac{1}{2}\sum_{\alpha,\beta} \frac{e^2 Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}$

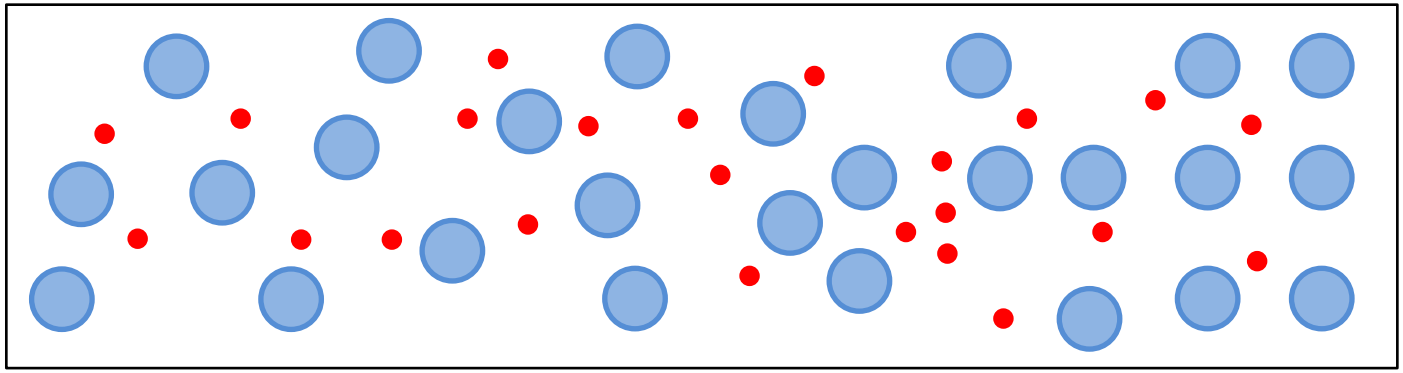
Coulomb interaction
Spin is ignored

An electron in condensed matter

A condensed matter sample

electrons

nuclei



$$H = K_e + K_n + V_{e-n} + V_{e-e} + V_{n-n}$$

- Born-Oppenheimer approximation
- Hartree-Fock approximation
- *Independent-electron approximation*

ab initio methods

empirical models

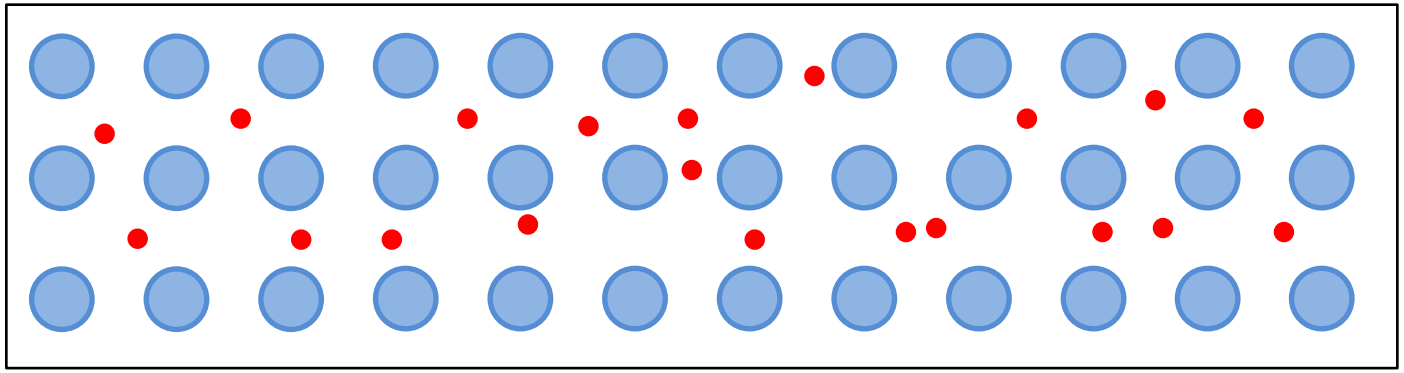
$$H = \sum_i H_i^e + H_{\text{correlations}} + H_{\text{e-vibrations}} + \sum_\alpha H_\alpha^n + H_{\text{anharm}}$$

An electron in condensed matter

A condensed matter sample : **crystalline solid**

electrons

nuclei

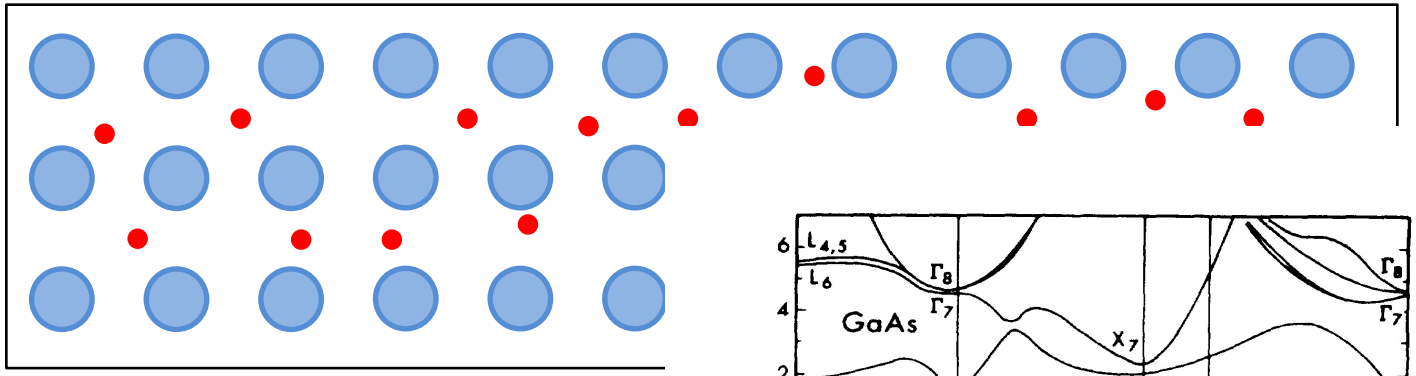


An electron in condensed matter

A condensed matter sample : **crystalline solid**

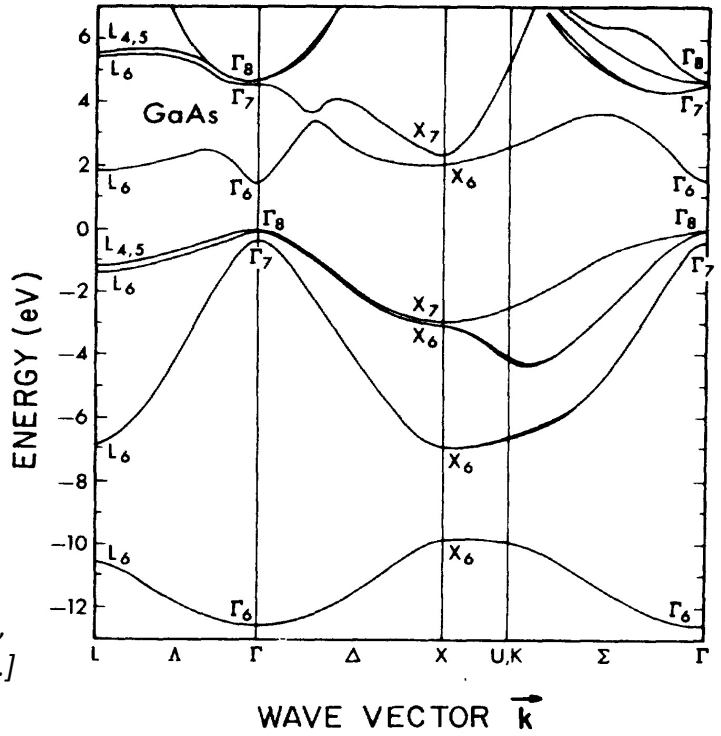
electrons

nuclei



Electronic properties

from ab initio calculations



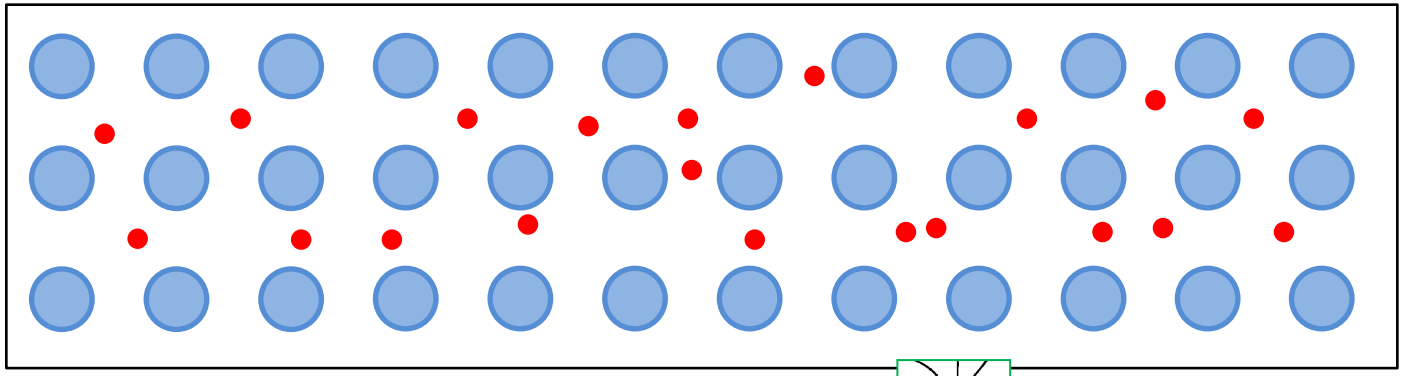
[from J. R. Chelikowski et al, Physical Review B 14 (1976).]

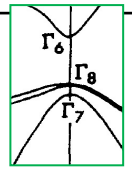
An electron in condensed matter

A condensed matter sample : **crystalline solid**

electrons

nuclei





ZOOM

Electronic properties

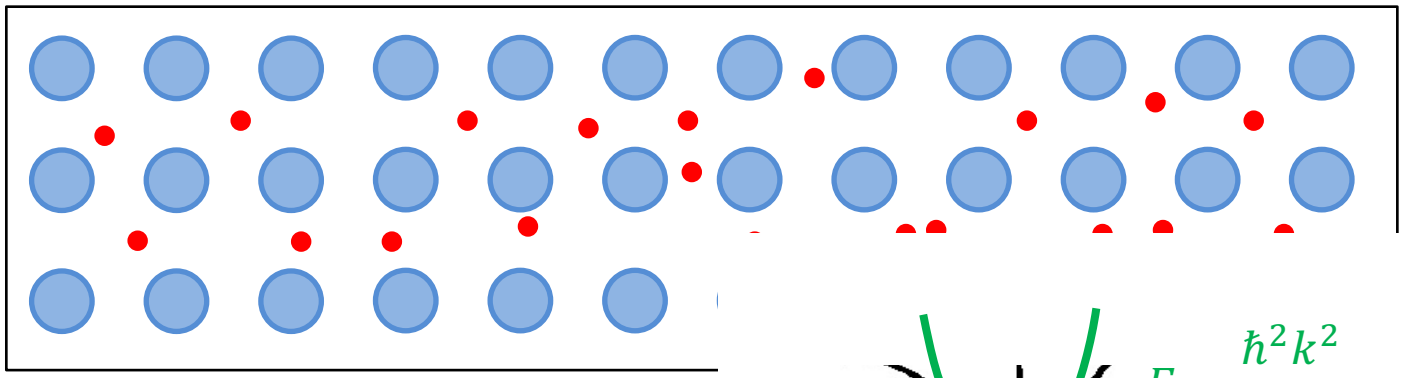
to empirical models

An electron in condensed matter

A condensed matter sample : **crystalline solid**

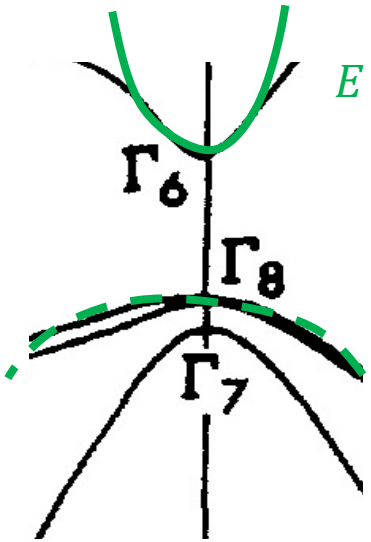
electrons

nuclei



Electronic properties

to empirical models



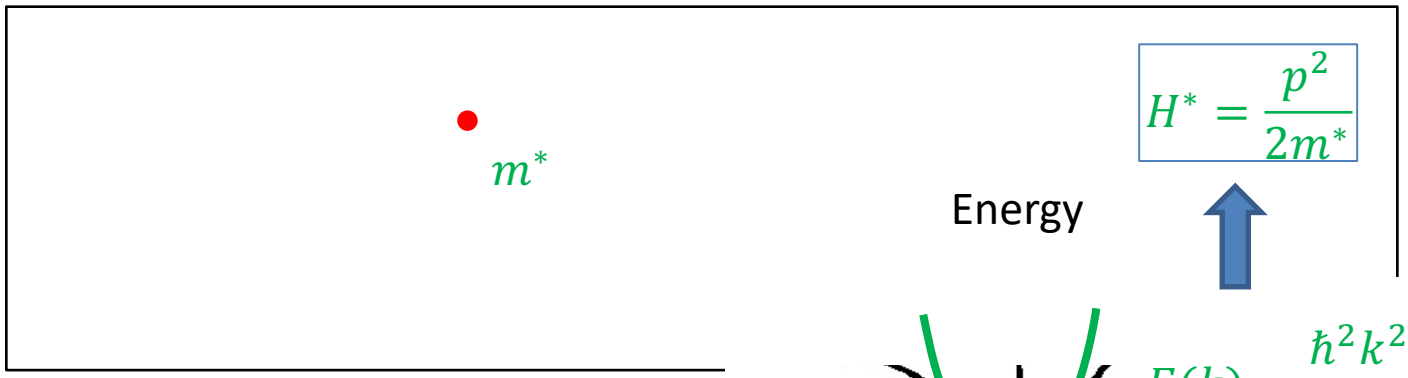
$$E = \frac{\hbar^2 k^2}{2m^*}$$

Effective mass approximation

An electron in condensed matter

- electron

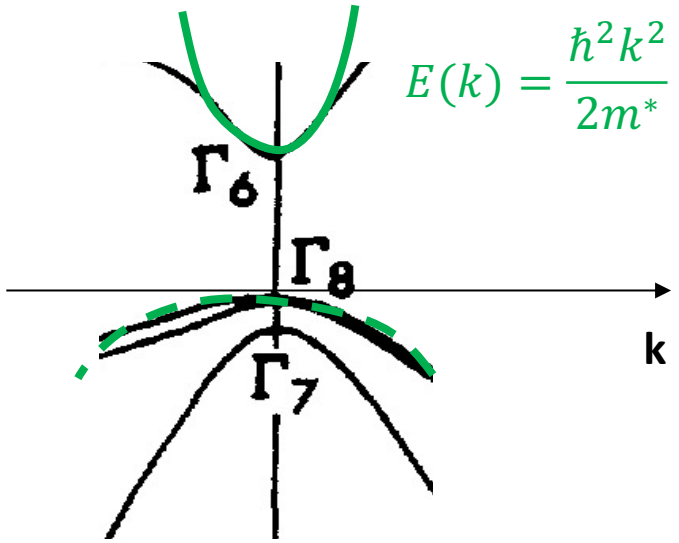
A condensed matter sample : **crystalline solid**



$$H^* = \frac{p^2}{2m^*}$$

Energy

$$E(k) = \frac{\hbar^2 k^2}{2m^*}$$



Electronic properties

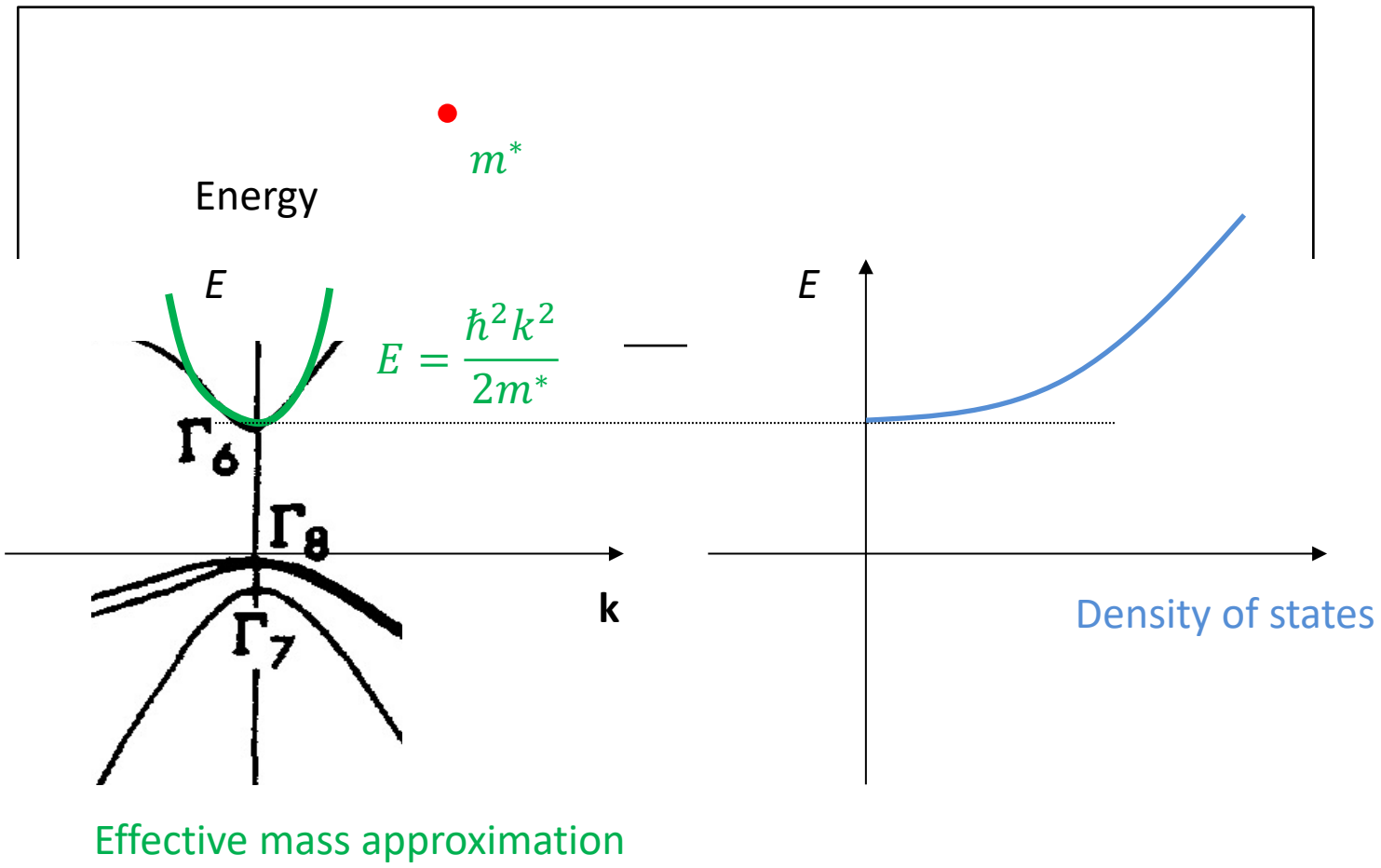
to empirical models

Effective mass approximation

An electron in condensed matter

A condensed matter sample : **crystalline solid**

- electron

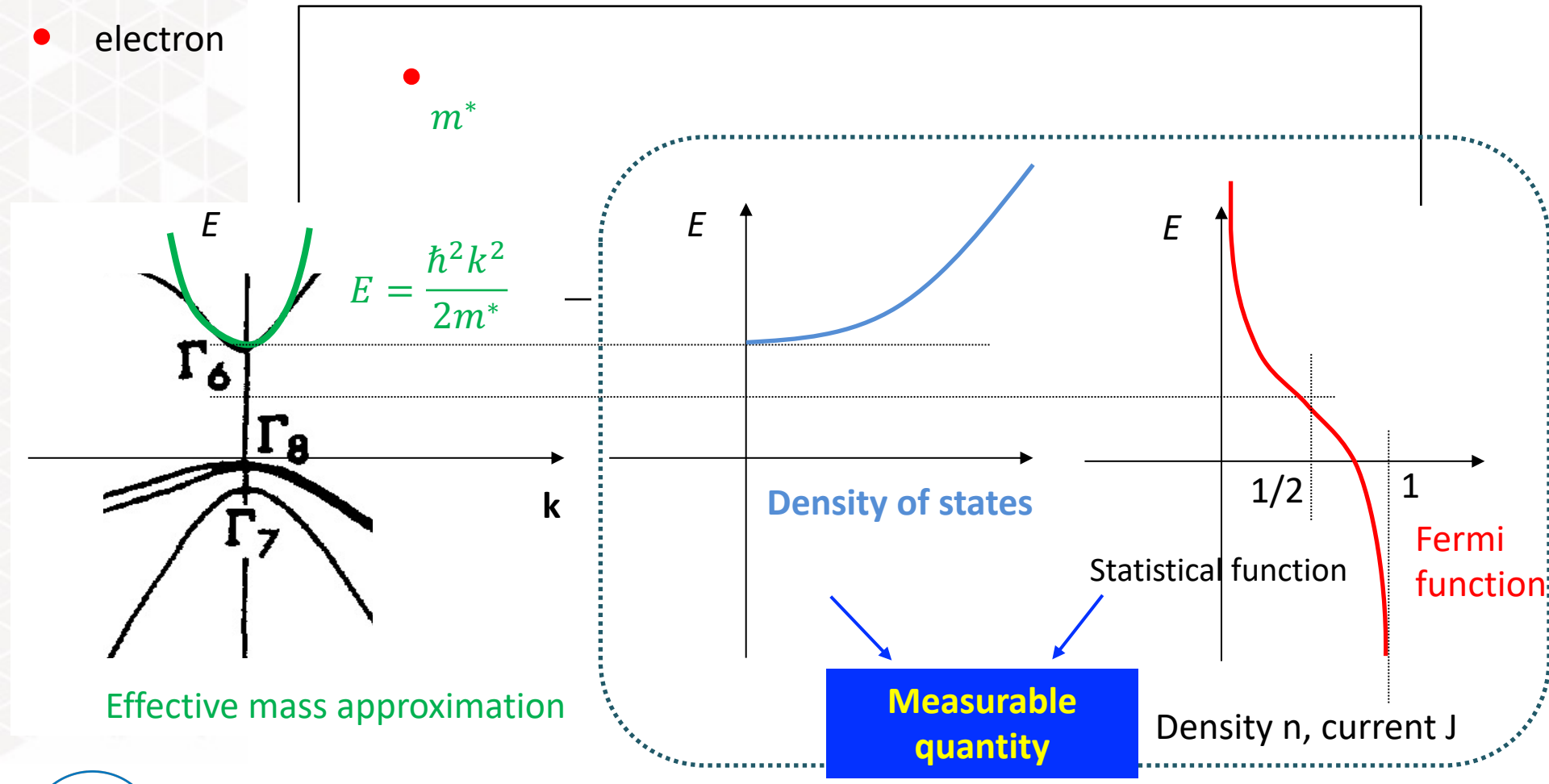


Effective mass approximation

An electron in condensed matter

A condensed matter sample : **crystalline solid**

- electron



Down to nanoscale

Nobel Prize in Physics 1973
with Ivar Giaever, Brian D. Josephson

Prize motivation: "for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors, respectively"

Leo ESAKI

Raphael TSU

IBM Thomas J. Watson Research Center
Yorktown Heights, NY, USA
1969

search & discovery

Man-made square wells offer insight and applications

Thanks to teams at two laboratories, that textbook abstraction of quantum mechanics, the one-dimensional square well, has become realized in a physical object. Known as a "heterostructure," this object consists of accurately deposited thin layers of two different semiconductors of matching lattice constants. When these man-made square wells are built up into stacks of 10–100 periods, they constitute essentially an infinite configuration (because of the finite mean free path of the carriers) known as a "superlattice" (PHYSICS TODAY, August 1973, page 20). These structures open the possibility of creating quantum states with predetermined energy levels and bandwidths.

Because of the unique characteristics of heterostructures and their related superlattices, including their unusual dimensions and negative-resistance regions, important devices are expected to result from this work, including terahertz oscillators, amplifiers, waveguides and greatly improved injection lasers. Laser oscillations from optically pumped multilayer structures of this type have already been reported.[1]

Considered as important as the potential applications, however, are the physical insights the study of these structures affords. These were explored in papers by Raphael Tsu, Leroy Chang, George Sai-Halasz and Leo Esaki[2] at the IBM Research Center, who investigated their transport properties, and by Raymond Dingle, Arthur Gossard and William Wiegmann[3] of Bell Laboratories (Murray Hill), who carried out a systematic determination of their energy levels by an optical-transmission method. Although much of this work was done at low temperatures (2–10 K), the IBM group studied photocurrents up to room temperature (300 K). Dingle told PHYSICS TODAY that the laser oscillations mentioned have also been observed at room temperature.

The techniques used by the two labs were similar in many respects: Both used gallium arsenide as the "well" material and gallium aluminum arsenide,

PHYSICS TODAY / AUGUST 1975 17

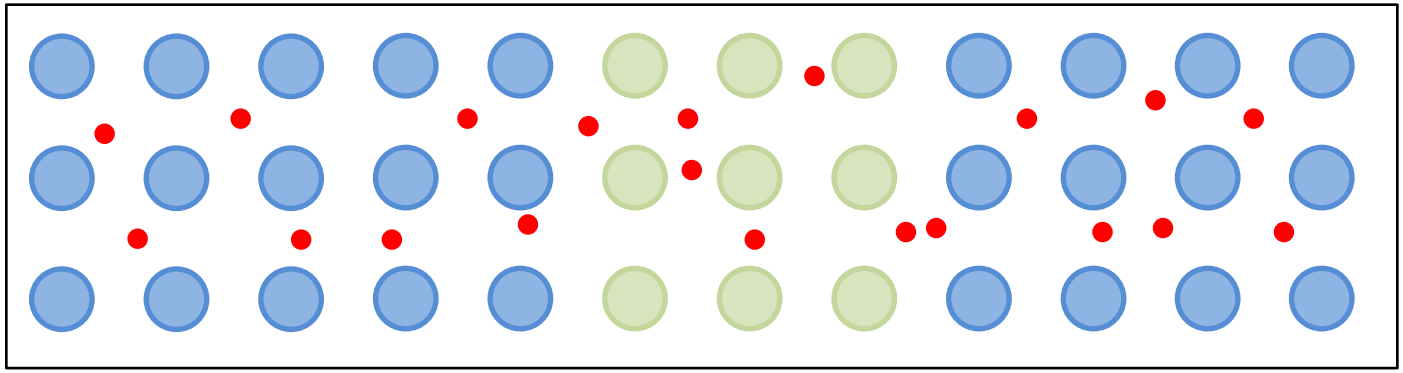
Physics Today, Search and Discovery,
Man-made square wells offer insight and applications, p.17, August 1975

Down to nanoscale

A condensed matter sample : **heterostructures**

electrons

nuclei

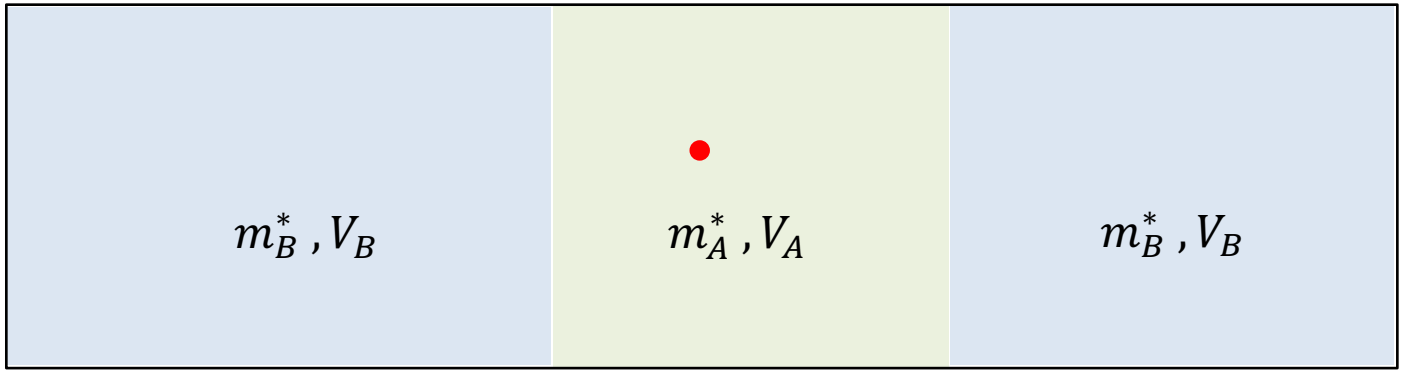


a few nanometers

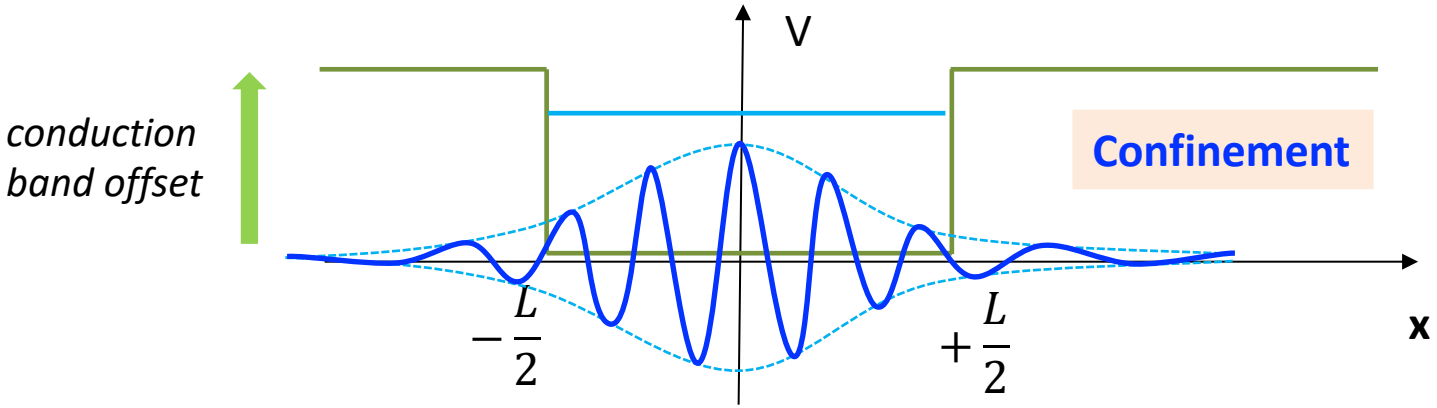
Down to nanoscale

A condensed matter sample : **heterostructures**

- electron

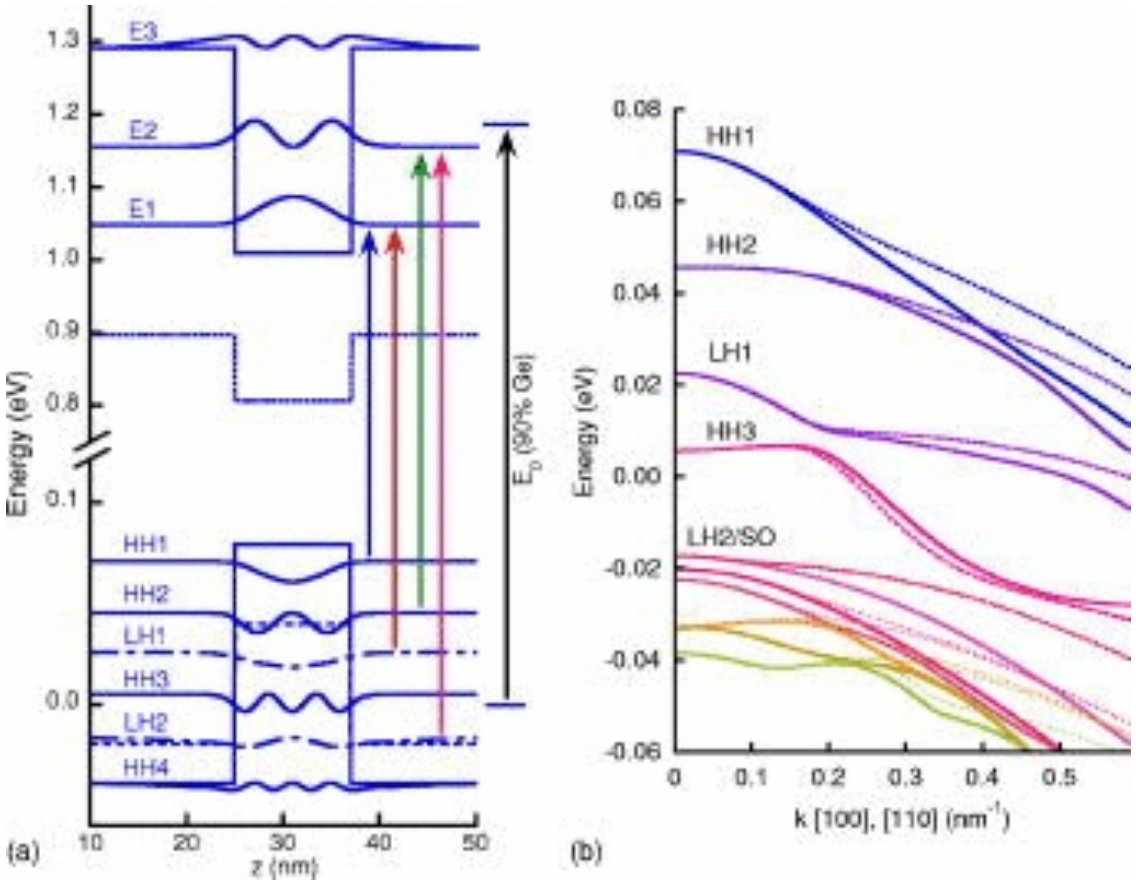


quantum well



Down to nanoscale

Subband structures in quantum wells

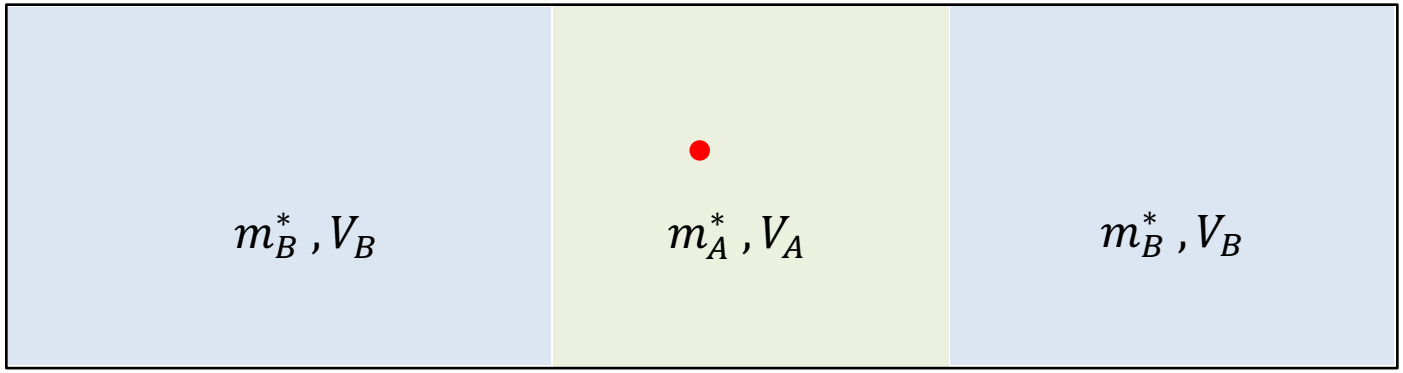


DOI:10.1063/1.2425032

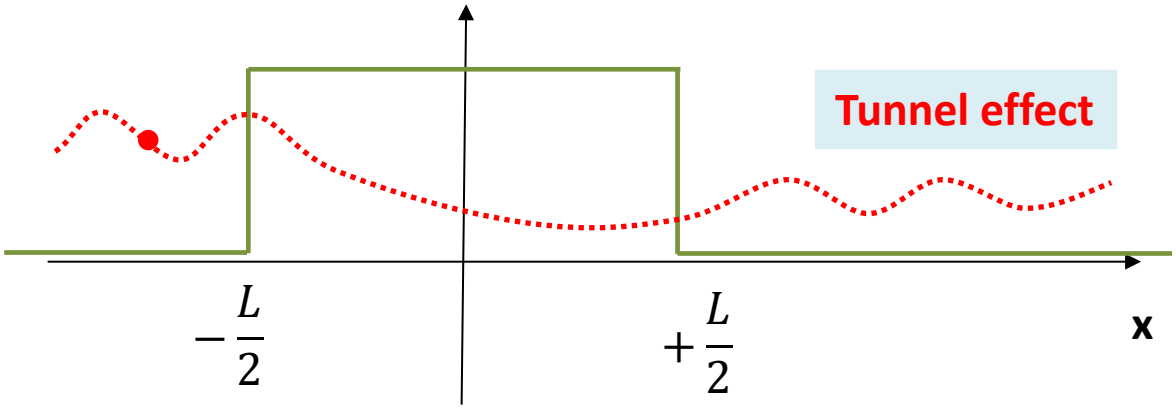
Down to nanoscale

A condensed matter sample : **heterostructures**

- electron



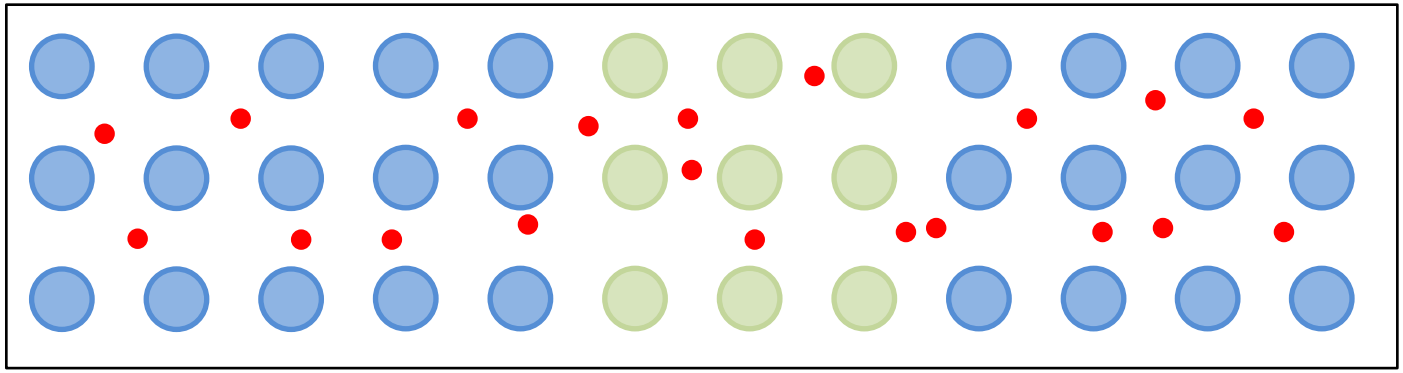
quantum barrier



Down to nanoscale

electrons

nuclei



a few nanometers

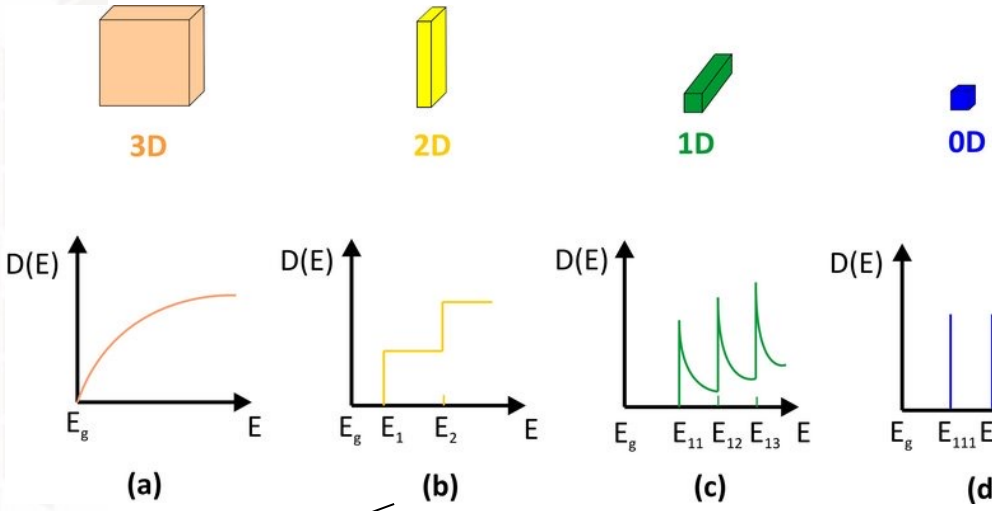
Properties at nanoscale are determined from

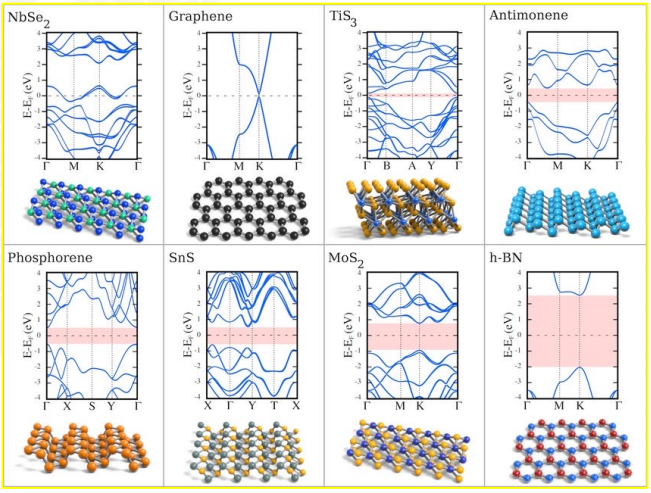
- empirical models,
- ab initio approaches,
- multi-scale & multi-physics methods.

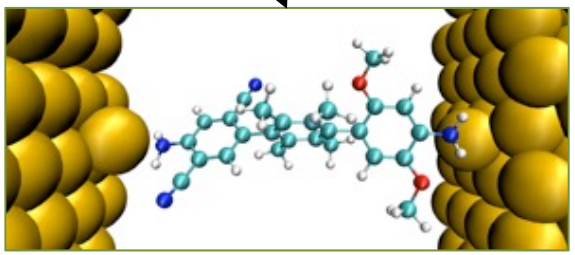
Down to nanoscale

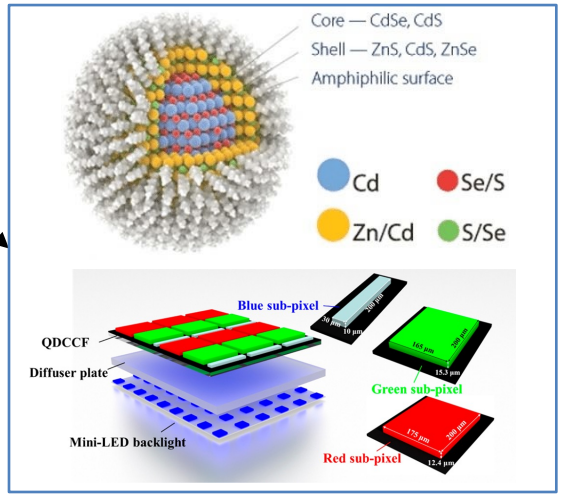
Density of states

DOI:10.14279/depositonce-7076









Down to nanoscale

Density of states

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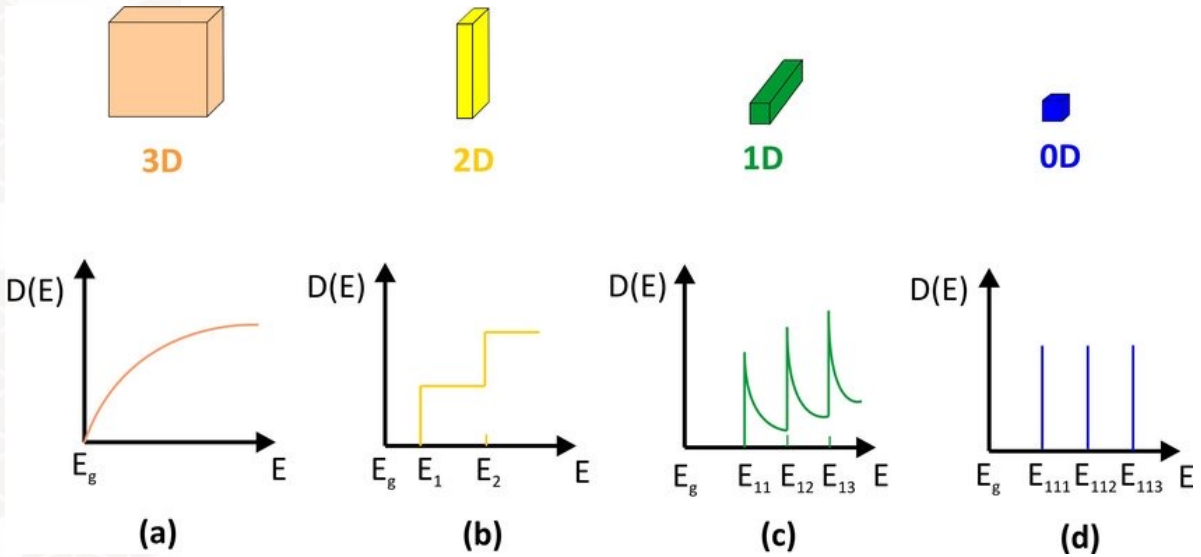
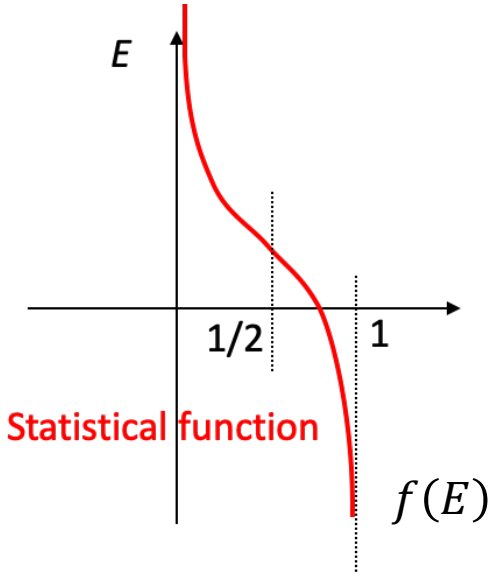




particle or charge density

$$n = \int dE\, f(E) \times D(E)$$

Observable, that is measure

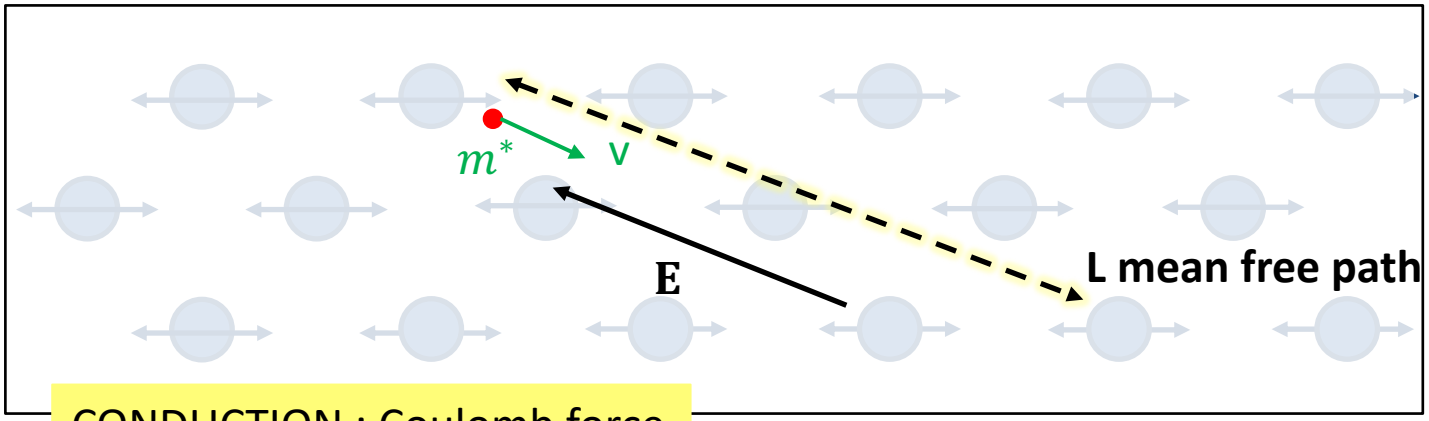
TRANSPORT

$$\frac{dN}{dt} ?$$

Transport: from classical to quantum

electron

vibration

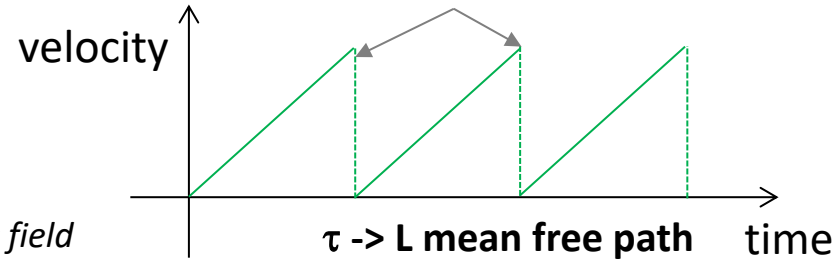


CONDUCTION : Coulomb force

Transport

electron-phonon interaction is mimicked by

collisions



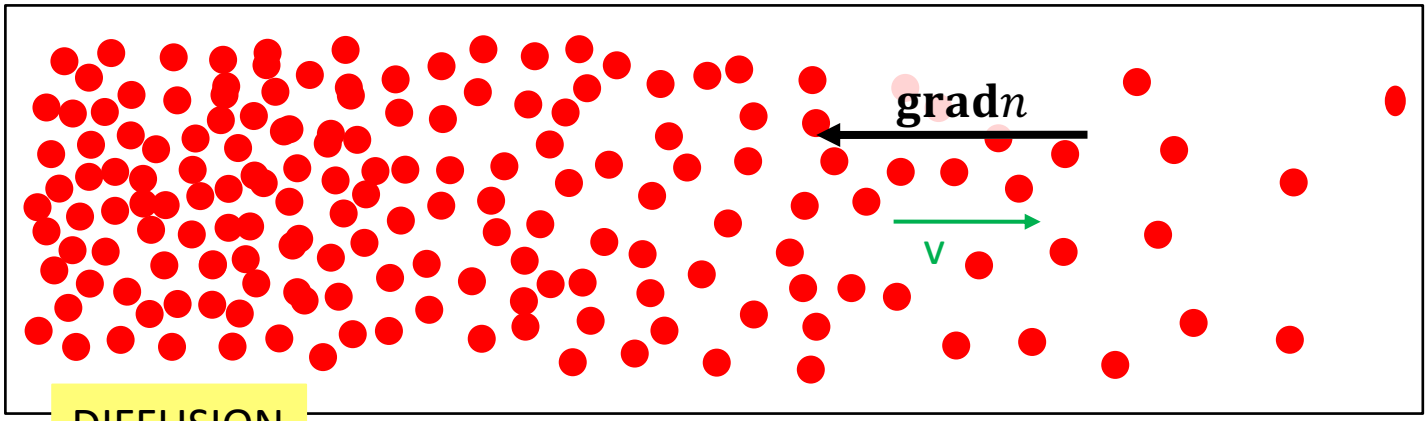
Drude model (1900)

Current density $J_{cond} = \frac{nq^2\tau}{m^*}\mathbf{E}$ *Electric field*

Electrical conductivity

Transport: from classical to quantum

- electrons



Particle transport

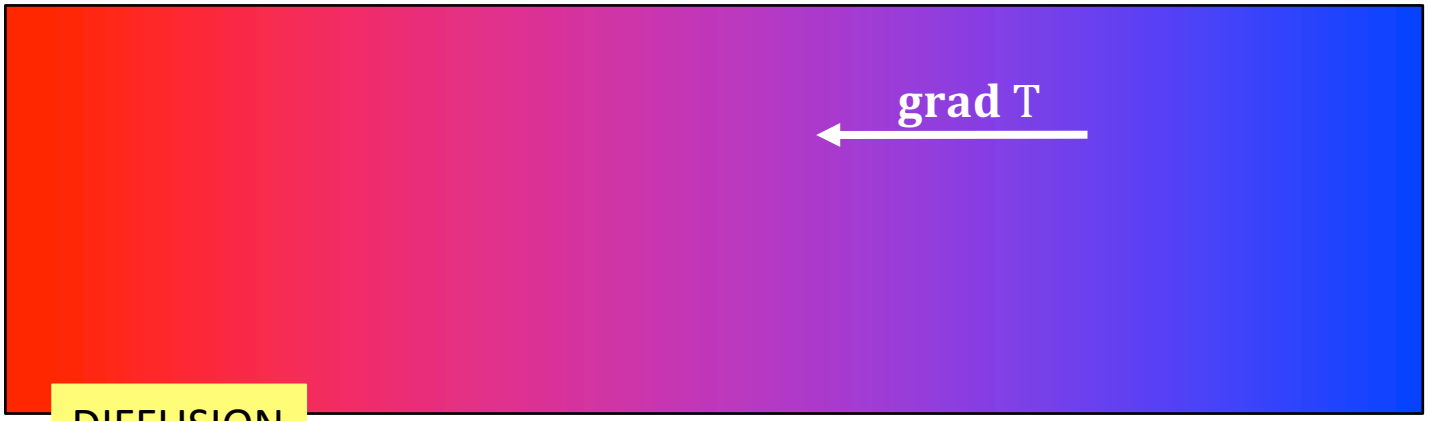
Fick's law (1855)

$$J_{diff} = -(-e)D\ \mathbf{grad}n$$

Current density — *Particle density*

diffusion coefficient

Transport: from classical to quantum



Particle transport

Fick's law (1855)

$$\mathbf{j} = -(-e)D\ \mathbf{grad} n$$

Current density — *Particle density*

diffusion coefficient

Heat Transport

Fourrier's law (1822)

$$\boldsymbol{\phi} = -\lambda\ \mathbf{grad}\ \mathrm{T}$$

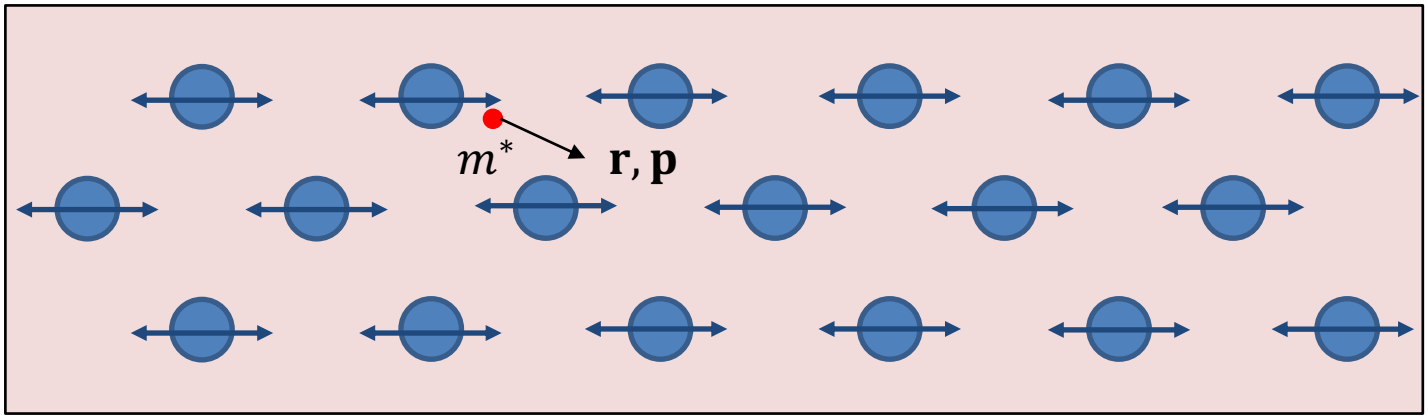
Heat flux — *Temperature*

Thermal conductivity

Transport: from classical to quantum

electron

vibration



Particle Transport

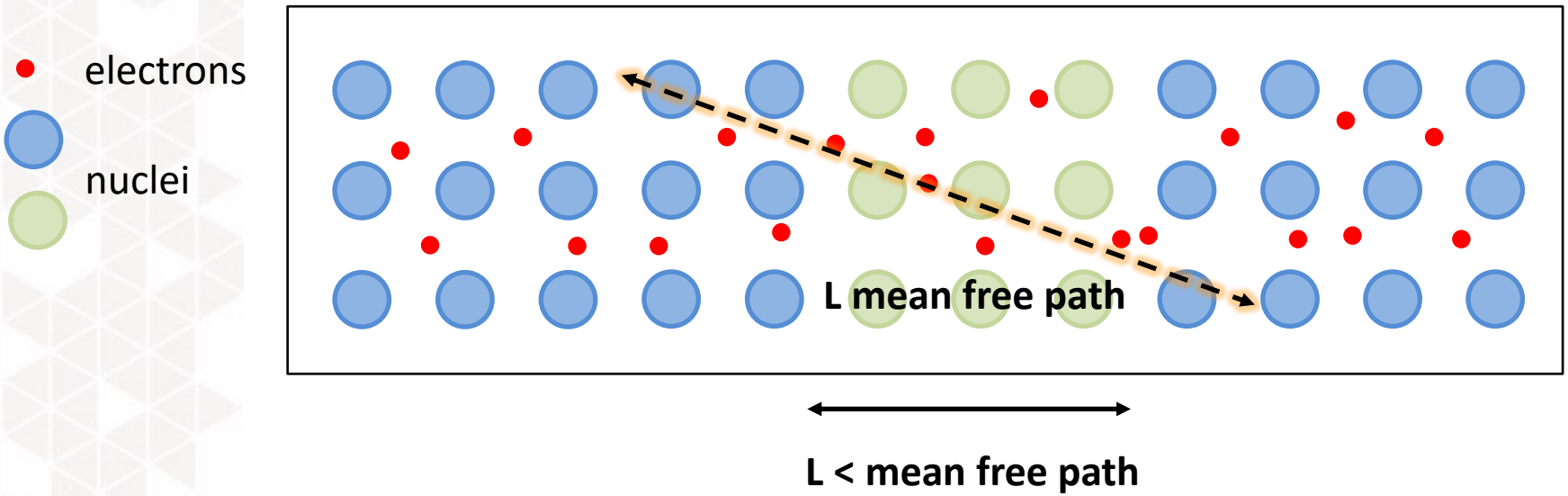
$f(\mathbf{r}, \mathbf{p}, t)$ is a probability density function, as $dN = f(\mathbf{r}, \mathbf{p}, t) d^3\mathbf{r} d^3\mathbf{p}$

Boltzmann's transport equation (1872)

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m^*} . \overrightarrow{\text{grad}}_{\mathbf{r}} f + \mathbf{F} . \overrightarrow{\text{grad}}_{\mathbf{p}} f = \frac{\partial f}{\partial t}\Big]_{coll}$$

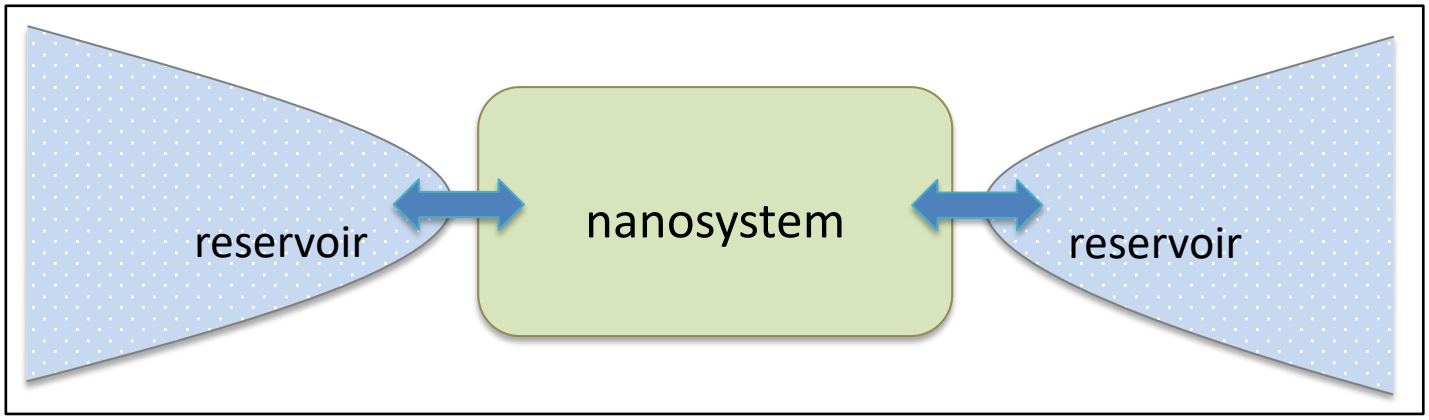
diffusion *force* *sources*

Transport: from classical to quantum



Semi-classical approaches are no longer valid.
They could be “quantum-like” transformed,
but it is easier to start from a quantum model.

Transport: from classical to quantum



a few nanometers

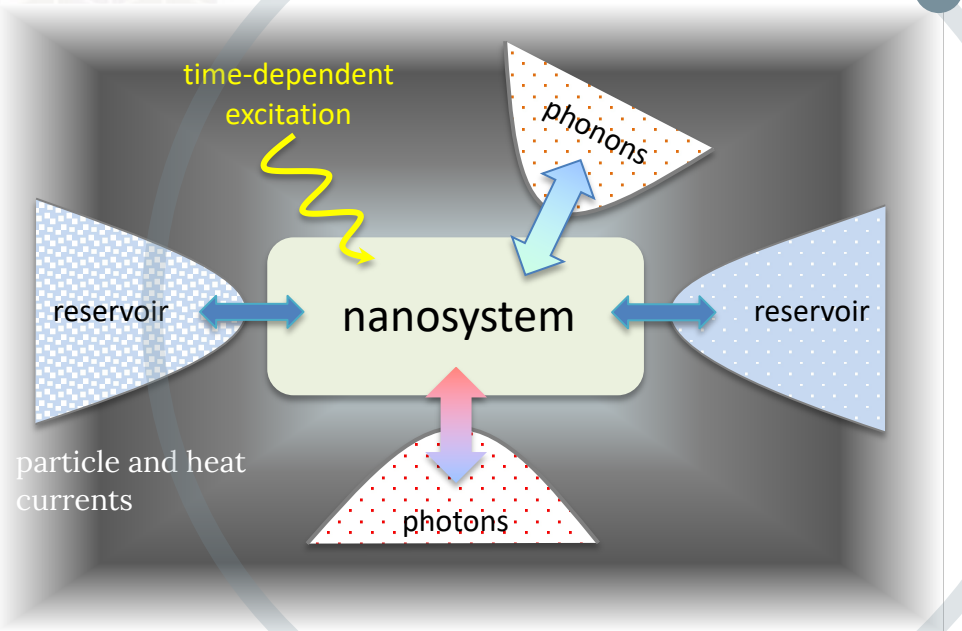
QUANTUM TRANSPORT

Quantum transport

HOW ?

With methods of quantum statistics

Today's choices



General framework: introduction to Nonequilibrium Green's functions

Interactions:
Marc Bescond's course

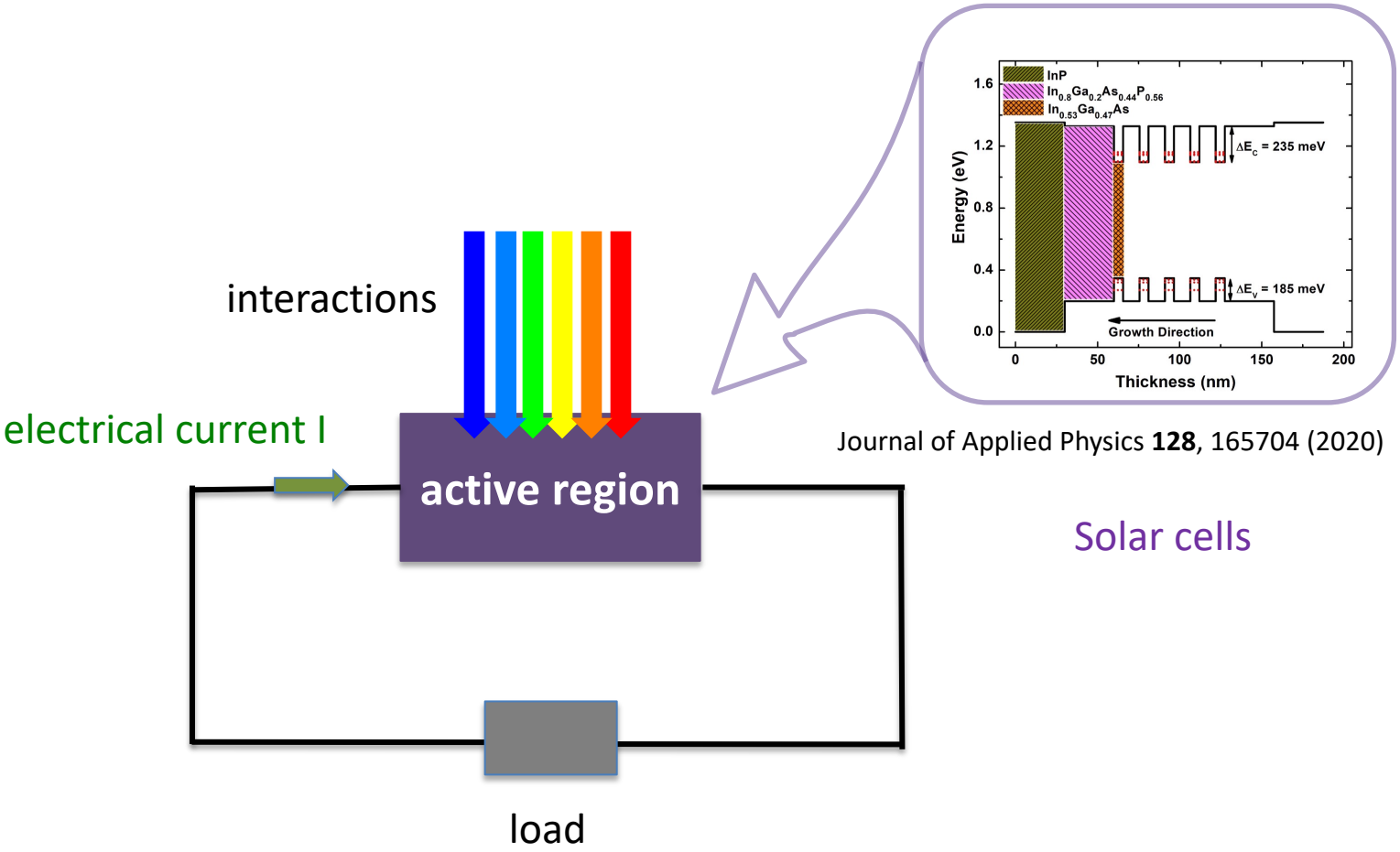
Without interaction

The Landauer formalism

Particle & heat currents

Issues in
quantum thermodynamics

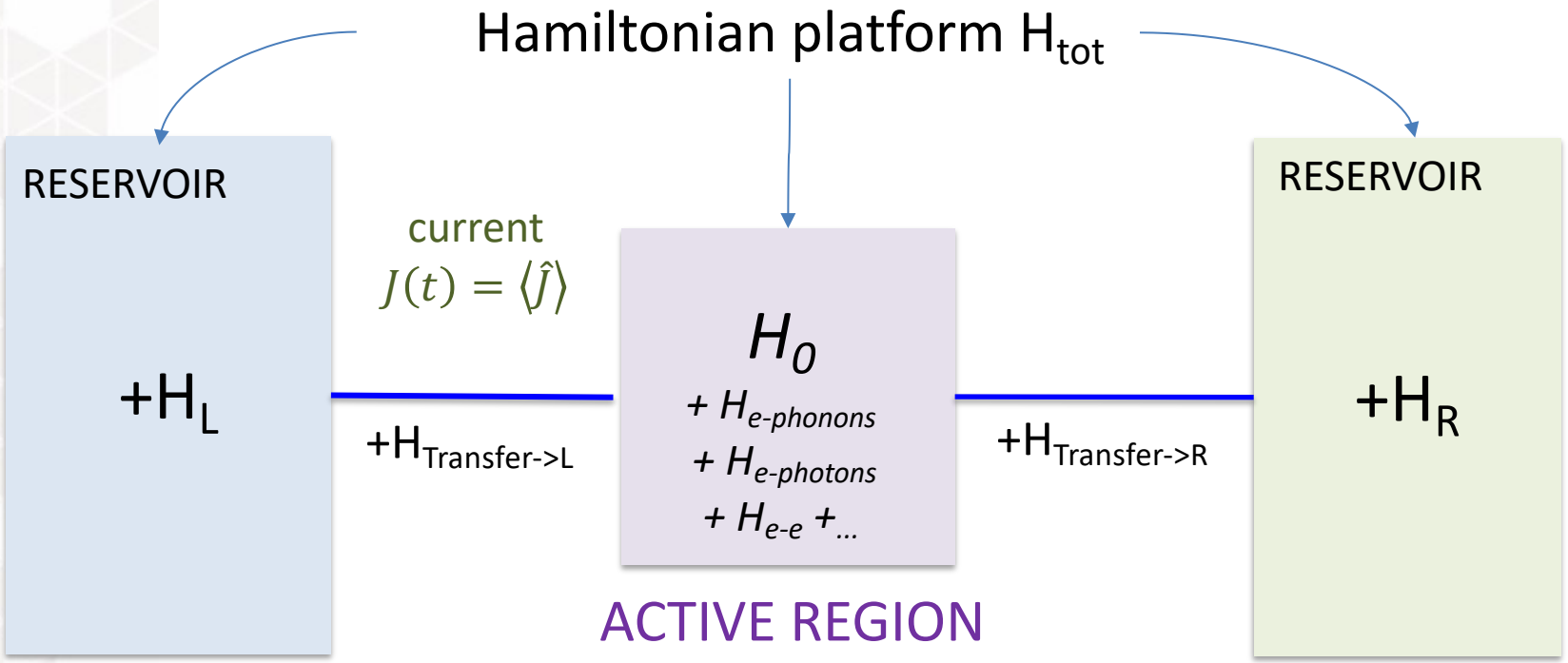
Methodology for quantum transport



Journal of Applied Physics **128**, 165704 (2020)

Solar cells

Methodology for quantum transport

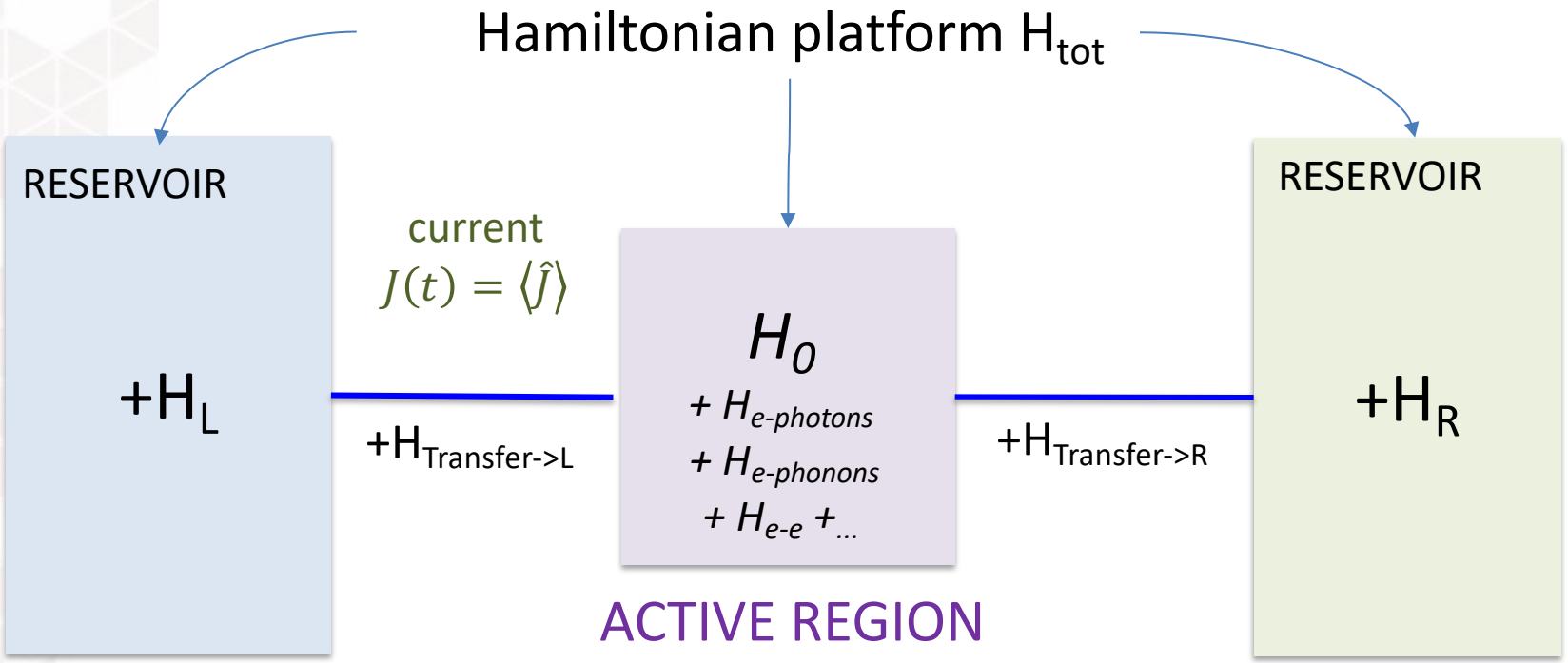


H_{tot} is build from

- empirical models,
- ab initio approaches,
- multi-scale & multi-physics methods.

😀 *Take your favorite!*

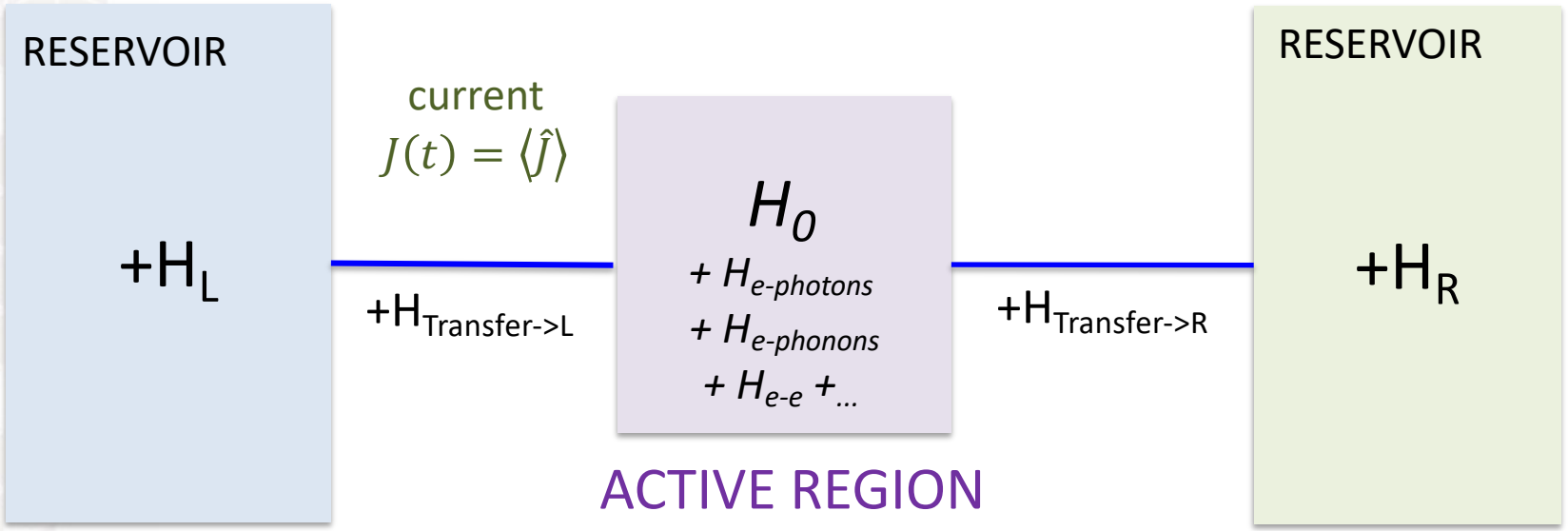
Methodology for quantum transport



😟 *It is not possible to solve the Schrödinger equation*

Methodology for quantum transport

Hamiltonian platform H_{tot}



Green's function of the active region

$$G(1,1') = -i\langle\phi_0|T\left[\Psi(1)\Psi^{\dagger}(1')\right]|\phi_0\rangle$$

$1 = \vec{r}, t$ time-ordering *fermion field* *ground state*

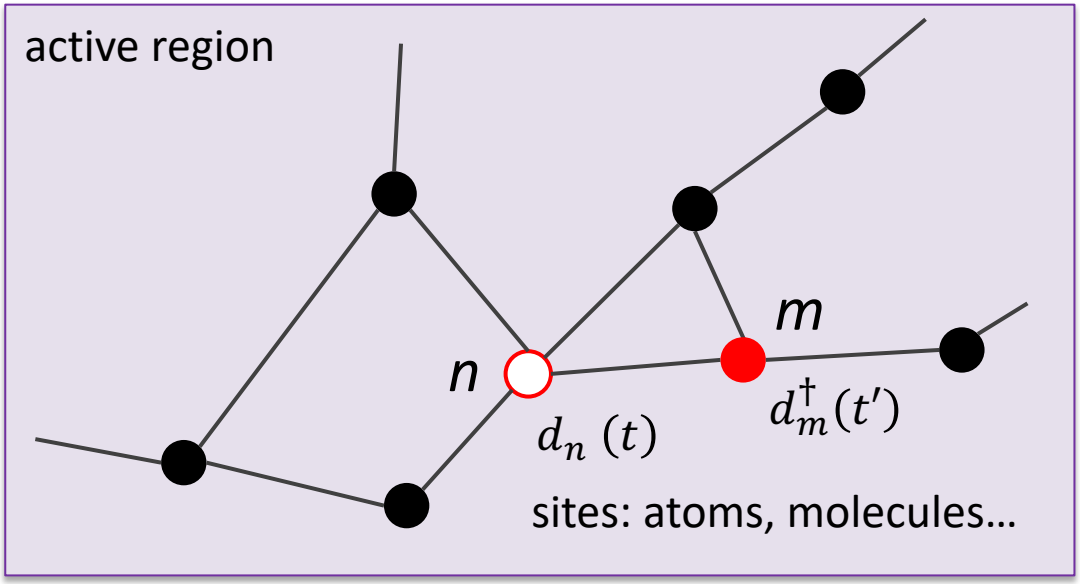
Non-Equilibrium Green's functions

Non-equilibrium Green's functions NEGF

elementary blocks

- retarded component: $G^r_{nm}(t,t') = -i\theta(t-t')\left\langle \left[d^\dagger_m(t'), d_n\ (t) \right]_+ \right\rangle$
- lesser component: $G^<_{nm}(t,t') = i\left\langle d^\dagger_m(t') d_n\ (t) \right\rangle$

T time-ordering



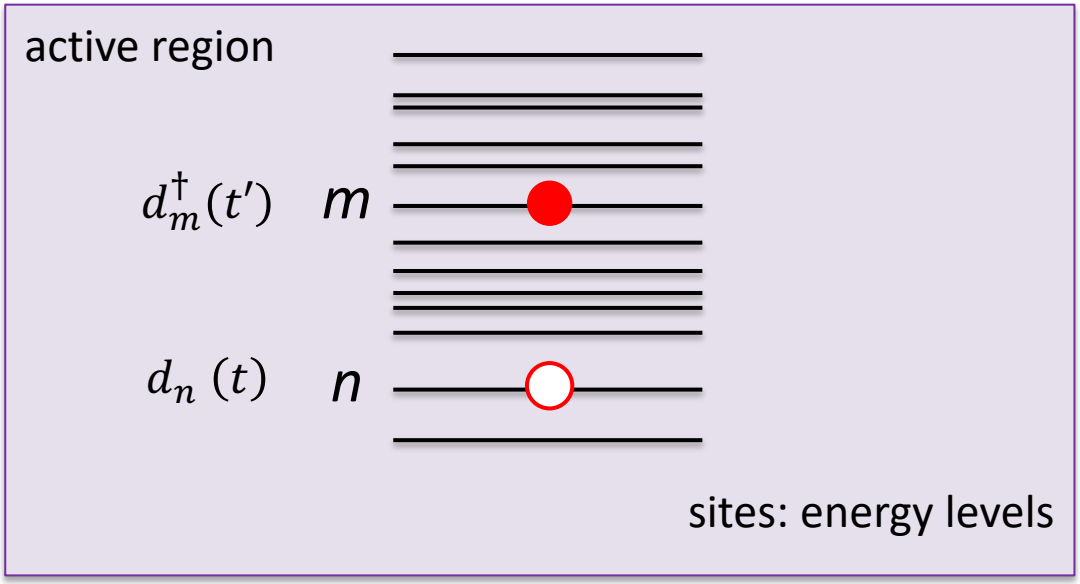
Non-Equilibrium Green's functions

Non-equilibrium Green's functions NEGF

elementary blocks

- retarded component: $G^r_{nm}(t,t') = -i\theta(t-t')\left\langle \left[d^\dagger_m(t'), d_n\ (t) \right]_+ \right\rangle$
- lesser component: $G^<_{nm}(t,t') = i\left\langle d^\dagger_m(t') d_n\ (t) \right\rangle$

T time-ordering



Stationary Spectral Formalism

H. Bruss and K. Flensberg, Many-body quantum theory in condensed matter physics, Oxford University Press (2004).

Heisenberg's equation for G

H. J. M. Haug and A.-P. Jauho, Quantum kinetics in Transport and Optics of Semiconductors 2nd edition, Springer (2008).

$$(t, t') \rightarrow (t - t') \rightarrow \varepsilon$$

$$G^r(\varepsilon) = G_0^r(\varepsilon) + G_0^r(\varepsilon)\Sigma^r(\varepsilon)G^r(\varepsilon)$$

$$G^<(\varepsilon) = G^r(\varepsilon)\Sigma^<(\varepsilon)G^a(\varepsilon)$$

G_0^r known Green's function: perturbative treatment

Σ SELF-ENERGIES

This course → **OPENNESS** contact to reservoir

Charge and heat transport in the Landauer formalism

Marc Bescond's course Thursday morning → **INTERACTION** ***electron-boson***

electron-electron:
out of the scope of the present course

Stationary Spectral Formalism

In fact, you already know $G^r(\varepsilon)$ and $G^<(\varepsilon)$

Spectral function: $A(\varepsilon) = -2\ \mathrm{Im}\ G^r(\varepsilon)$

Occupation number: $n(\varepsilon) = -iG^<(\varepsilon)$

At equilibrium

$A(\varepsilon) \rightarrow$ **Density of states**

$n(\varepsilon) \rightarrow$ **Fermi function**

$$G^<(\varepsilon) = if(\varepsilon)\left(-2\mathrm{Im}\ G^r(\varepsilon)\right)$$

Fluctuation-dissipation relation

$$n = \int d\varepsilon\ f(\varepsilon) \times DOS(\varepsilon)$$

Stationary Spectral Formalism

In fact, you already know $G^r(\varepsilon)$ and $G^<(\varepsilon)$

Spectral function: $A(\varepsilon) = -2\ \mathrm{Im}\ G^r(\varepsilon)$

Occupation number: $n(\varepsilon) = -iG^<(\varepsilon)$

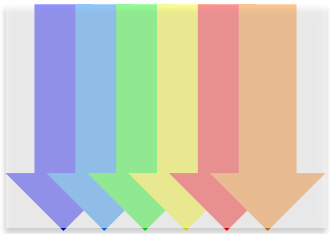
Out-of equilibrium

It is no longer possible to split density of states and statistical function in $G^r(\varepsilon)$ and $G^<(\varepsilon)$

$$n = \int d\varepsilon\, f(\varepsilon) \times DOS(\varepsilon)$$

$$= -i \int d\varepsilon\, G^<(\varepsilon)$$

CURRENTS



Σ_{int}

$G^{r,a,\gtrless}$ Green's function

Observable A

G

Σ_R

Σ_L

spectral response $\mathcal{A}$

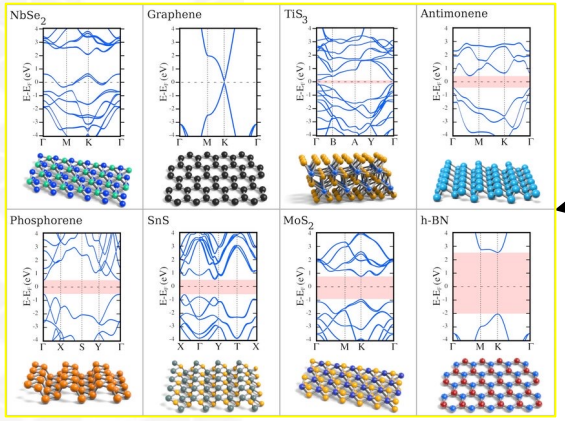
$\Sigma^{r,a,\gtrless}$ self-energy functions

Openness
Interactions

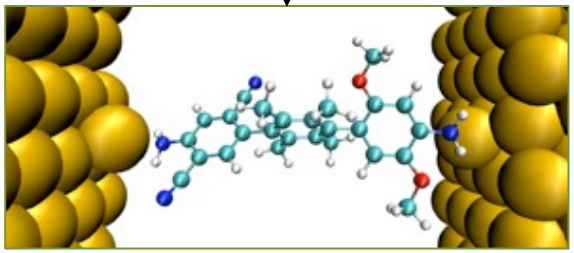
Measure a $\Longleftarrow \int d\varepsilon \, \mathcal{A}(\varepsilon)$

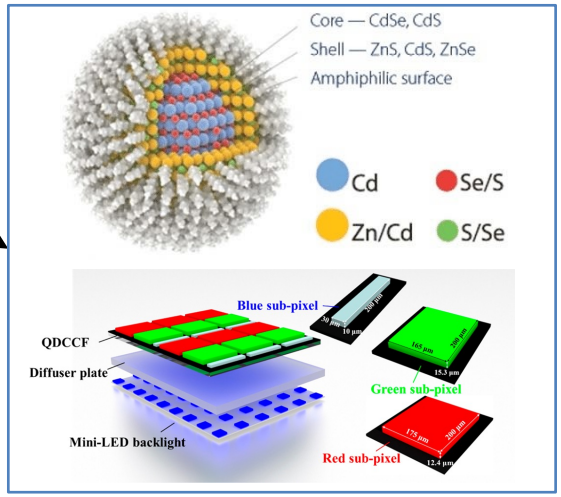
In Schrödinger formalism

In NEGF formalism



Regarding a nanosystem

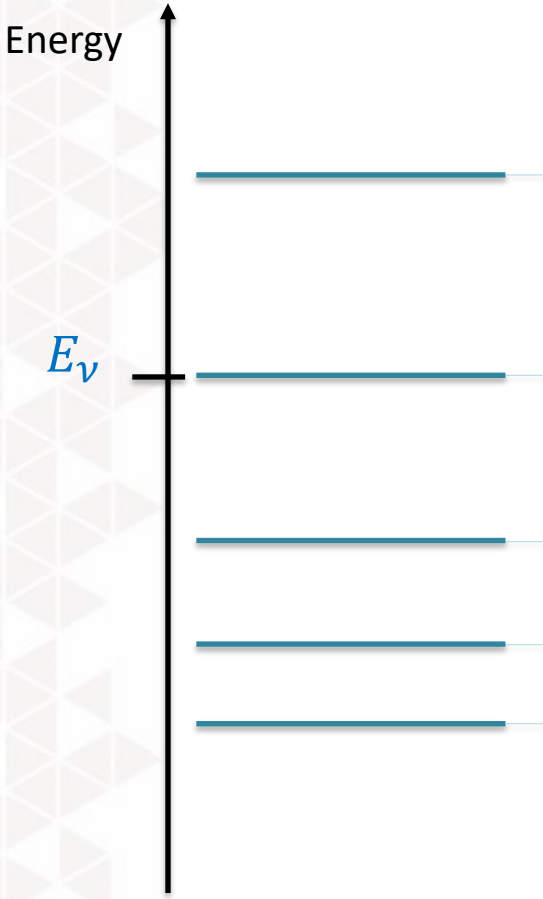




In Schrödinger formalism

Eigenvalue problem

$$[H_0]\psi = E\psi$$

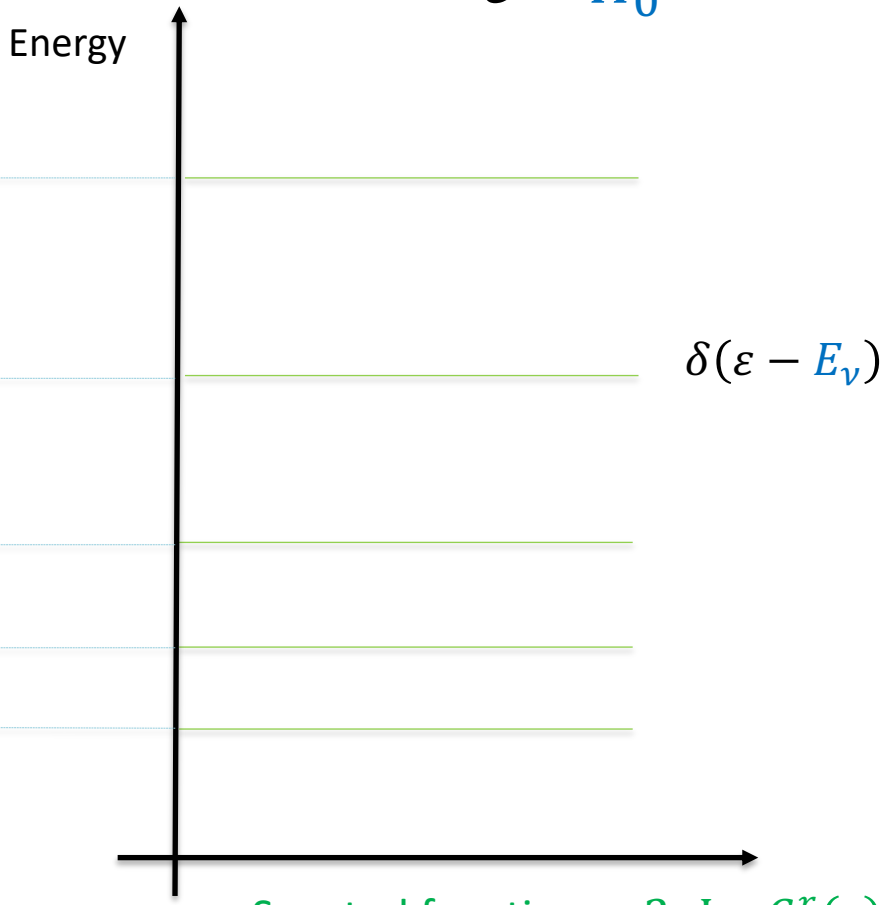


Level structure

In NEGF formalism

Distributions

$$G^r(\varepsilon) = \frac{1}{\varepsilon - H_0}$$

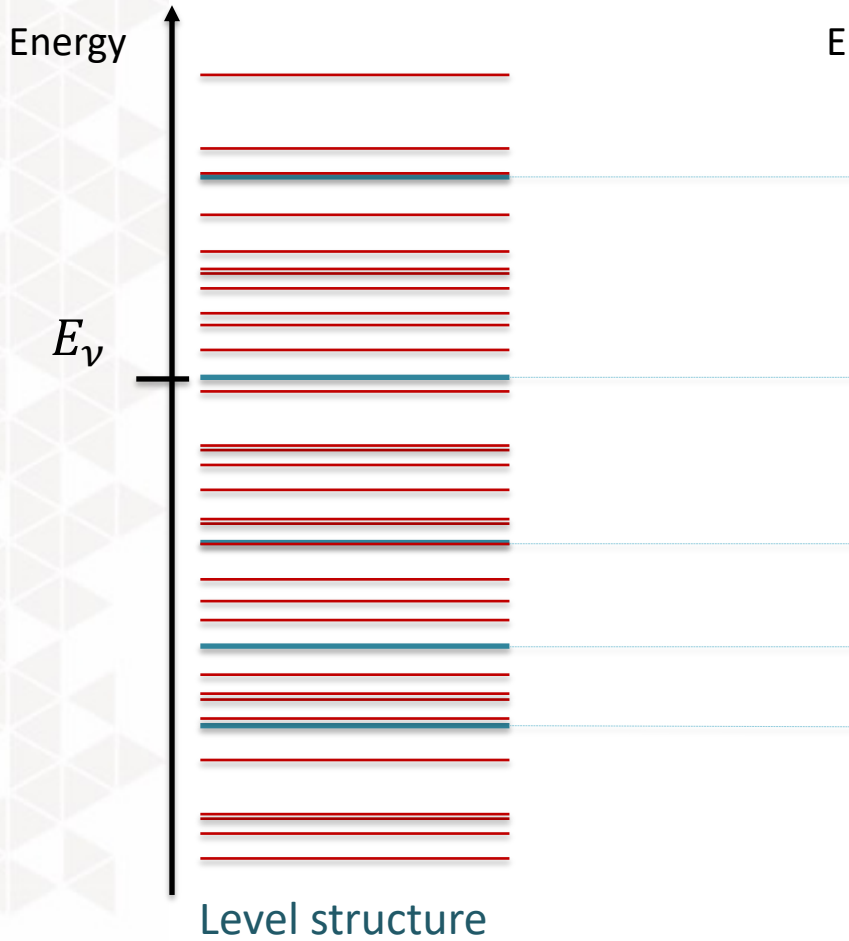


Spectral function: $-2\pi \mathrm{Im}\, G^r(\varepsilon)$

In Schrödinger formalism

Eigenvalue problem

$$[H_0 + H_{res} + H_{int}]\psi = E\psi$$

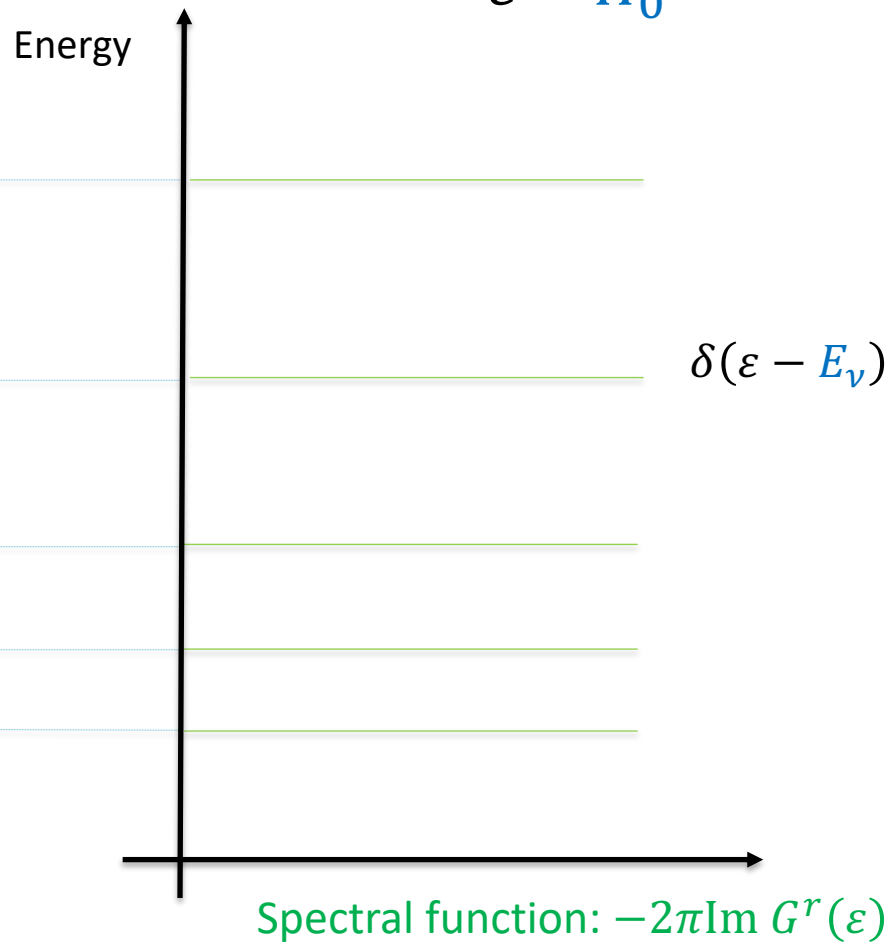


Level structure

In NEGF formalism

Distributions

$$G^r(\varepsilon) = \frac{1}{\varepsilon - H_0}$$

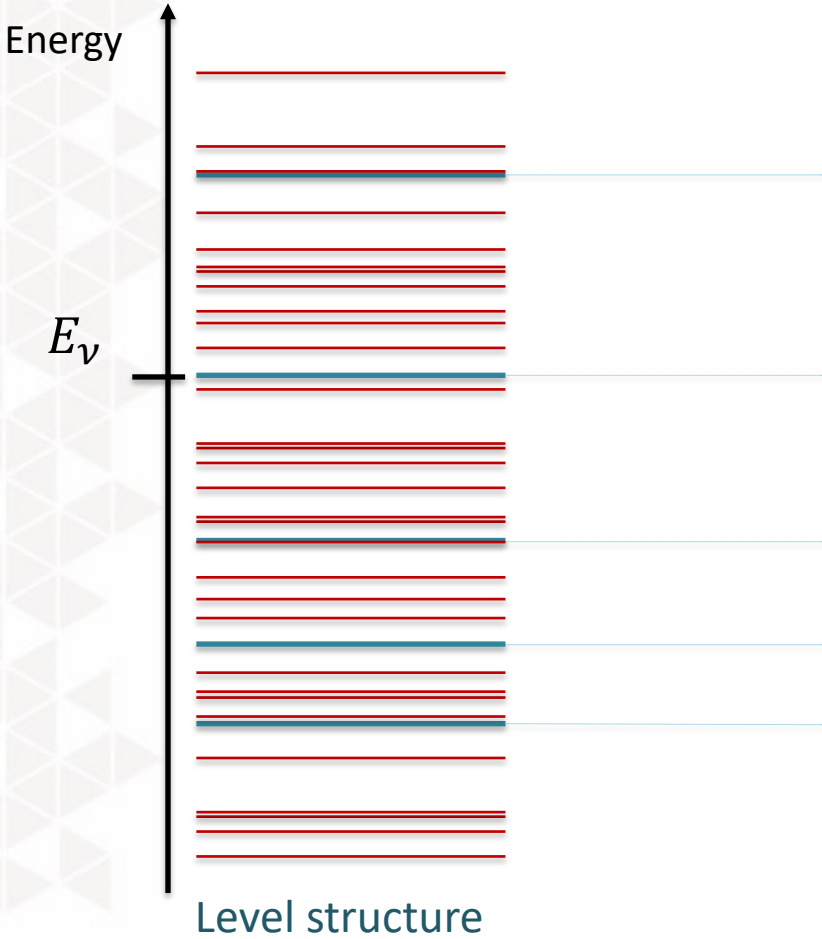


Spectral function: $-2\pi \mathrm{Im}\, G^r(\varepsilon)$

In Schrödinger formalism

Eigenvalue problem

$$[H_0 + H_{res} + H_{int}]\psi = E\psi$$

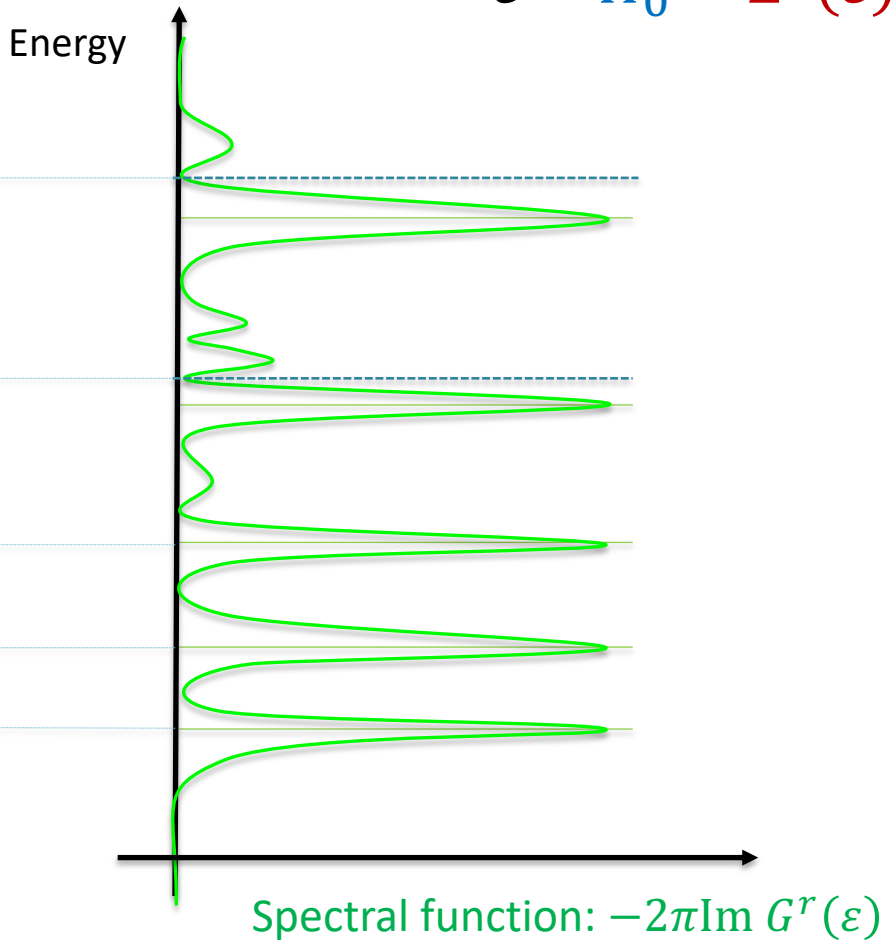


Level structure

In NEGF formalism

Distributions

$$G^r(\varepsilon) = \frac{1}{\varepsilon - H_0 - \Sigma^r(\varepsilon)}$$

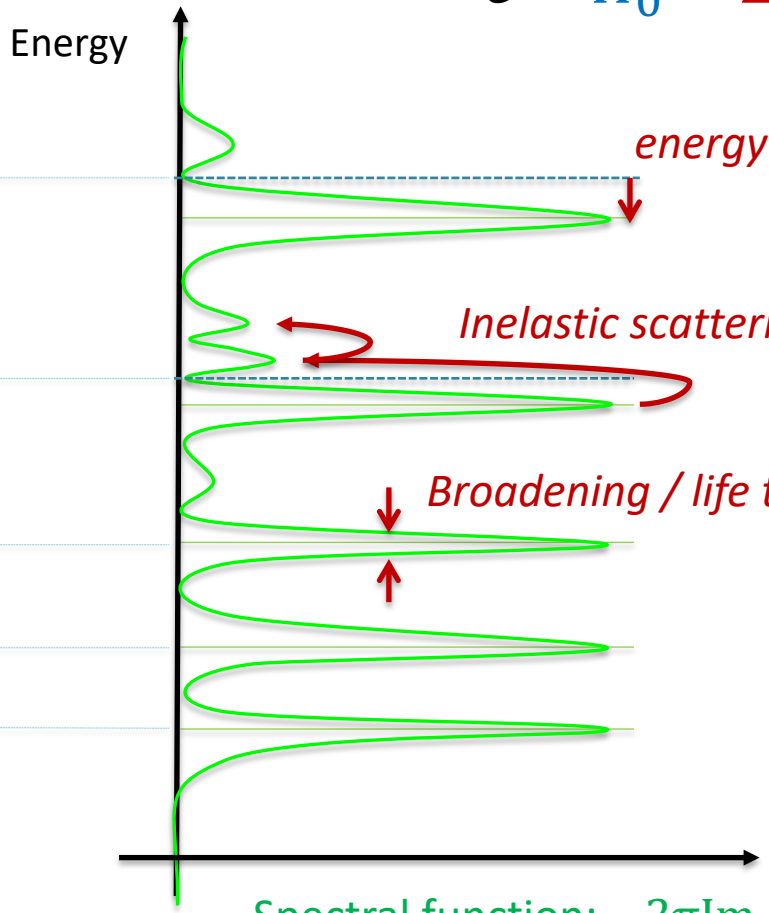


Spectral function: $-2\pi \mathrm{Im}\, G^r(\varepsilon)$

In NEGF formalism

Distributions

$$G^r(\varepsilon) = \frac{1}{\varepsilon - H_0 - \Sigma^r(\varepsilon)}$$



energy shift ← *real part of* Σ^r

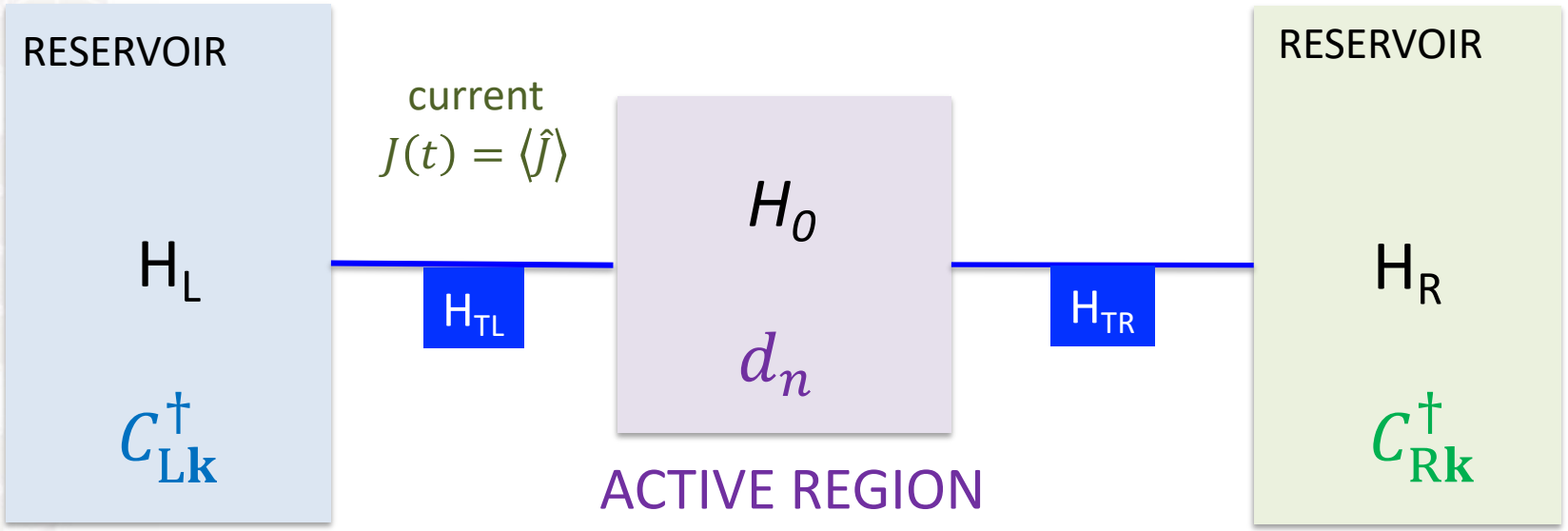
Inelastic scattering ← *energy-dependence of* Σ^r in terms $G^{\gtrless}(\varepsilon \pm \hbar\omega_{\xi\mathbf{q}})$

Broadening / life time ← *imaginary part of* Σ^r

Spectral function: $-2\pi \mathrm{Im}\, G^r(\varepsilon)$

OPENNESS: contact self-energy (exact)

H. J. M. Haug and A.-P. Jauho, Quantum kinetics in Transport and Optics of Semiconductors 2nd edition, Springer (2008).

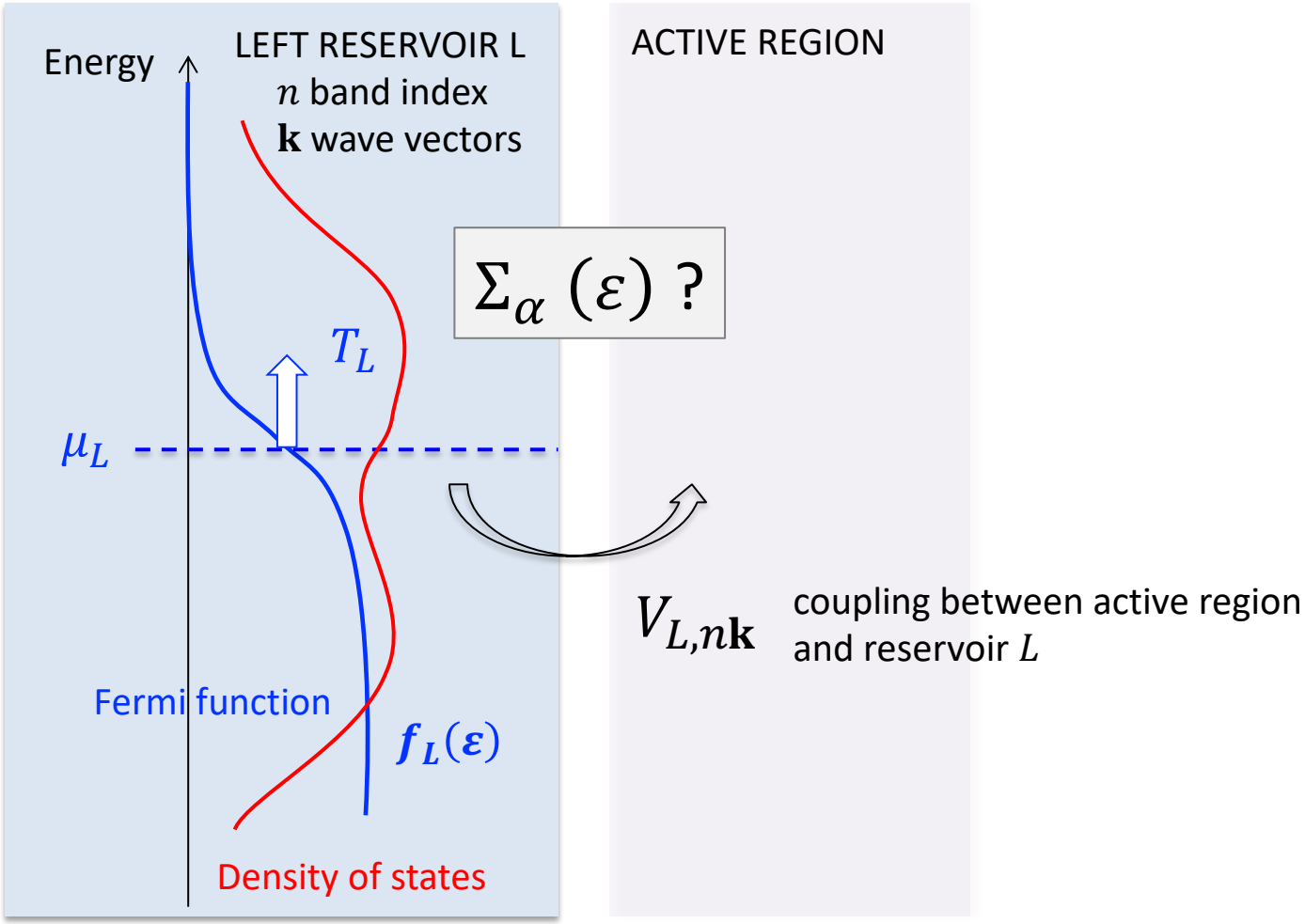


$$H_{T\alpha} = \sum_{n,\mathbf{k}} V_{\alpha n \mathbf{k}} C^{\dagger}_{\alpha \mathbf{k}} d_n + h.c. \quad \text{with} \quad \alpha \in \{L, R\}$$

$h.c.$ for hermitian conjugated

OPENNESS: contact self-energy (exact)

H. J. M. Haug and A.-P. Jauho, Quantum kinetics in Transport and Optics of Semiconductors 2nd edition, Springer (2008).



OPENNESS: contact self-energy (exact)

H. J. M. Haug and A.-P. Jauho, Quantum kinetics in Transport and Optics of Semiconductors 2nd edition, Springer (2008).

$$\Sigma_{\alpha}^{\gtrless}(\varepsilon) = \sum_{\alpha,n\mathbf{k}} \left|V_{\alpha,n\mathbf{k}}\right|^2 g_{\alpha,n\mathbf{k}}^{\gtrless}(\varepsilon)$$

- $V_{\alpha,n\mathbf{k}}$ coupling between active region and reservoir $\alpha \in \{L, R\}$
- $g_{\alpha,n\mathbf{k}}^{\gtrless}(\varepsilon)$ Green's function of reservoir α

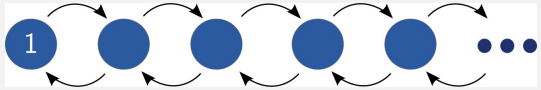
OPENNESS: contact self-energy (exact)

OPENNESS: contact to reservoir (exact)

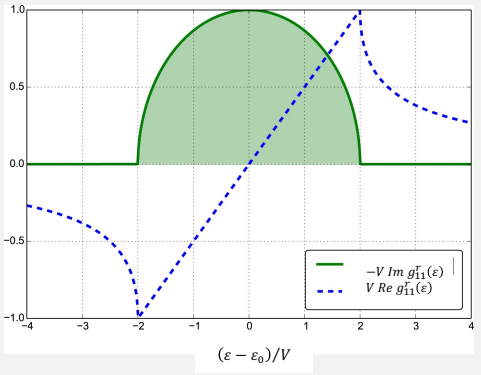
H. J. M. Haug and A.-P. Jauho, Quantum kinetics in Transport and Optics of Semiconductors 2nd edition, Springer (2008).

$$\Sigma_{\alpha}^{\gtrless}(\varepsilon) = \sum_{\alpha,n\mathbf{k}} \left|V_{\alpha,n\mathbf{k}}\right|^2 g_{\alpha,n\mathbf{k}}^{\gtrless}(\varepsilon)$$

- General expression : $\Sigma_{\alpha}^{r,a}(\varepsilon) = \Lambda_{\alpha}(\varepsilon) \pm i\frac{1}{2}\Gamma_{\alpha}(\varepsilon)$
- Semi-infinite chain model for reservoir



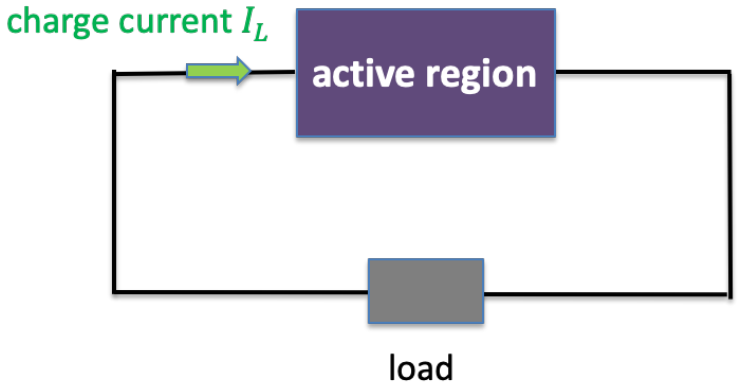
Pedagogical introduction to equilibrium Green's functions: condensed-matter examples with numerical implementations
DOI: 10.1590/1806-9126-RBEF-2016-0087



- Wide band limit approximation: $\Sigma_{\alpha}^{r,a}(\varepsilon) = \pm i\frac{1}{2}\Gamma_{\alpha}$

Charge current in ballistic regime

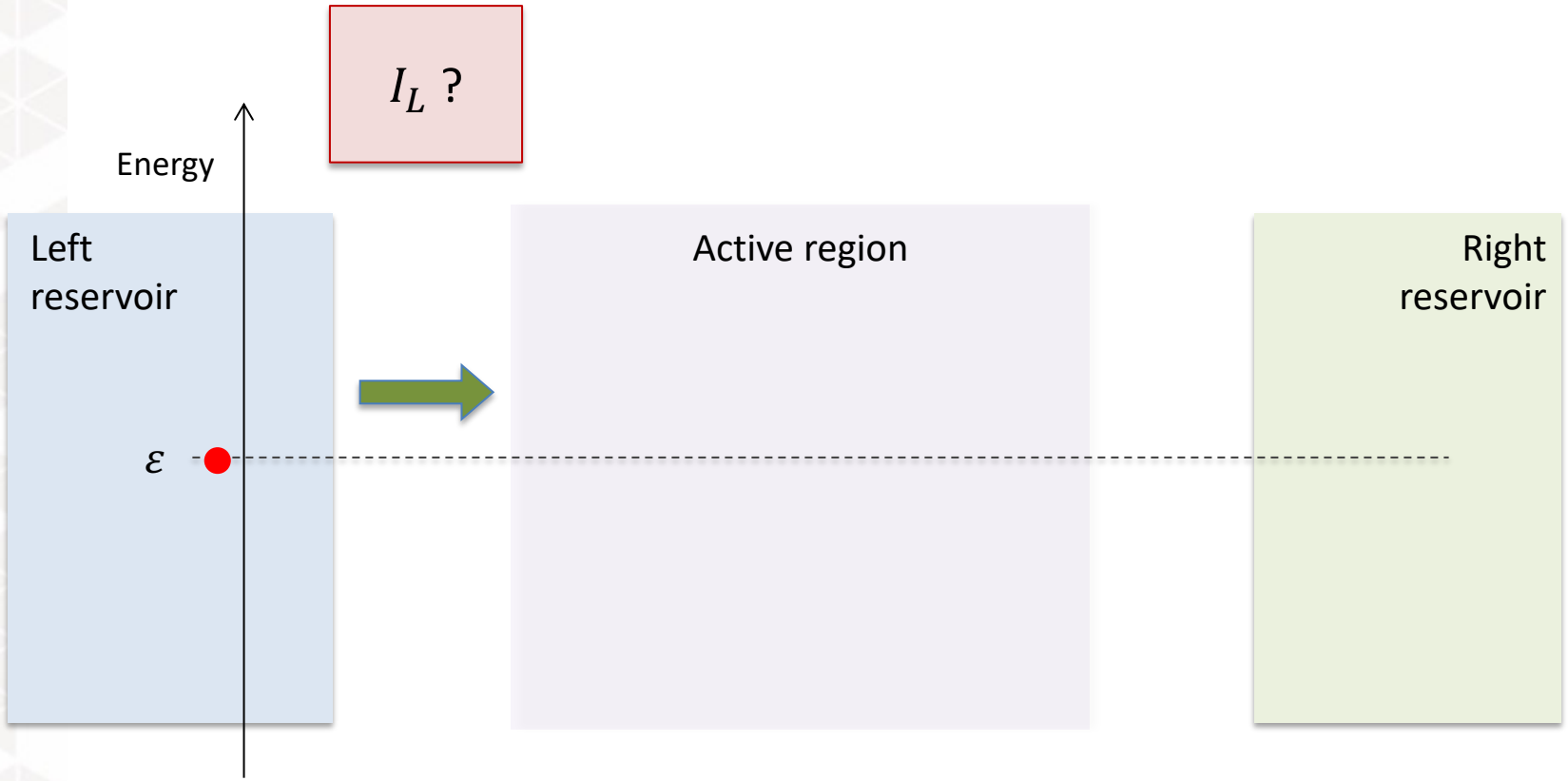
Ballistic regime: *without interactions*



Observable I_L

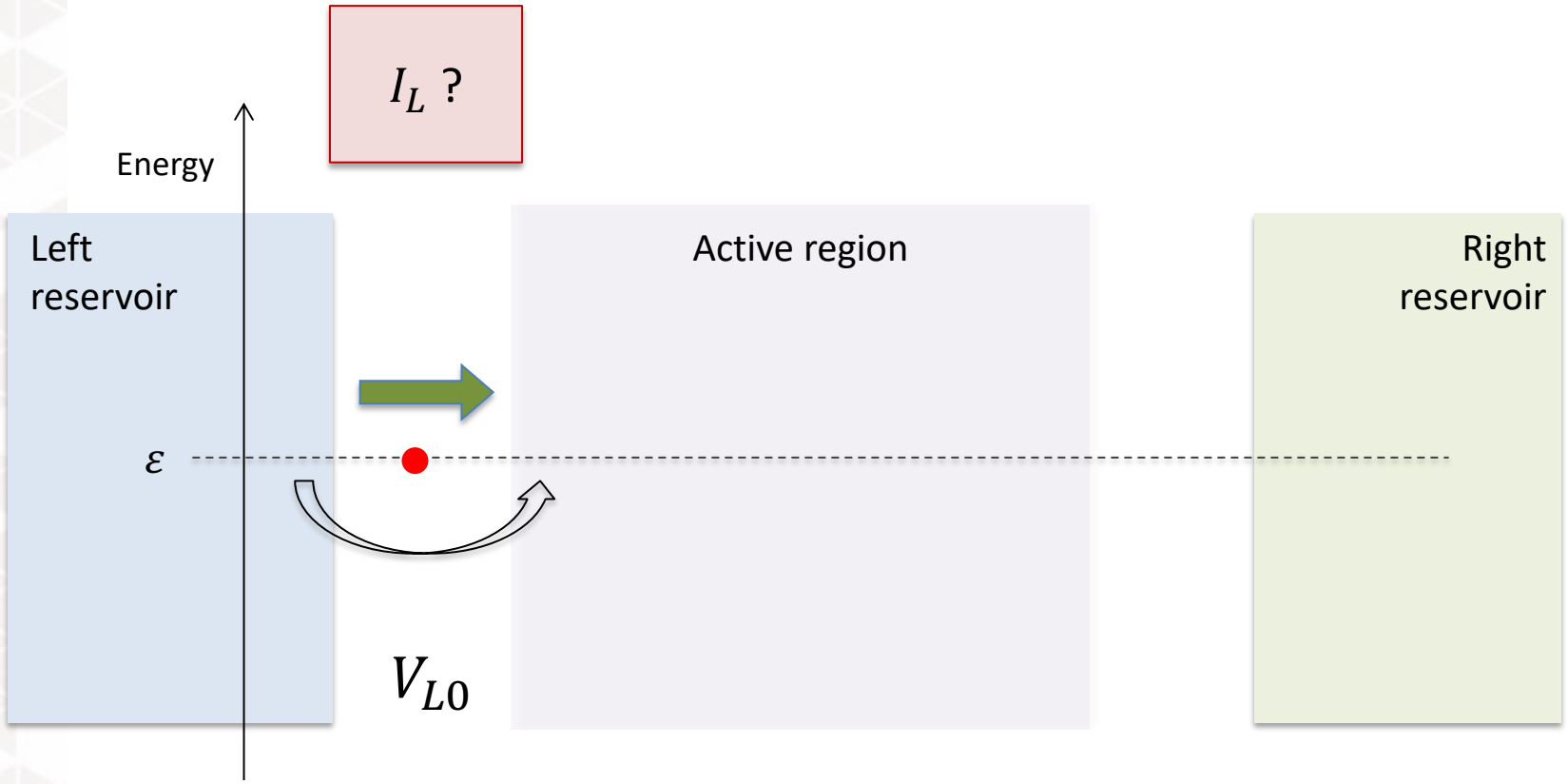
$$I_L = q\left\langle \frac{dN_L}{dt} \right\rangle$$

I_L ?



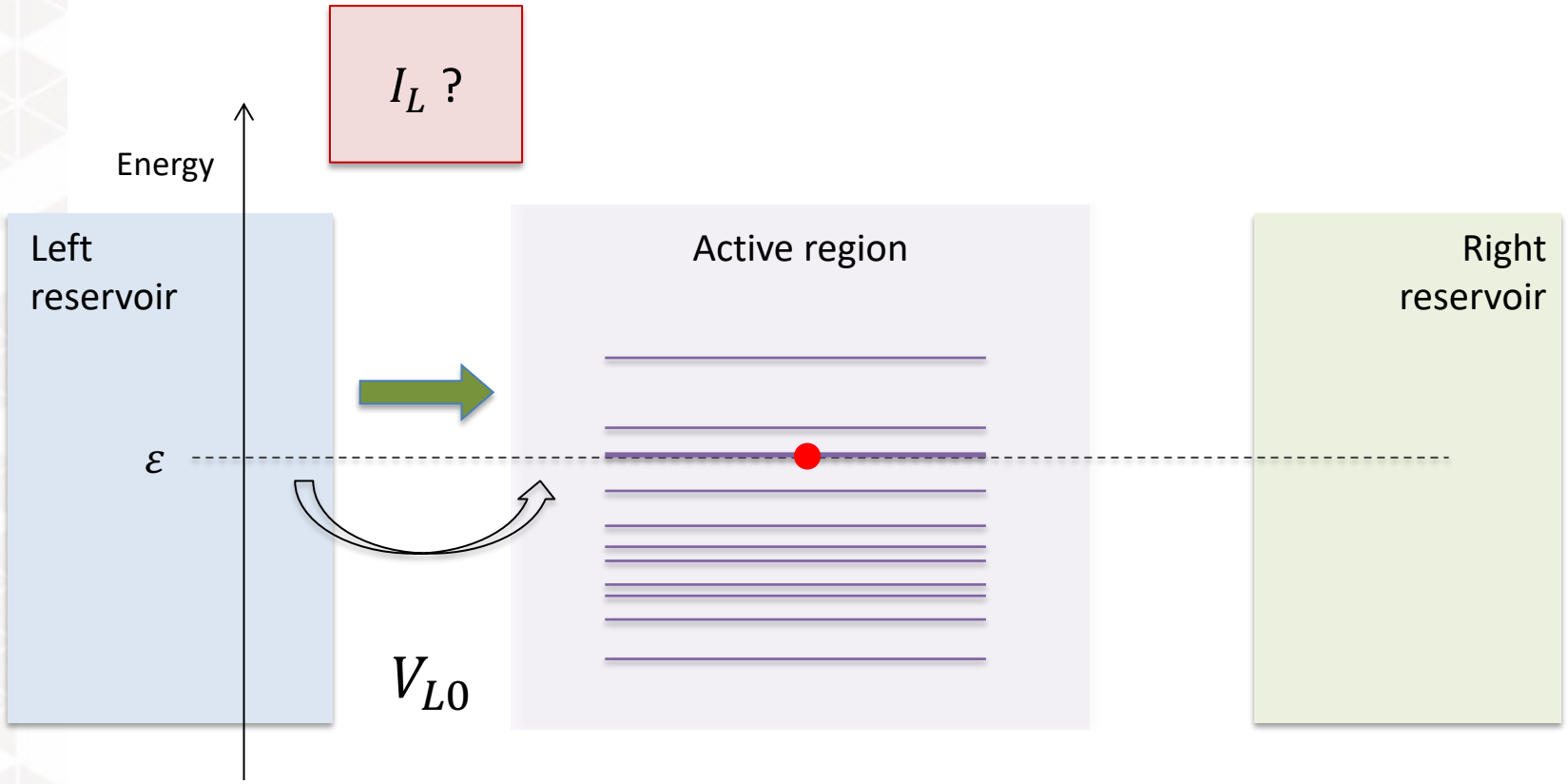
Transport will depend on *(from left to right)*

- presence of an electron inside left reservoir



Transport will depend on *(from left to right)*

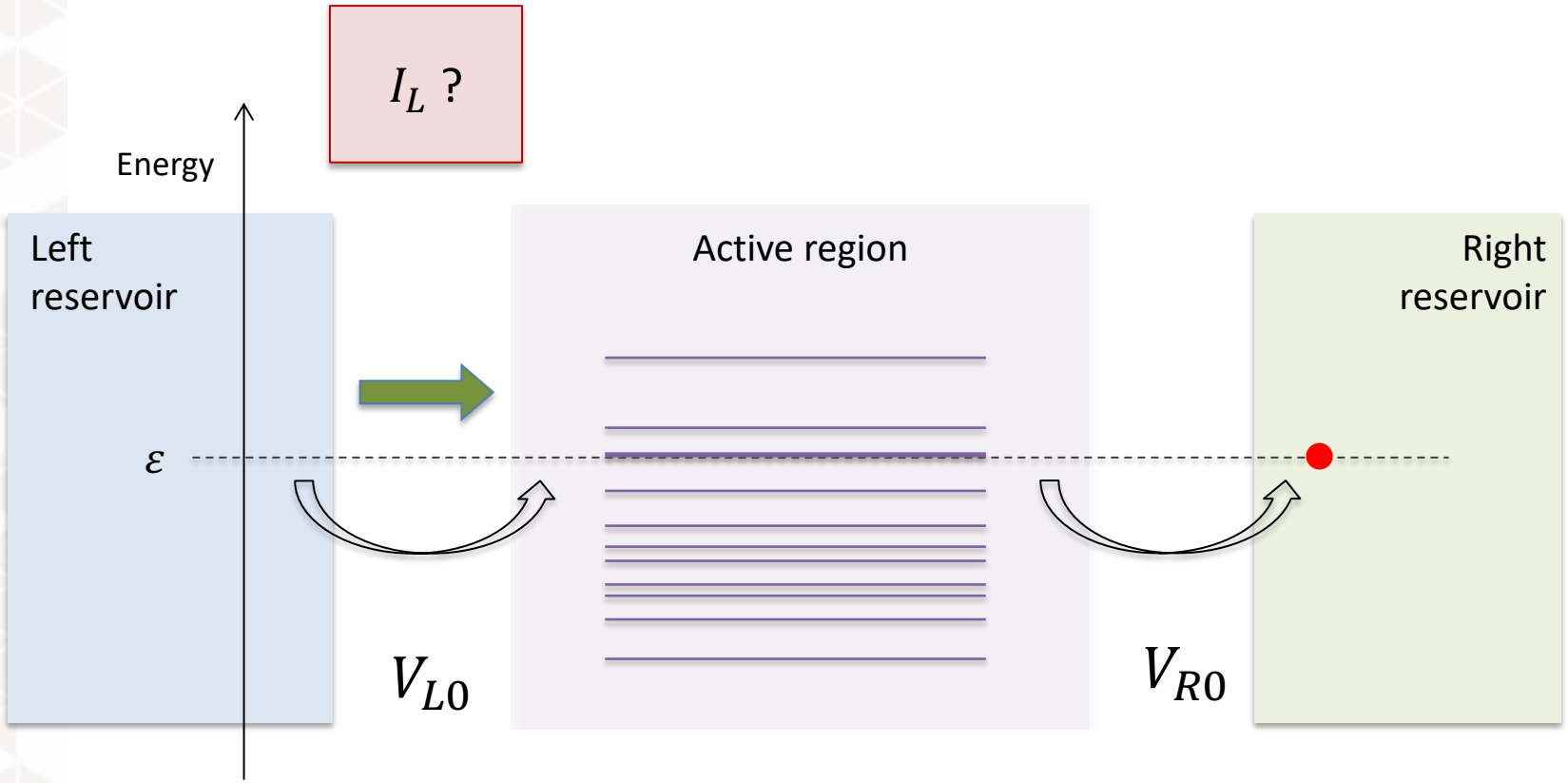
- presence of an electron inside left reservoir
- non-zero coupling between central region and reservoirs V_{L0}



Transport will depend on *(from left to right)*

- presence of an electron inside left reservoir

- non-zero coupling between central region and reservoirs V_{L0}
- available states inside active region (density of states)



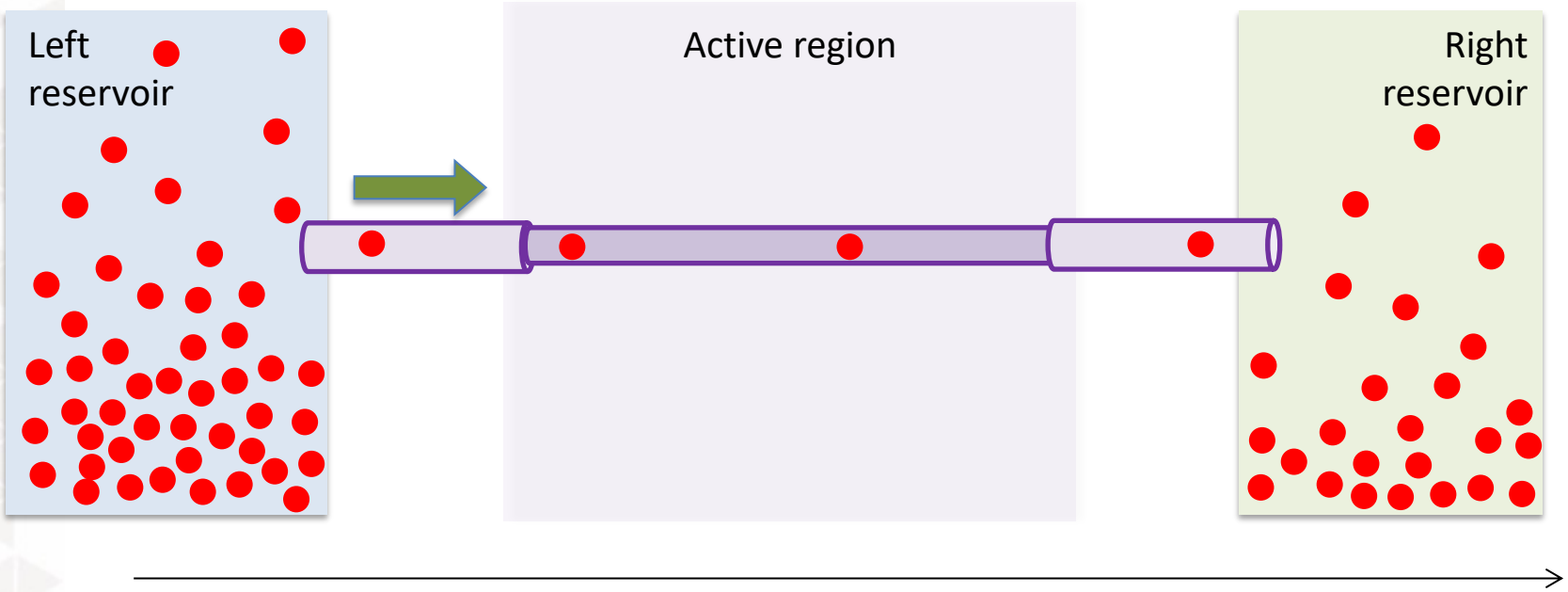
Transport will depend on *(from left to right)*

- presence of an electron inside left reservoir and a vacancy in right reservoir

- non-zero coupling between central region and reservoirs V_{L0} and V_{R0}
- available states inside active region (density of states)

$$J(\varepsilon) = \frac{2q}{h}\,\mathcal{T}(\varepsilon)\times[f_L(\varepsilon) - f_R(\varepsilon)]$$

spectral current



Transport will depend on *(from left to right)*

- presence of an electron inside left reservoir and a vacancy in right reservoir

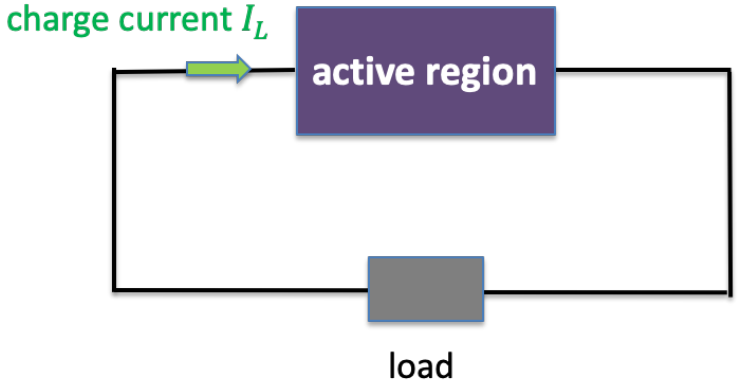
$$f_L(\varepsilon) > f_R(\varepsilon)$$

- non-zero coupling between central region and reservoirs V_{L0} and V_{R0}
- available states inside active region (density of states)

$$\mathcal{T}(\varepsilon) = \mathrm{Tr}\left[\mathbf{\Gamma}_L\ \mathbf{G}^{\mathbf{r}}\mathbf{\Gamma}_R\ \mathbf{G}^{\mathbf{a}}\right]$$

Charge current in ballistic regime

Ballistic regime: *without interactions*



$$J(\varepsilon) = \frac{2q}{h}\,\mathcal{T}(\varepsilon)\times[f_L(\varepsilon) - f_R(\varepsilon)]$$

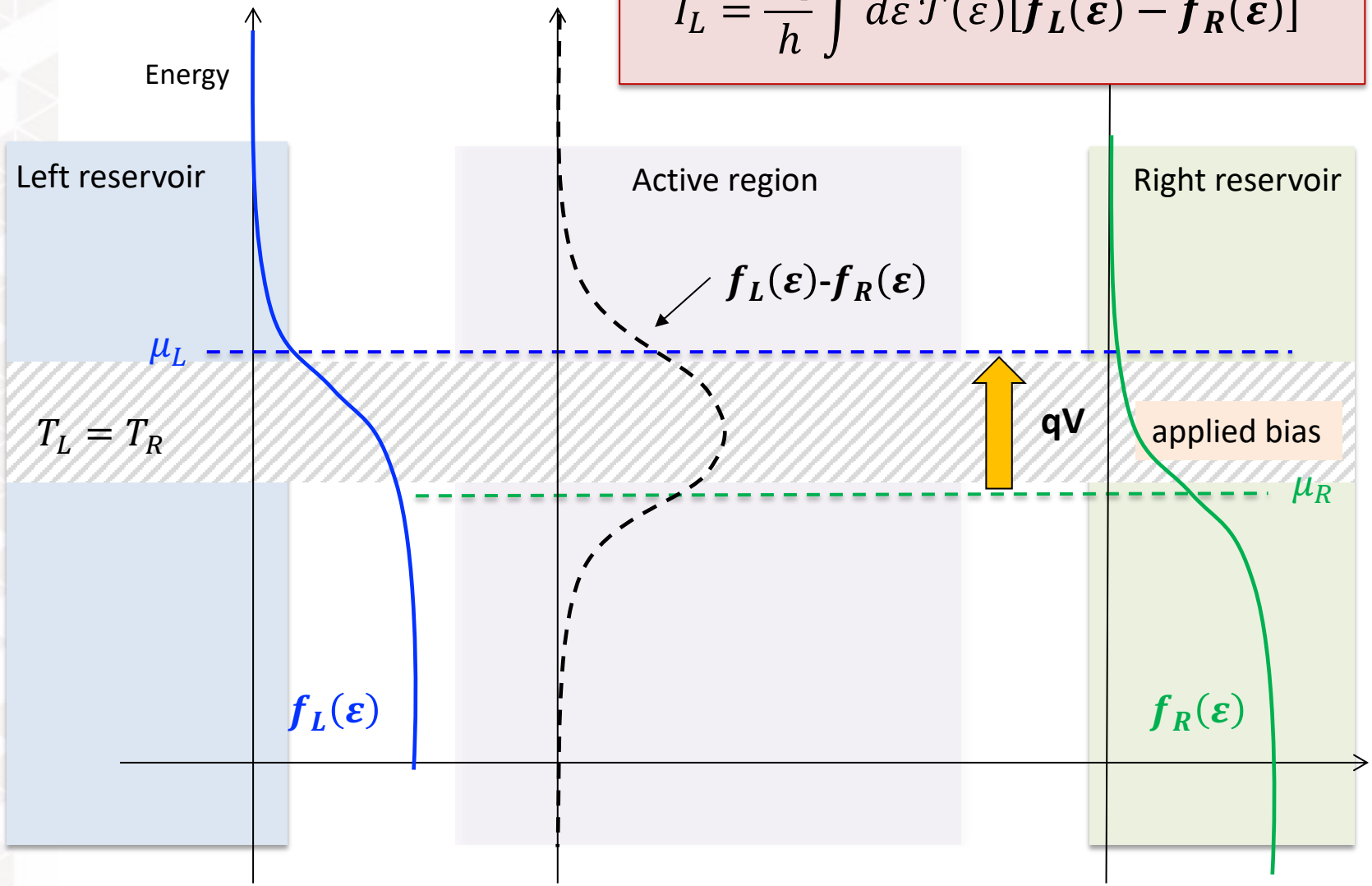
This is the famous LANDAUER formula for the current

$$I_L = \frac{2q}{h}\int d\varepsilon\,\mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$

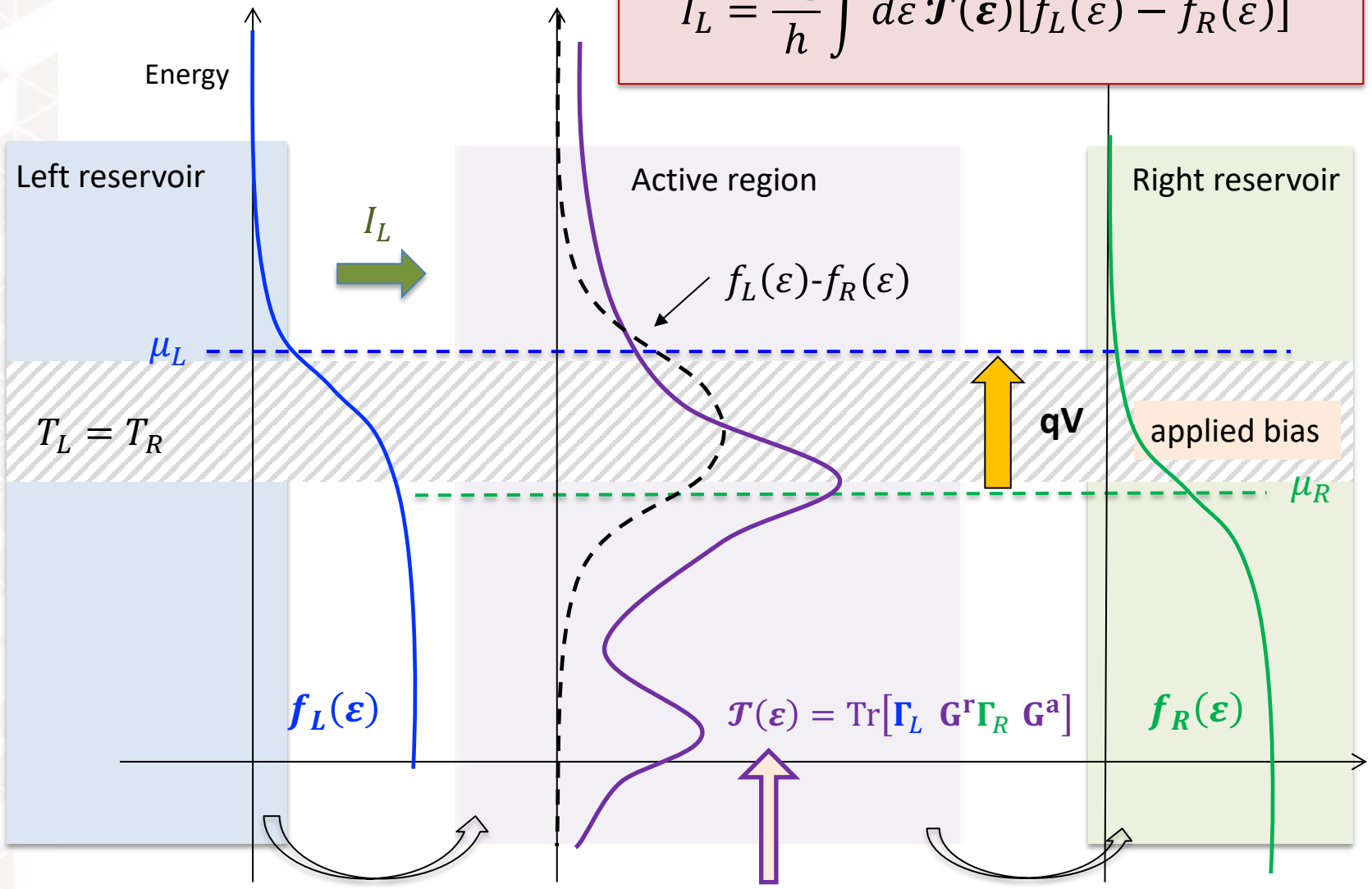
with **transmission** $\mathcal{T}(\varepsilon) = \mathrm{Tr}\left[\mathbf{\Gamma}_L\ \mathbf{G^r}\mathbf{\Gamma}_R\ \mathbf{G^a}\right]$

$$\Gamma_\alpha\ (\varepsilon) = -2\mathrm{Im}\,\Sigma^r_\alpha(\varepsilon)$$

$$I_L = \frac{2q}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)[\boldsymbol{f_L(\varepsilon) - f_R(\varepsilon)}]$$

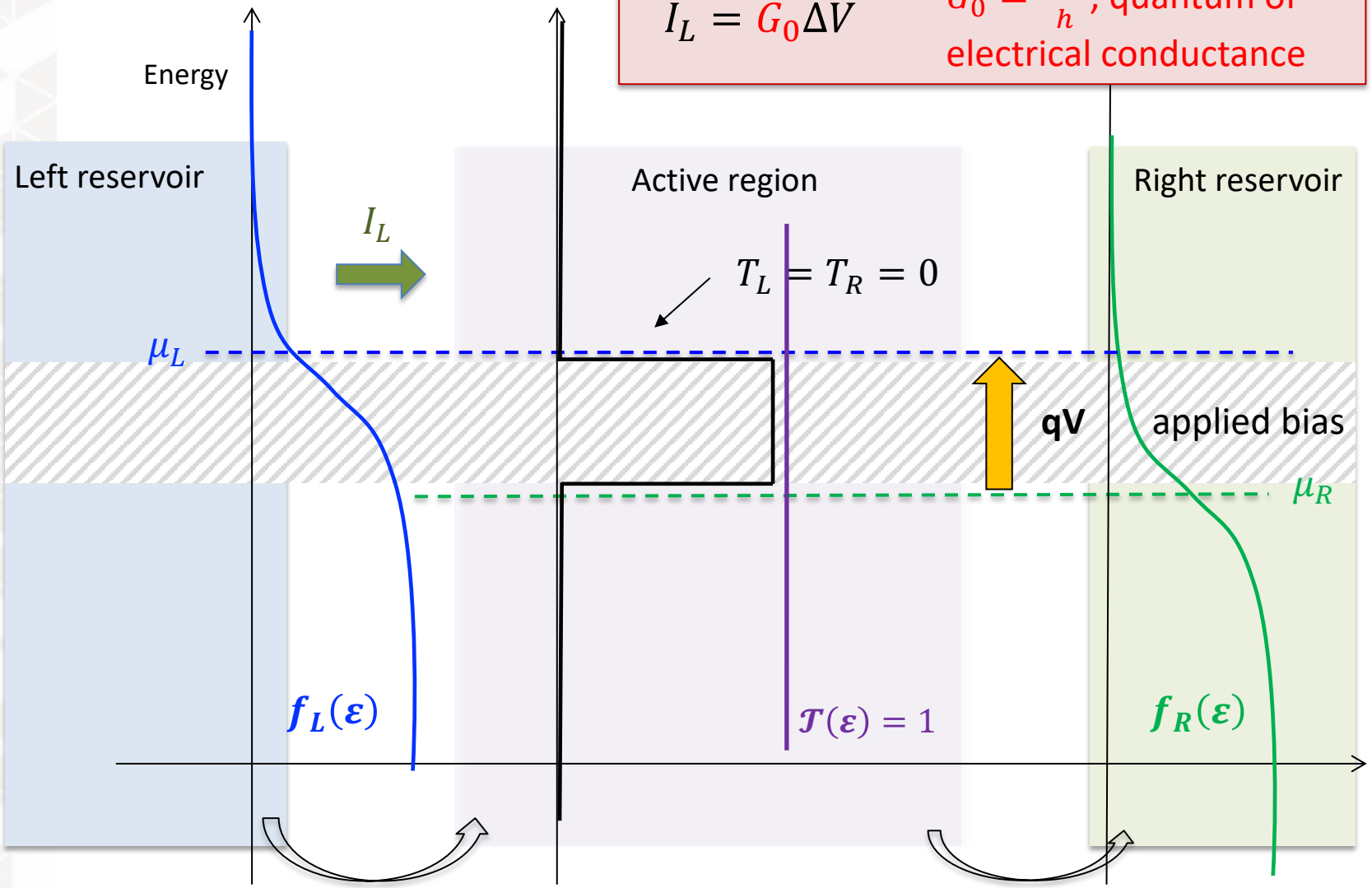


$$I_L = \frac{2q}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$



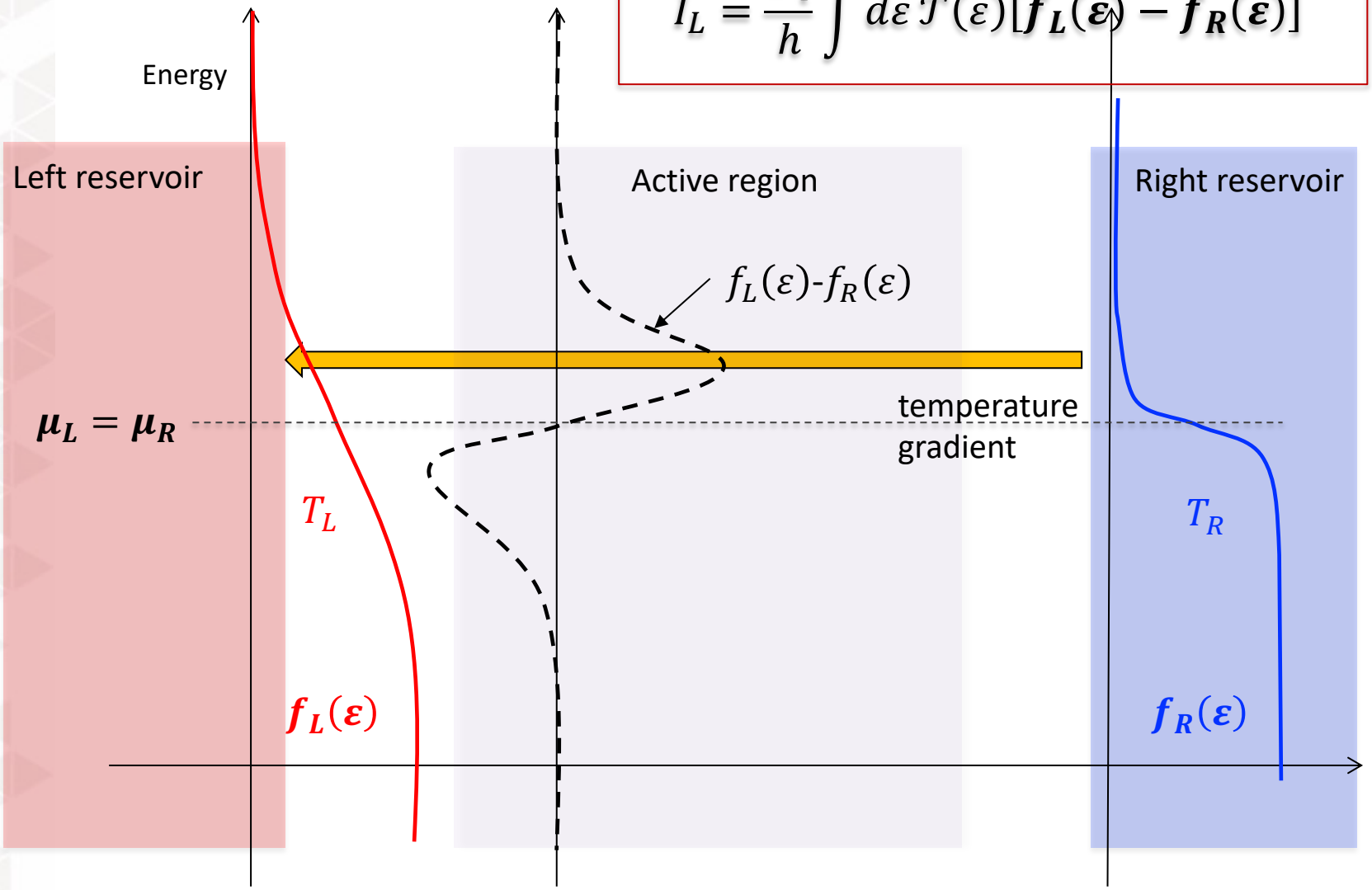
Densities of states of active region and reservoirs
Couplings to reservoir

$I_L = G_0 \Delta V$ $G_0 = \frac{2q^2}{h}$, quantum of electrical conductance



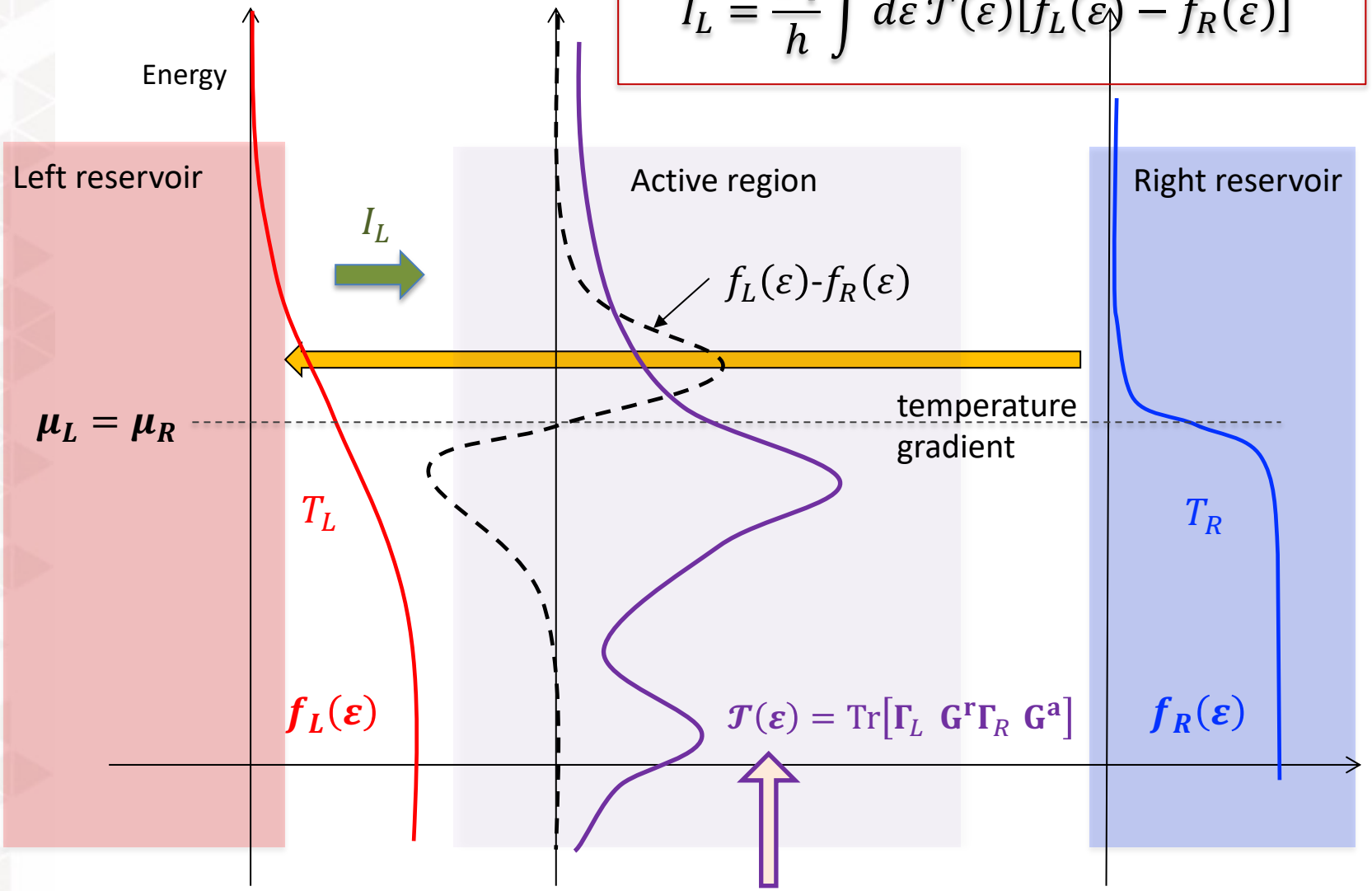
Thermolectricity

$$I_L = \frac{2q}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)[\boldsymbol{f_L(\varepsilon)} - \boldsymbol{f_R(\varepsilon)}]$$



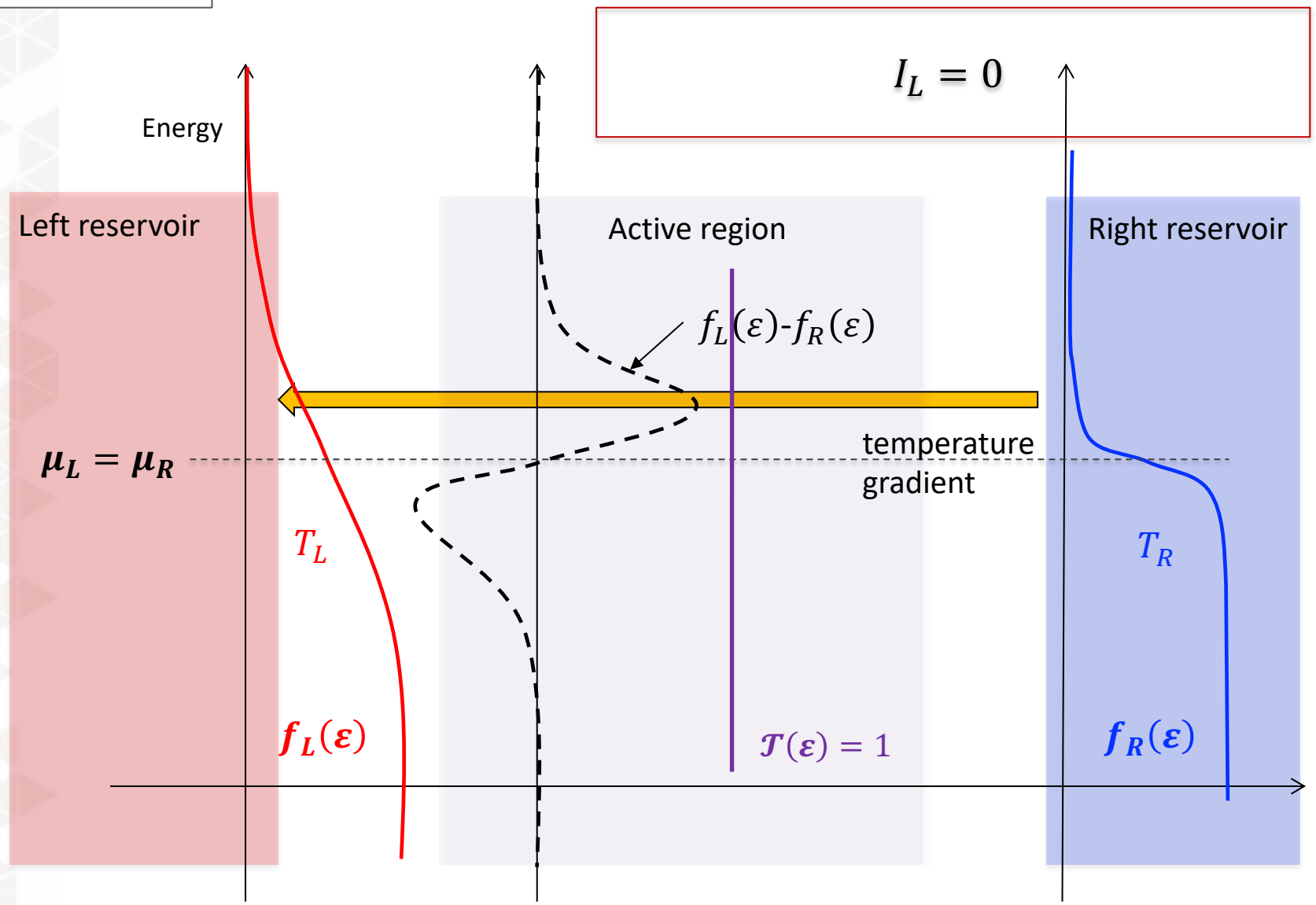
Thermolectricity

$$I_L = \frac{2q}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$



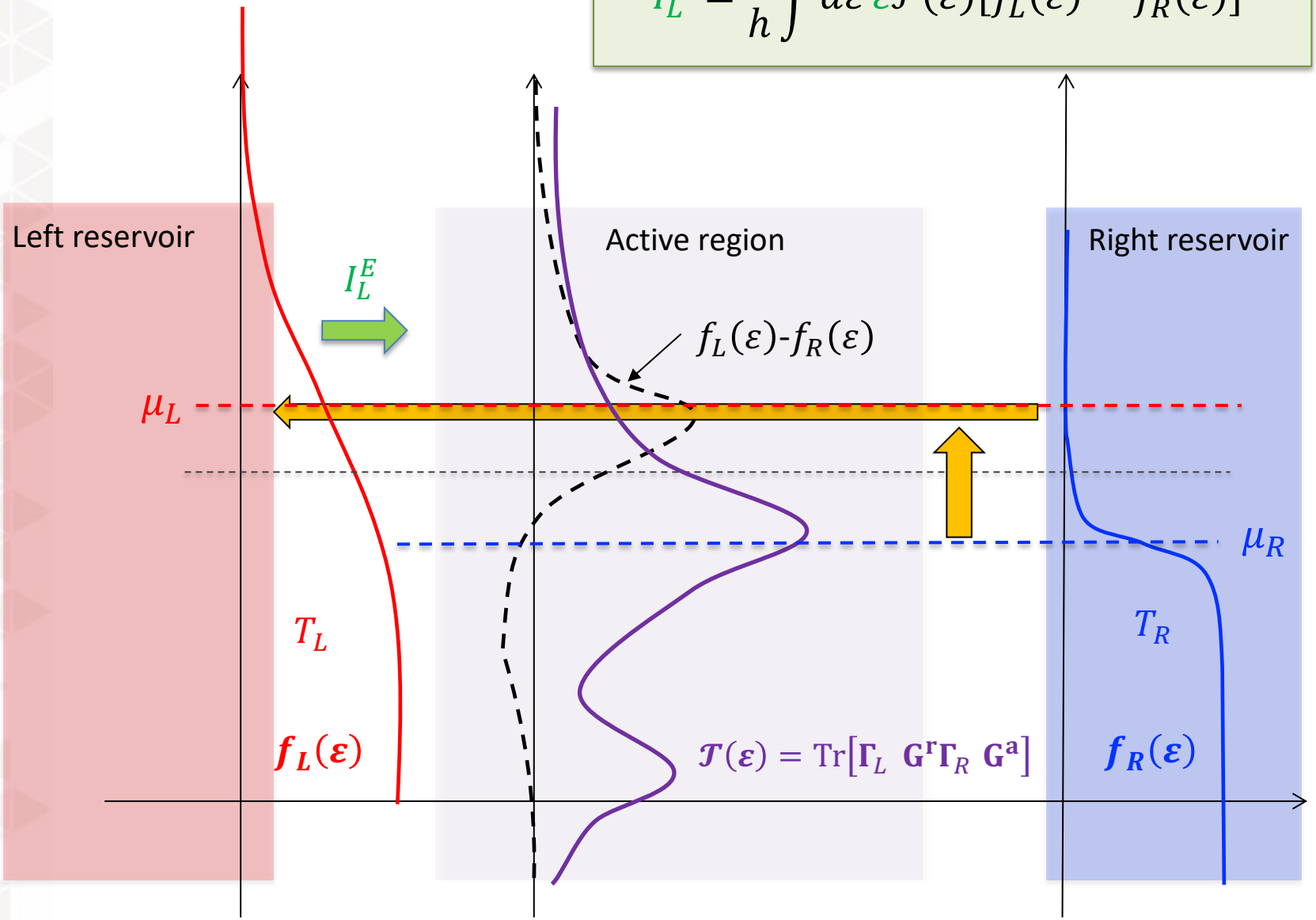
Densities of states of active region and reservoirs
Couplings to reservoir

Thermolectricity



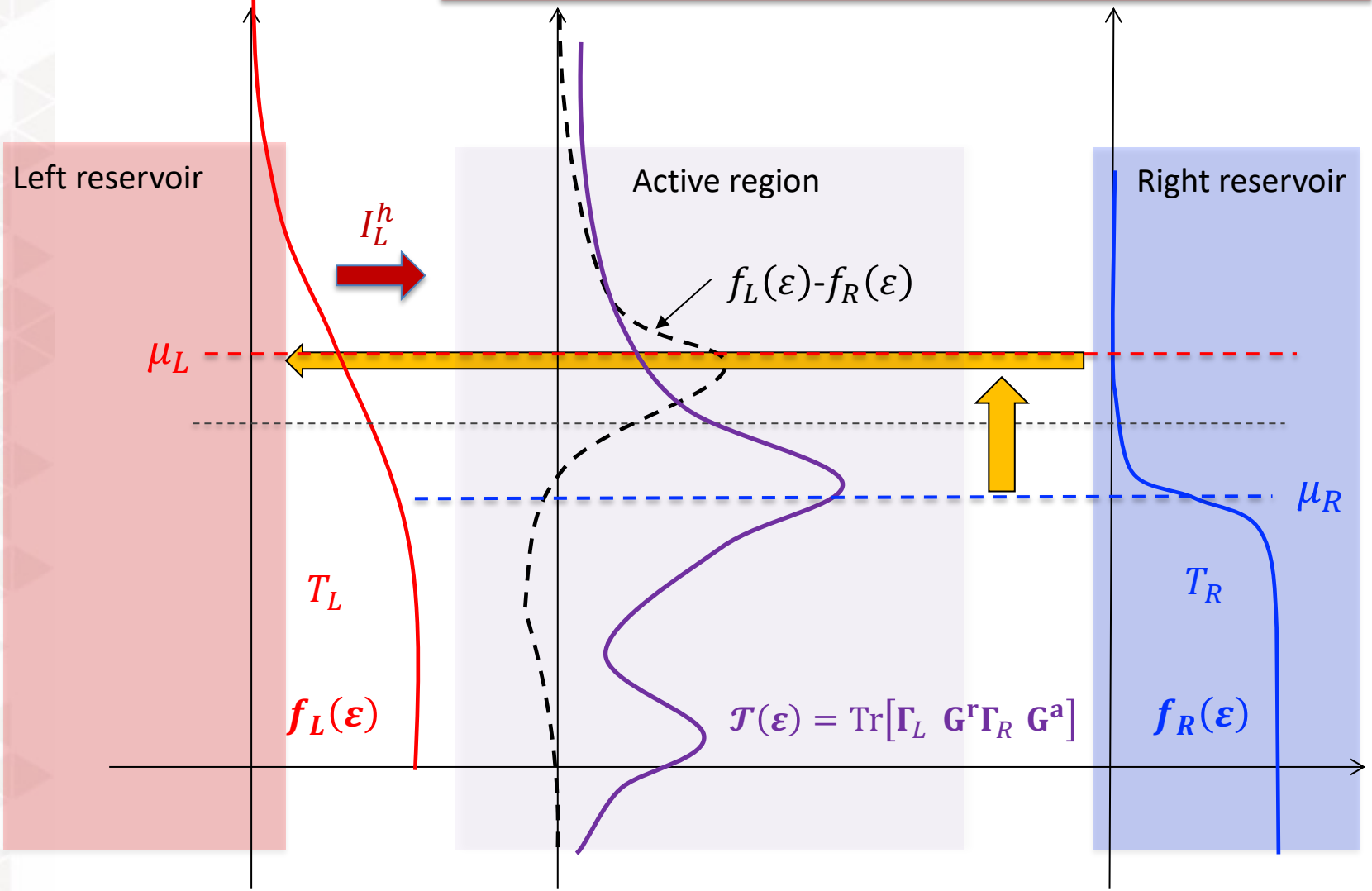
Energy current

$$I_L^E = \frac{2}{h}\int d\varepsilon\, \varepsilon \mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$



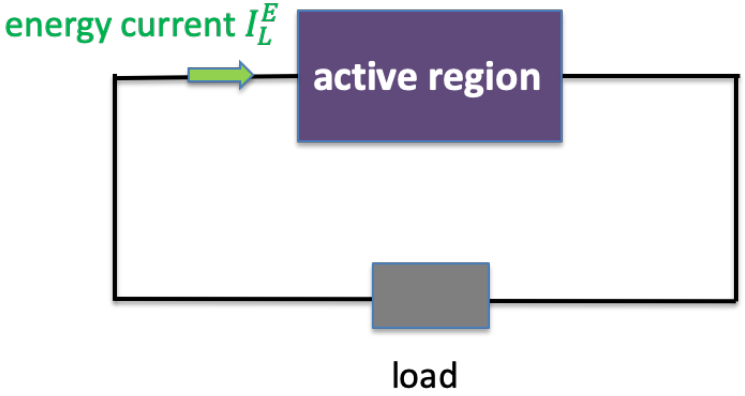
Heat current

$$I_L^h = \frac{2}{h}\int d\varepsilon\,[\varepsilon - \mu_L]\mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$



Energy & Heat currents in ballistic regime

Ballistic regime: *without interactions*



Observable I_L^E

$$I_L^E = -\left\langle \frac{dH_L}{dt} \right\rangle$$

Energy current

$$I_L^E = \frac{2}{h}\int d\varepsilon\, \varepsilon \mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$

Heat current

$$I_L^h = \frac{2}{h}\int d\varepsilon\, [\varepsilon - \mu_L]\mathcal{T}(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)]$$

Quantum of thermal conductance $\kappa = \frac{\pi^2 {k_B}^2 T_L^2}{3h}$

Thermoelectric coefficents (linear response)

$$\begin{pmatrix} V \\ J \end{pmatrix} = \begin{pmatrix} G^{-1} & -S \\ \pi & \kappa \end{pmatrix} \begin{pmatrix} I \\ \Delta T \end{pmatrix}$$

I particle current
J heat current

G electrical conductance
S Seebeck coefficient (or thermopower)
π *Peltier coefficient*
κ *thermal conductance*

Onsager relation: $\pi = ST_0$
Figure of merit: $ZT_0 = S\pi G/\kappa$

Relation to NOISE

$$ZT_0 = \frac{S_{IJ}^2}{S_{II}\,S_{JJ} - S_{JJ}^2}$$

S_{IJ} *current-current particle I or heat J correlations* $\langle I(t)J(t')\rangle$

J. Phys.: Condens. Matter **27** (2015) 015302

Energy issues @nanoscale

Challenges for energy

Thermodynamics in the quantum regime

- Definition of energy, heat, temperature, potentials
- Heat and laws of thermodynamics

Energy current operator

Discrete nanocircuit model

Lattice Hamiltonian (non-interacting)

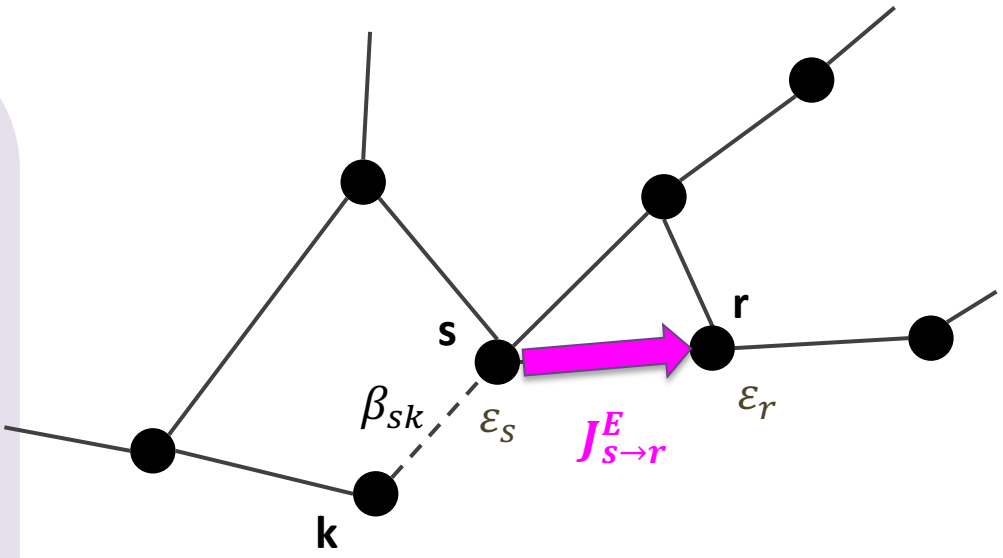
$$H_{tot} = \sum_s h_s^0 + \sum_{\langle i,s \rangle} V(s,i)$$

$$h_s^0 = \varepsilon_s n_s$$

$$V(s,i) = \beta_{si} a_s^+ a_i + h.c.$$

β_{si} is the coupling parameter

$a_s^+ (a_i)$ is the creation (annihilation) operator at site *s(i)*



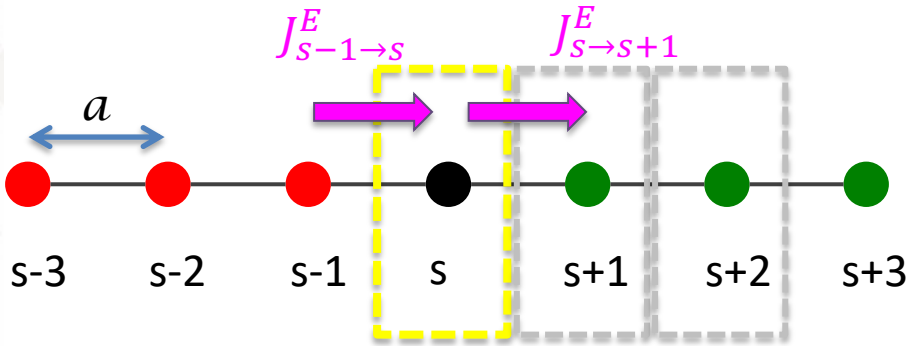
*We want to define the energy current operator in the **general** discrete ballistic case*

1D problem [Wu and Segal 2009, J. Phys. A: Math Theor. 42]

Energy current operator

As for the charge current operator [Caroli et al. 1971, J. Phys. C: Solid State Phys. 4…]

We want to calculate $J_s^E \Leftarrow \dot{h}_s + \mathrm{div} J_s^E = \partial_t h_s$ *continuity equation*



$$\mathrm{div} J_s^E = \frac{J_{s\to s+1}^E - J_{s-1\to s}^E}{a}$$

Energy current operator

As for the charge current operator [Caroli et al. 1971, J. Phys. C: Solid State Phys. 4…]

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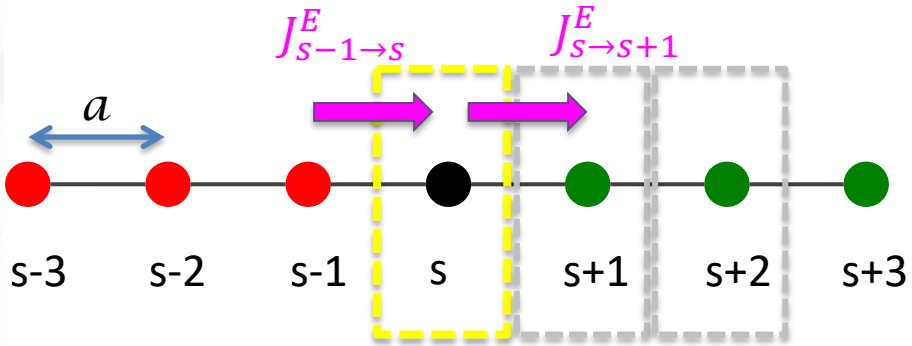

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The problem is the sub-system definition

In contrast with

$N = \sum_s n_s$

↓

charge current

$H = \sum_s h_s^0 + \sum_{\langle i,s\rangle} V(s,i)$

$H = \sum_s h_s$

$$h_s = h_s^0 + \frac{1}{2}\sum_{\langle i,s\rangle} V(s,i)$$

Energy current

We define the **energy current operator** in the general (3D) discrete case

$$J^E_{s\to r} = \frac{a_{is}}{i\hbar}[h_r, h_s]$$

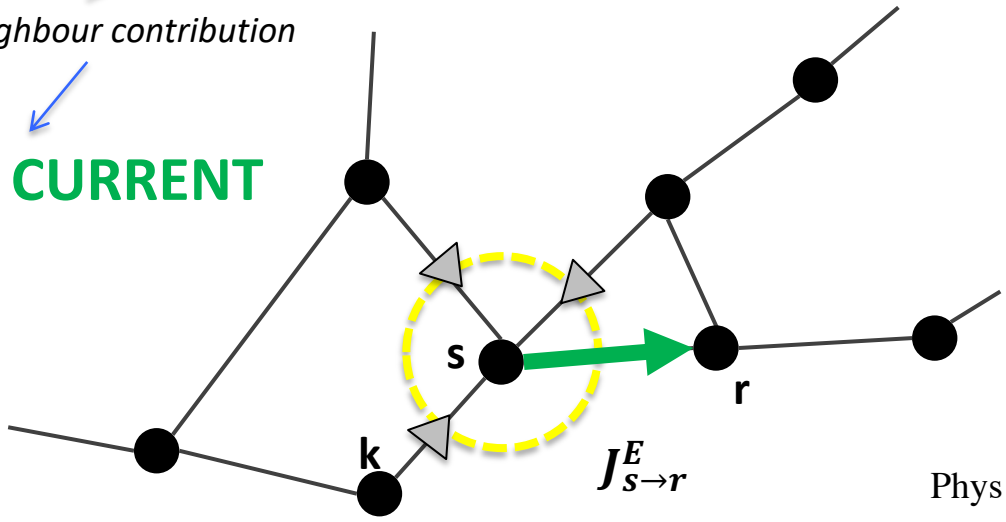
- ❑ Exchange symmetry $J^E_{s\to r} = -J^E_{r\to s}$
- ❑ Energy conservation law

➔ We deduce the **energy current** in terms of NEGFs **G**

$$< \mathbf{j^E_{s\to r}} > (\mathbf{t}) = \frac{1}{\hbar}\mathrm{Im}\left[\frac{\epsilon_s + \epsilon_r}{2}\beta_{rs}\mathbf{G^<_{rs}}(\mathbf{t},\mathbf{t}) + \frac{1}{4}\sum_k \beta_{rs}\beta_{sk}\mathbf{G^<_{kr}}(\mathbf{t},\mathbf{t}) + \beta_{kr}\beta_{rs}\mathbf{G^<_{sk}}(\mathbf{t},\mathbf{t}) + \beta_{rk}\beta_{ks}\mathbf{G^<_{sr}}(\mathbf{t},\mathbf{t})\right]$$

first-neighbour contribution

particle CURRENT



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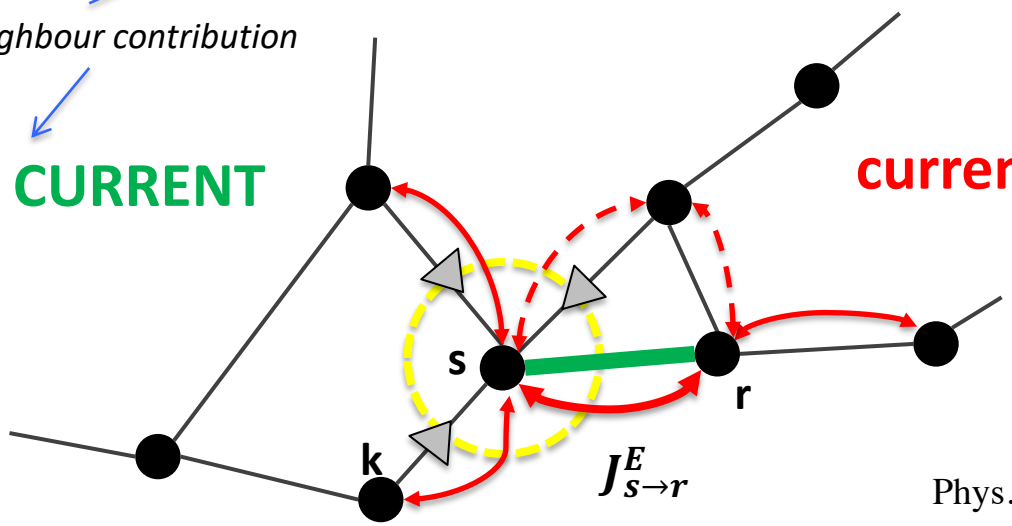
first-neighbour contribution

second-neighbour contributions

particle CURRENT

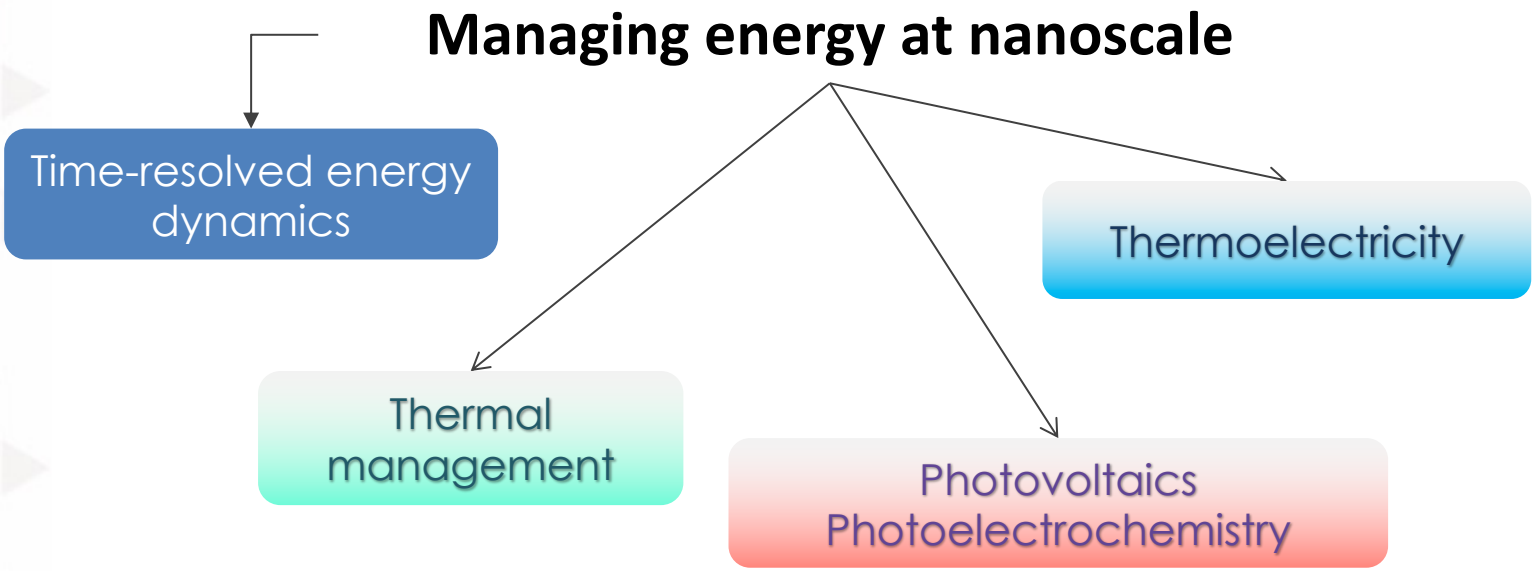
current CORRELATIONS

$\langle J_{s\to r}(t) J_{r\to k}(t)\rangle$

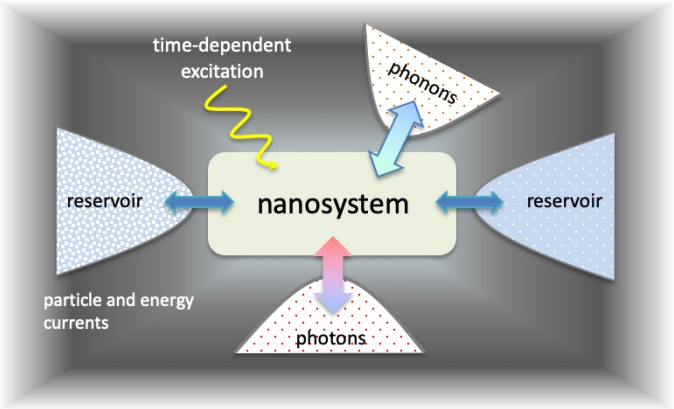


Quantum electron transport

FOR WHAT ?



Main messages



- When the system size is lower than the mean free path, semi-classical approaches are no longer valid
  Quantum transport is needed
- Non-equilibrium Green's functions currently form a powerful and flexible method for quantum transport modelling & simulations
- Without interaction, the framework simplifies into the meaningful Landauer formalism
- At the nanoscale, energy transport is still not completly elaborated