ECE 656: Electronic Transport in Semiconductors Fall 2017

Transport in Devices: the ballistic BTE

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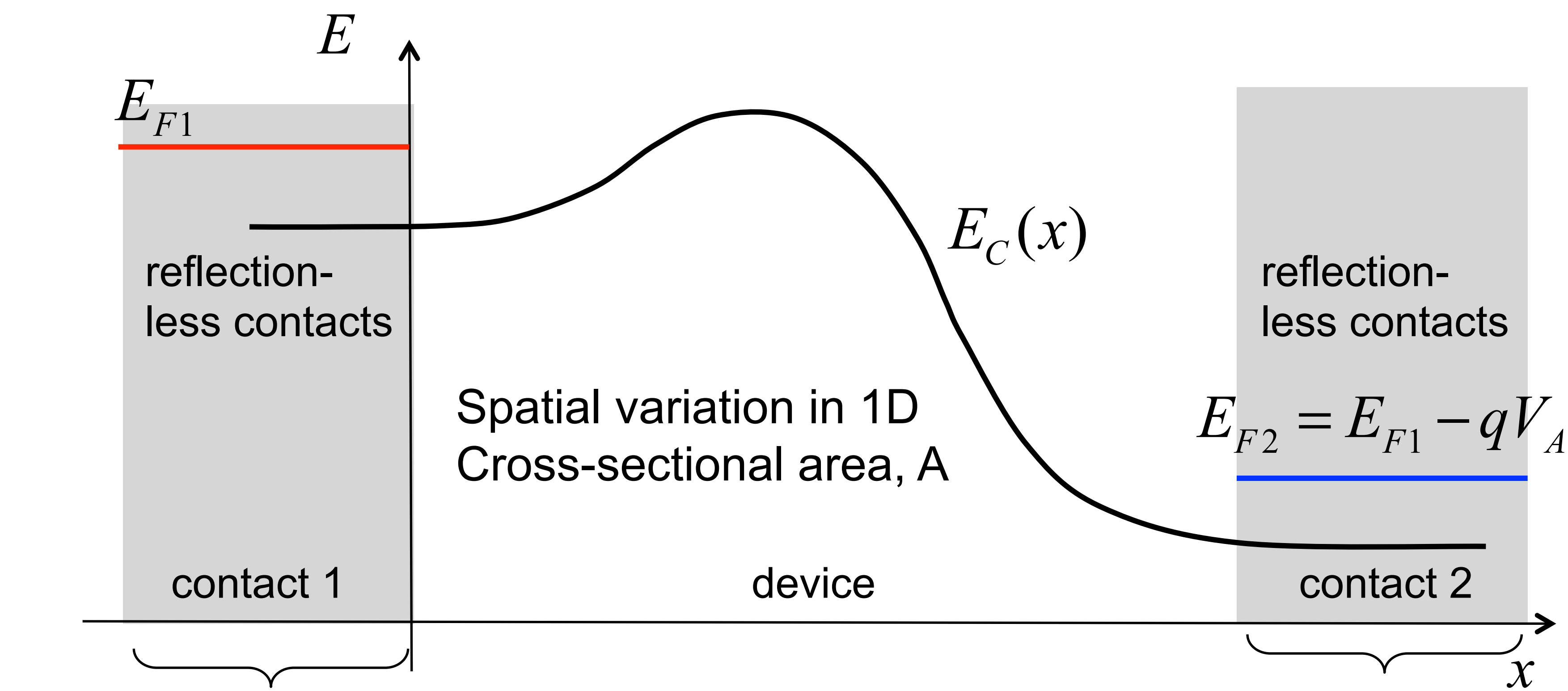
Goal: Solve the BTE for a ballistic device



thermal equilibrium reservoir

ballistic

thermal equilibrium reservoir

$f(\vec{r},\vec{p},t) = f(E) = f_0(E_{F1})$

$f(E) \neq f_0(E)$

$f(\vec{r},\vec{p},t) = f(E) = f_0(E_{F2})$

Outline

1) Goal
2) **General solution**
3) Boundary conditions
4**)** Example solution
5) Discussion
6) Summary

BTE

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f$$

$\hat{C} f = 0$ in two cases:

-equilibrium - - - - - - - - > $f_0 = \dfrac{1}{1 + e^{(E - E_F)/k_B T}}$

-ballistic transport - - - - - - - - > $f(\vec{r}, \vec{p}, t) = ?$

BTE with Cf = 0

$$\vec{\upsilon} \bullet \nabla_r f_0 + \vec{F}_e \bullet \nabla_p f_0 = 0$$

assume:

$$f_0 = g\left(E_{TOT}\right) = g\left[E_C(\vec{r}) + E(\vec{k})\right]$$

$$\vec{\upsilon} \bullet \frac{dg}{dE_{TOT}} \nabla_r E_{TOT} + \vec{F}_e \bullet \frac{dg}{dE_{TOT}} \nabla_p E_{TOT} = 0$$

$$\vec{\upsilon} \bullet \nabla_r E_C(\vec{r}) + \vec{F}_e \bullet \nabla_p E(\vec{k}) = 0$$

$$\vec{\upsilon} \bullet \left(-\vec{F}_e\right) + \vec{F}_e \bullet \vec{\upsilon} = 0$$

Any function of total energy satisfies the equilibrium BTE!

And the ballistic BTE!!

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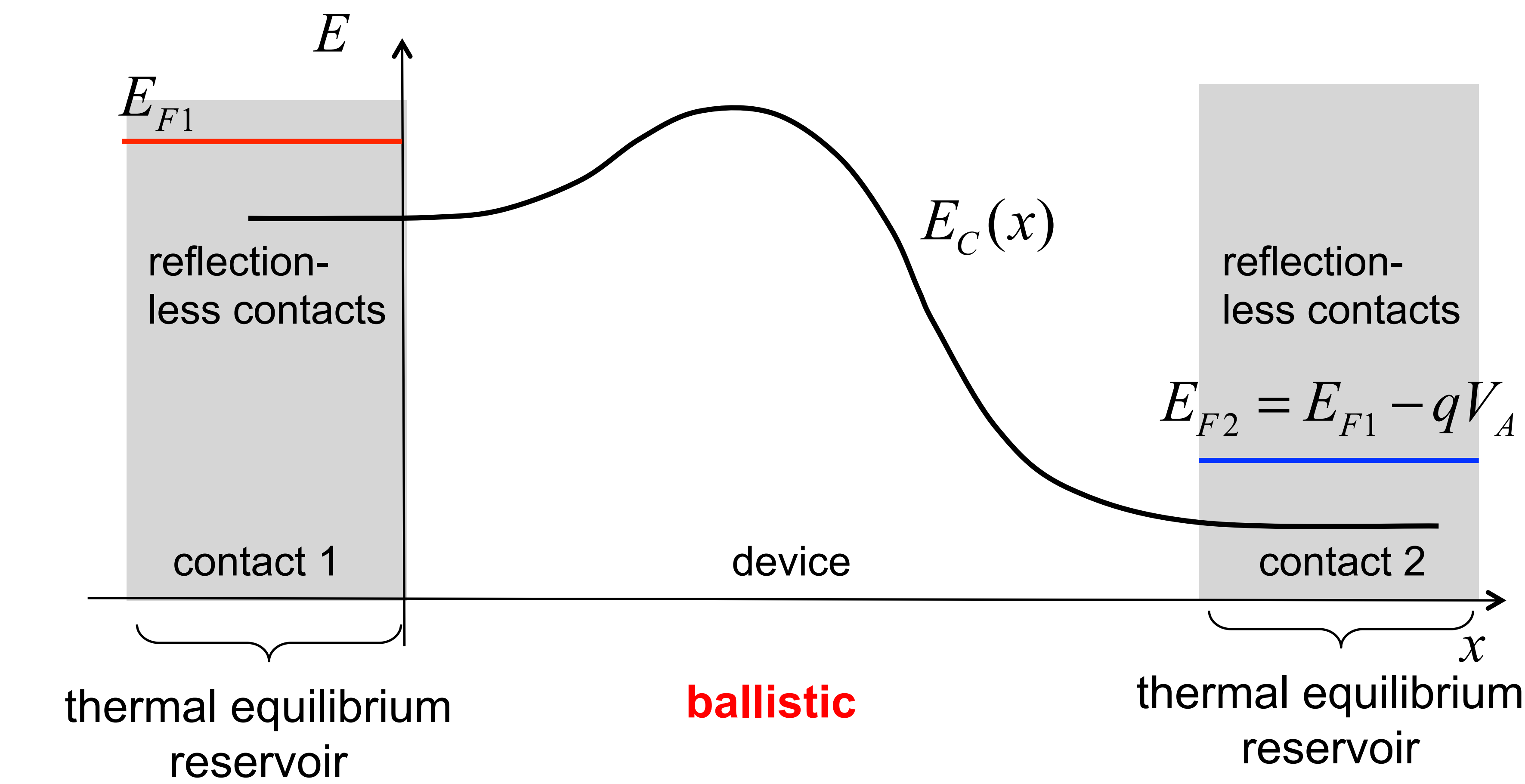
Goal: Solve the BTR for a 1D ballistic device



$$f(\vec{r}, \vec{p}, t) = f(E) = f_0(E_{F1})$$

$$f(E) \neq f_0(E)$$

$$f(\vec{r}, \vec{p}, t) = f(E) = f_0(E_{F2})$$

Solution for a ballistic device

Steady-state ballistic BTE:

$$\upsilon_x \frac{\partial f(x,p_x)}{\partial x} - q\mathcal{E}_x \frac{\partial f(x,p_x)}{\partial p_x} = 0$$

Solution:

$$f(x,p_x) = g\left(E\right) = g\left[E_C(x) + E(k_x)\right]$$

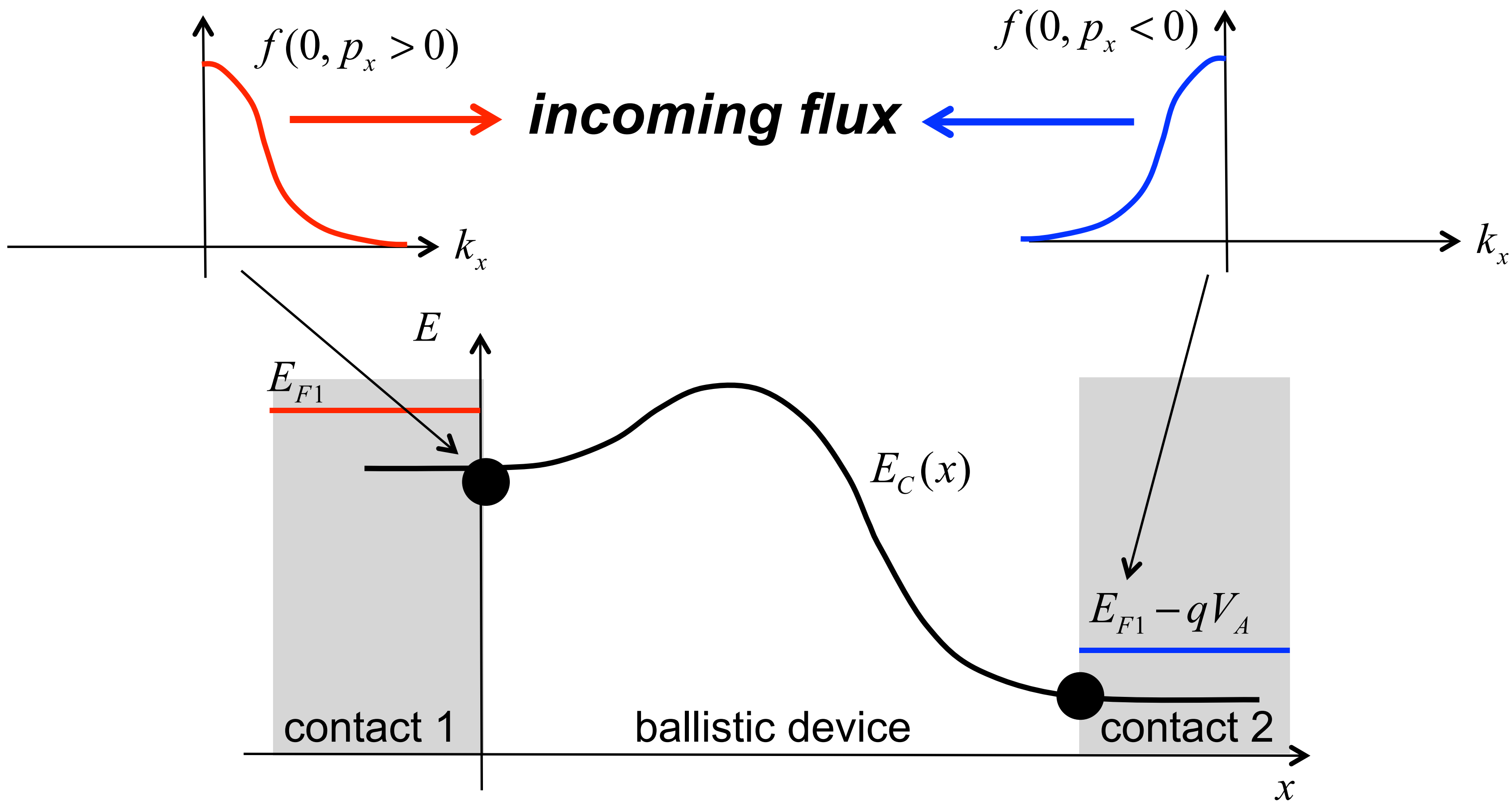
Boundary conditions:

First-order equation in space --> one boundary condition, but we have two contacts!

Boundary conditions

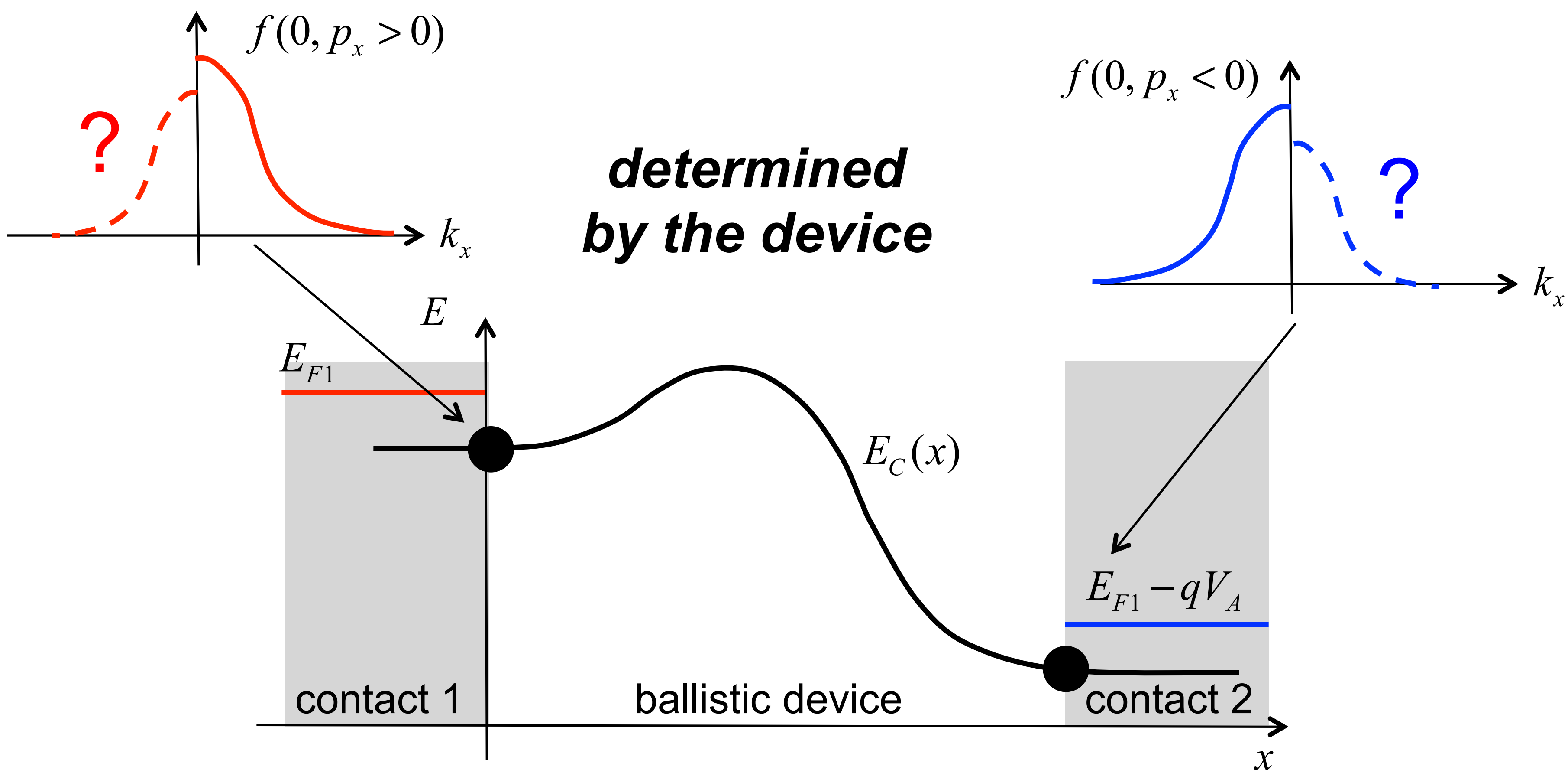
Solution:

Apply one-half of the boundary condition to each contact.

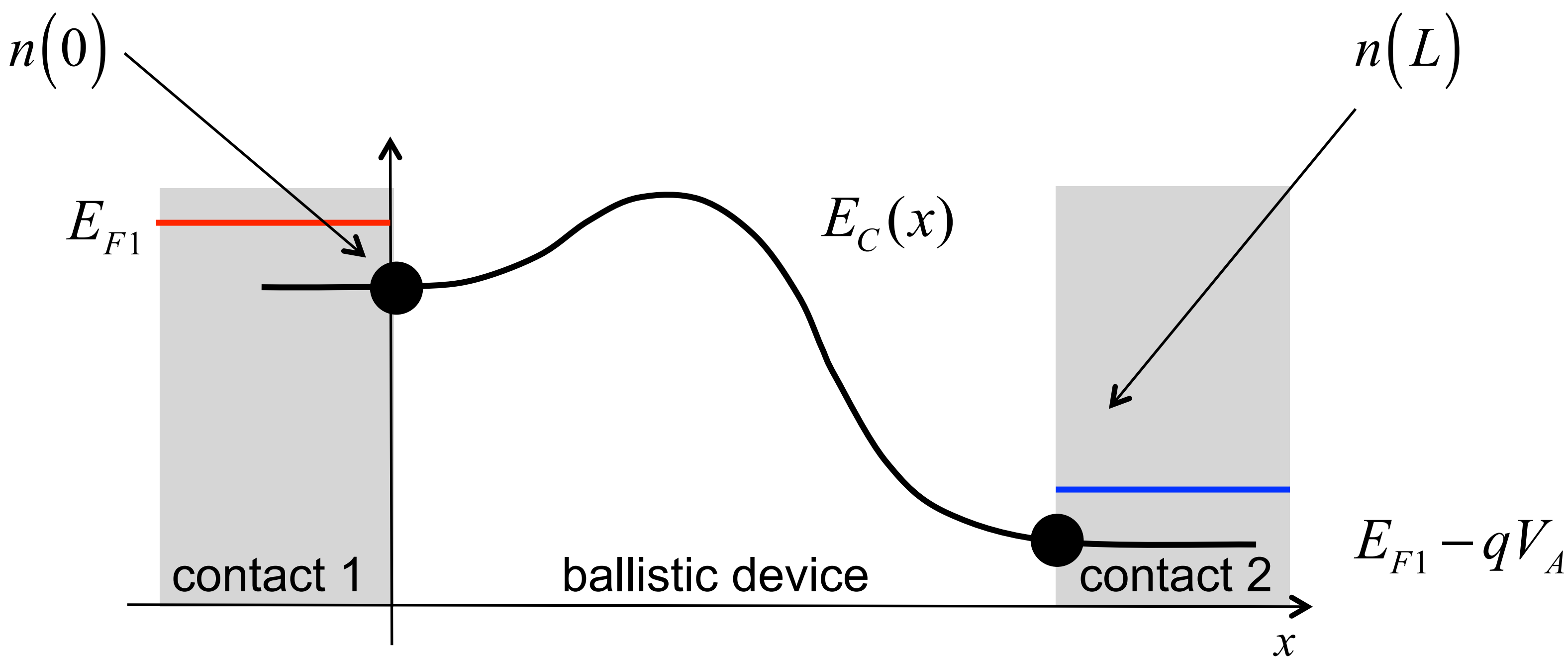


Boundary conditions for the BTE

What about the exiting flux?



Carrier densities at the contacts



$$n(0) = \frac{1}{\Omega}\sum_{\vec{p}} f(x=0,\vec{p}) \qquad n(L) = \frac{1}{\Omega}\sum_{\vec{p}} f(x=0,\vec{p})$$

Specifying the carrier densities at both contacts is not correct, in general.

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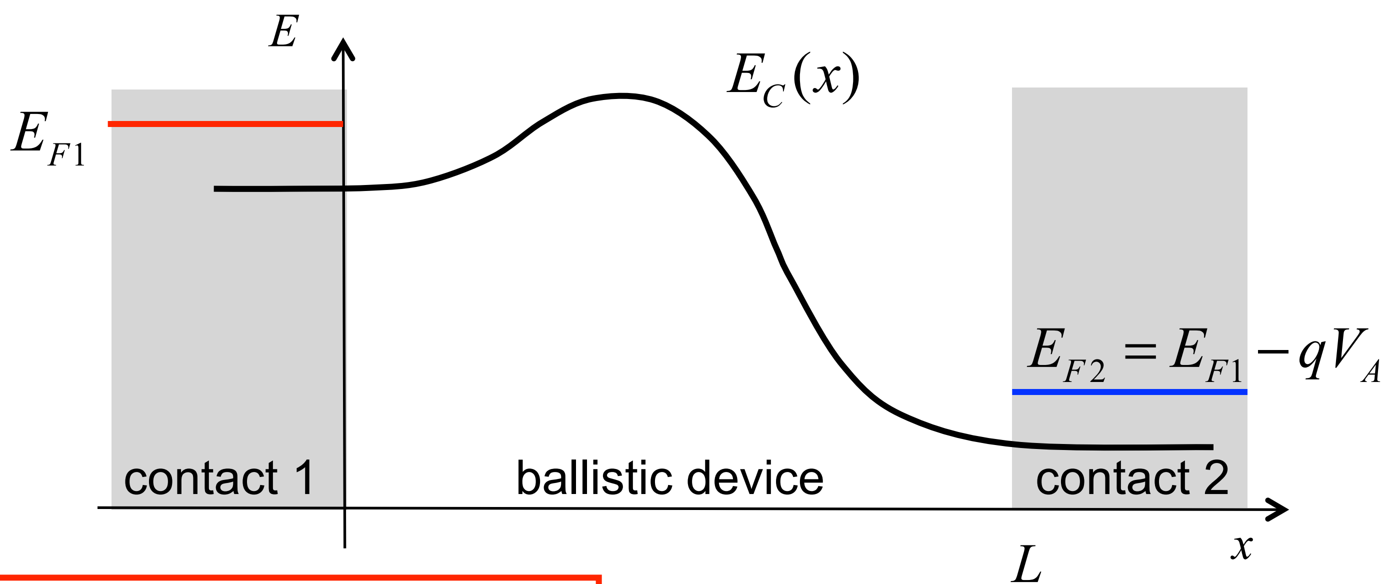
Solution to the s.s. ballistic BTE



$$\upsilon_x \frac{\partial f(x,p_x)}{\partial x} - q\mathcal{E}_x \frac{\partial f(x,p_x)}{\partial p_x} = 0$$

$$f(0, p_x > 0) = \frac{1}{1 + e^{(E - E_{F1})/k_B T}}$$

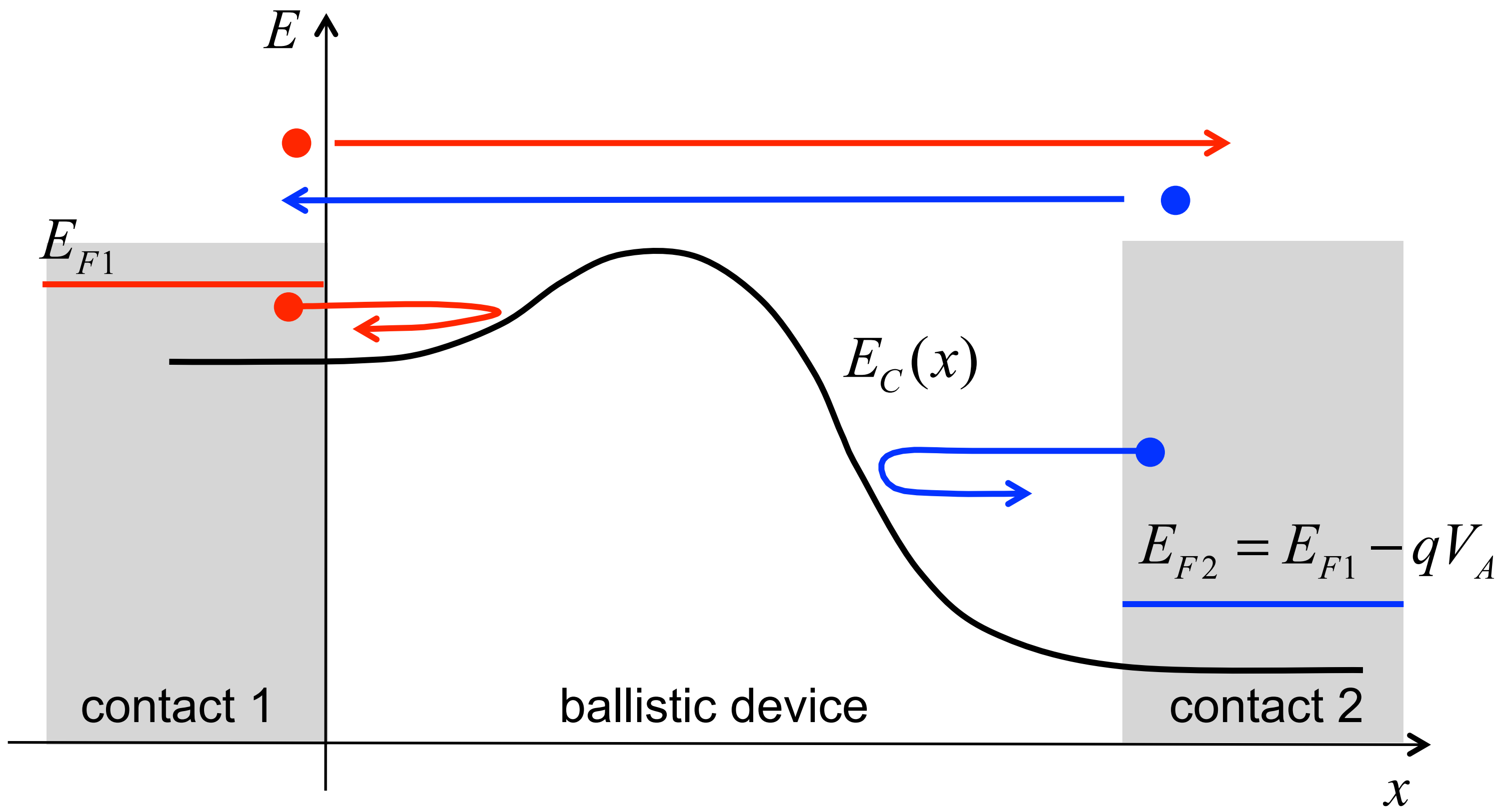
$$f(L, p_x < 0) = \frac{1}{1 + e^{(E - E_{F2})/k_B T}}$$

$$f(x,p_x) = g\left[E_C(x) + E(k_x)\right]$$

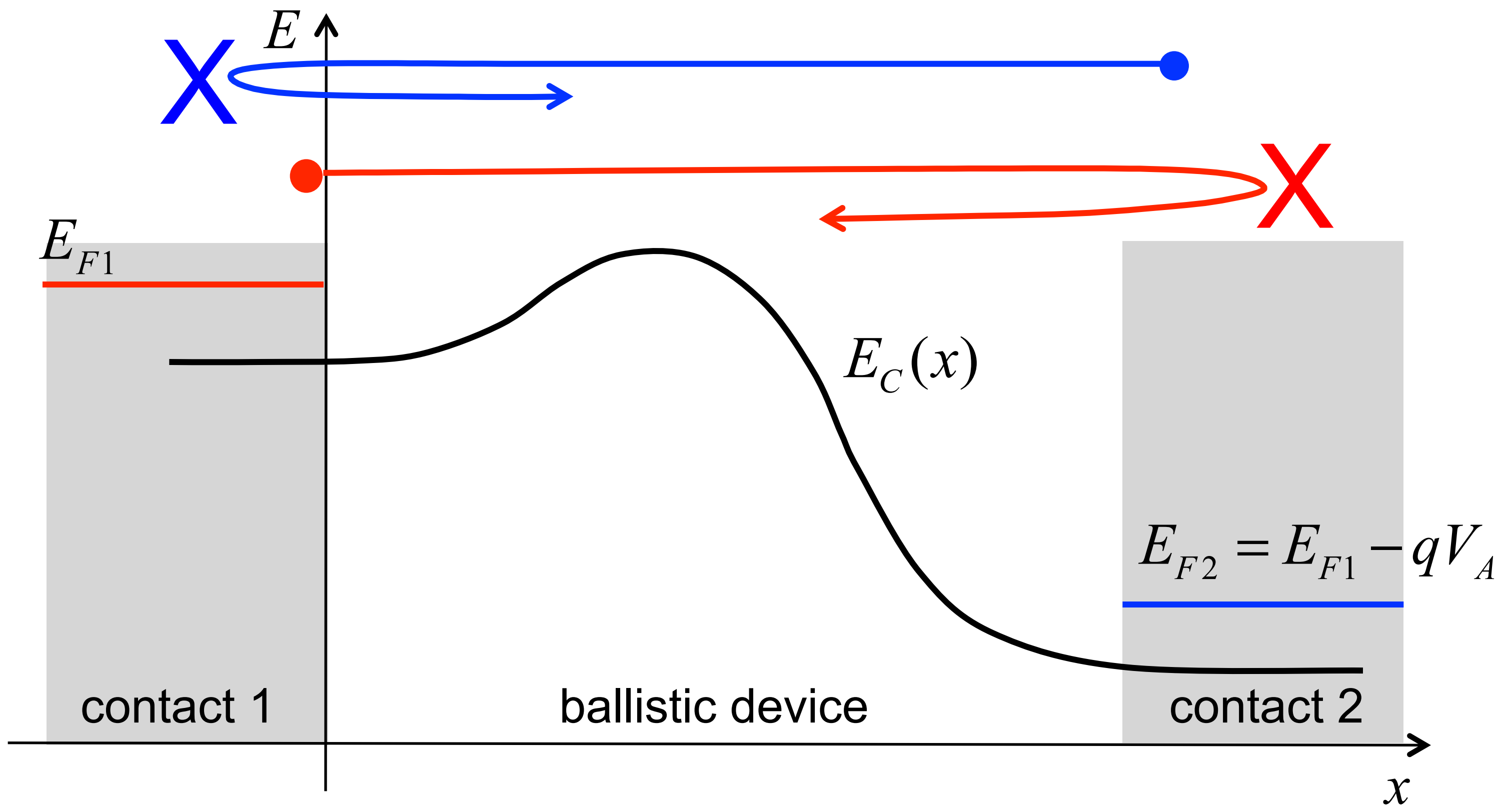
$$f(x,p_x) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$E_F = E_{F1} \text{ or } E_{F2}\,?$$

Follow trajectories in phase space



Importance of reflection-less contacts



"reflection-less"
or
"absorbing" contacts

"reflection-less"
or
"absorbing" contacts

To determine the appropriate Fermi level

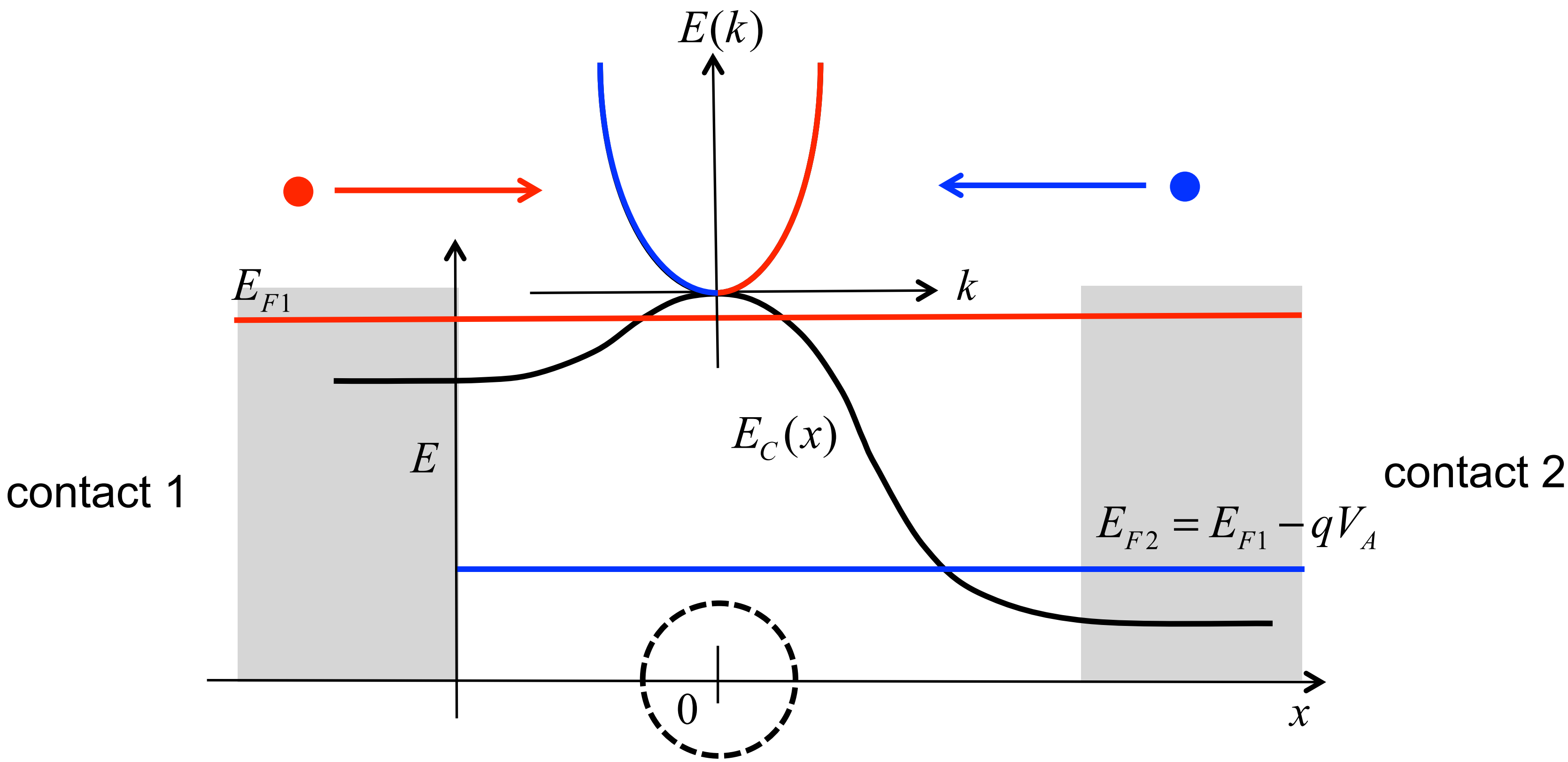
Within a ballistic device, the probability that a *k*-state is occupied is given by an equilibrium Fermi function.

For a given state at a given location, the Fermi level to use is the one from the contact that populated the *k*-state.

Within a ballistic device, each *k*-state is in **equilibrium** with one contact or the other.

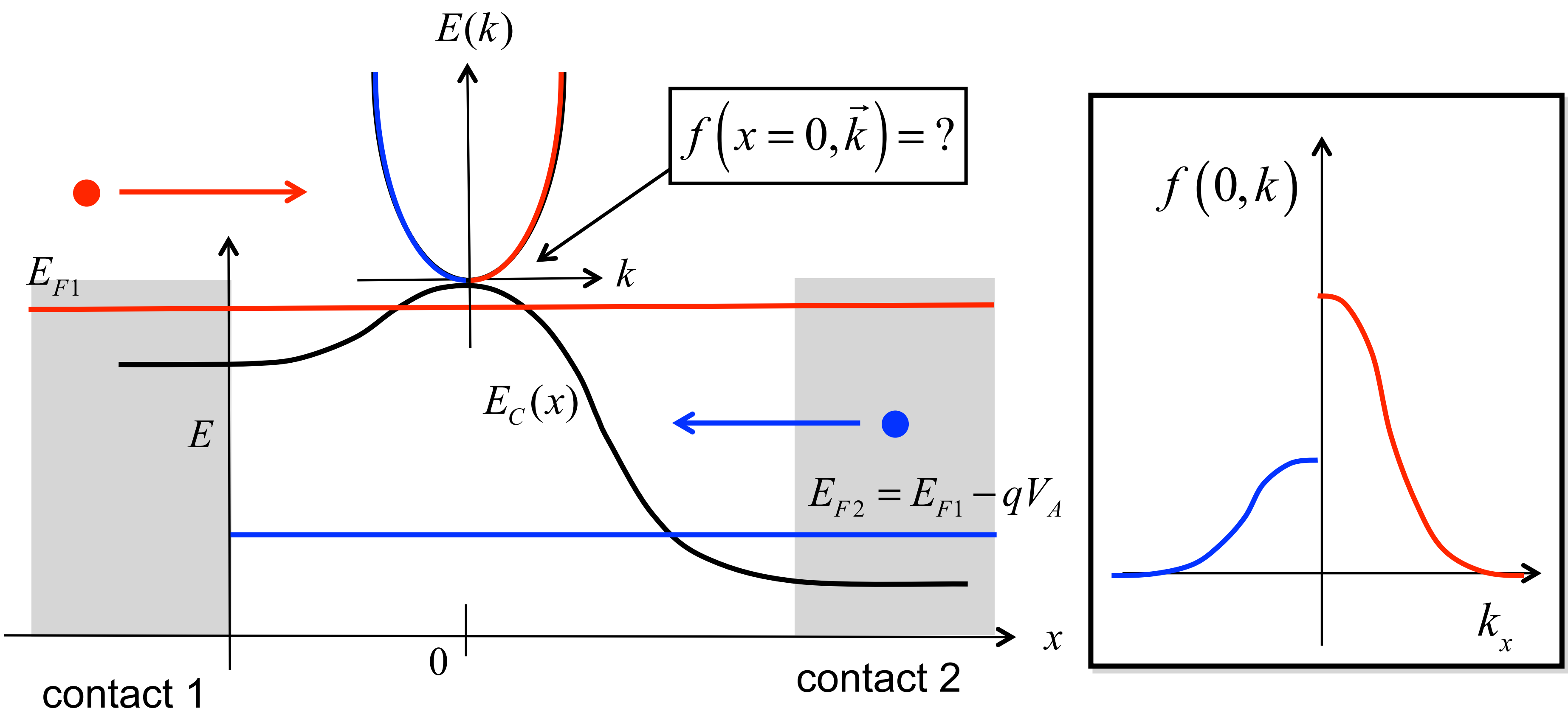
The overall distribution, however, is as far from equilibrium as it can be.

The solution at x = 0

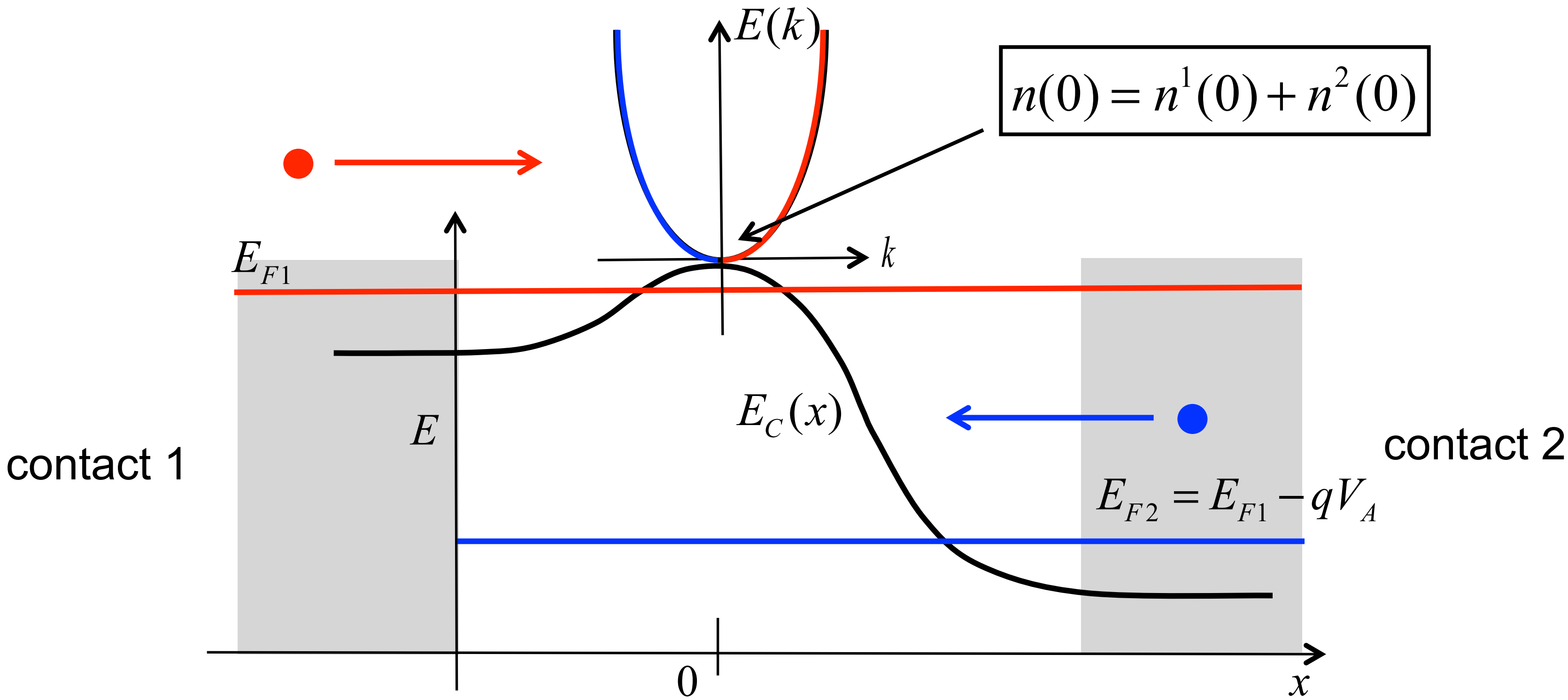


$$f\left(x=0,\vec{k}\right)=?$$

Distribution function



Carrier density



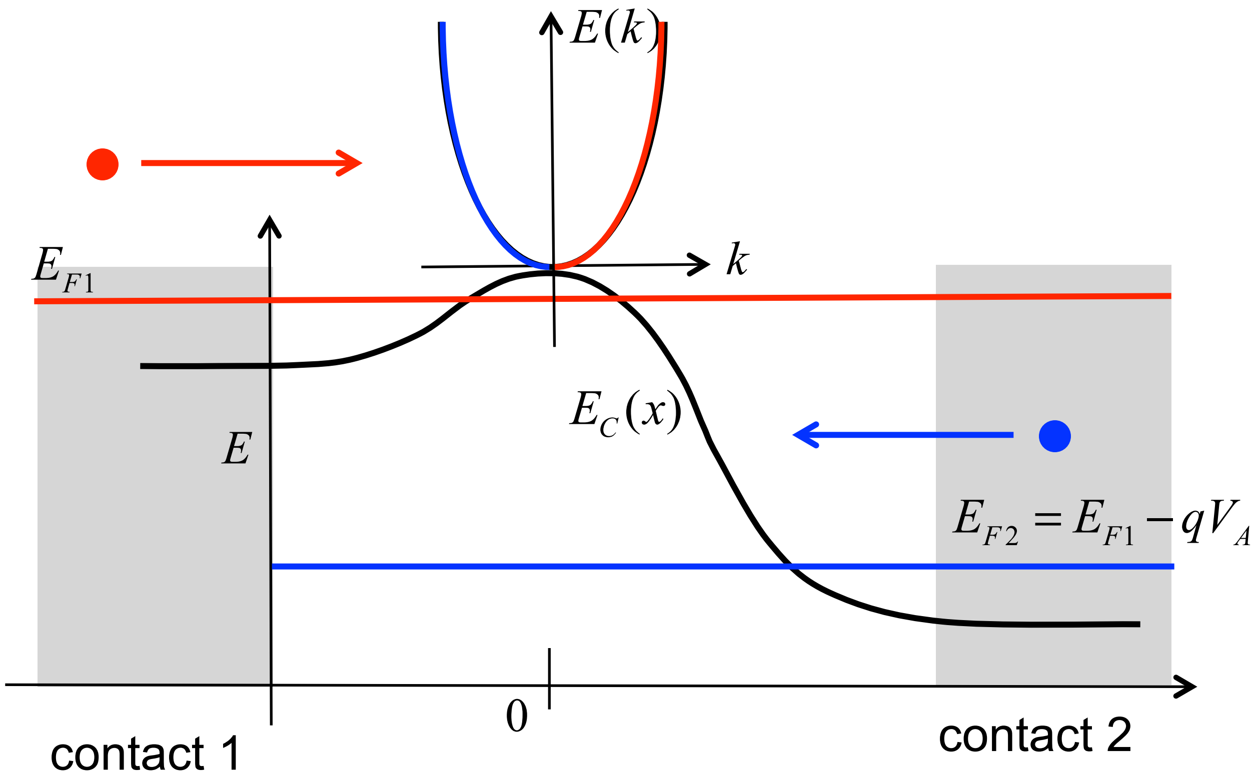
$$n^1\left(0\right) = n^+(0) = \frac{1}{\Omega}\sum_{k_x>0} f_0(E_{F1})$$

$$n^2(0) = n^-(0) = \frac{1}{\Omega}\sum_{k_x<0} f_0(E_{F2})$$

$$n(0) = \int D^1(0,E) f_0(E_{F1}) dE$$

$$n^2(0) = \int D^2(0,E) f_0(E_{F2}) dE$$

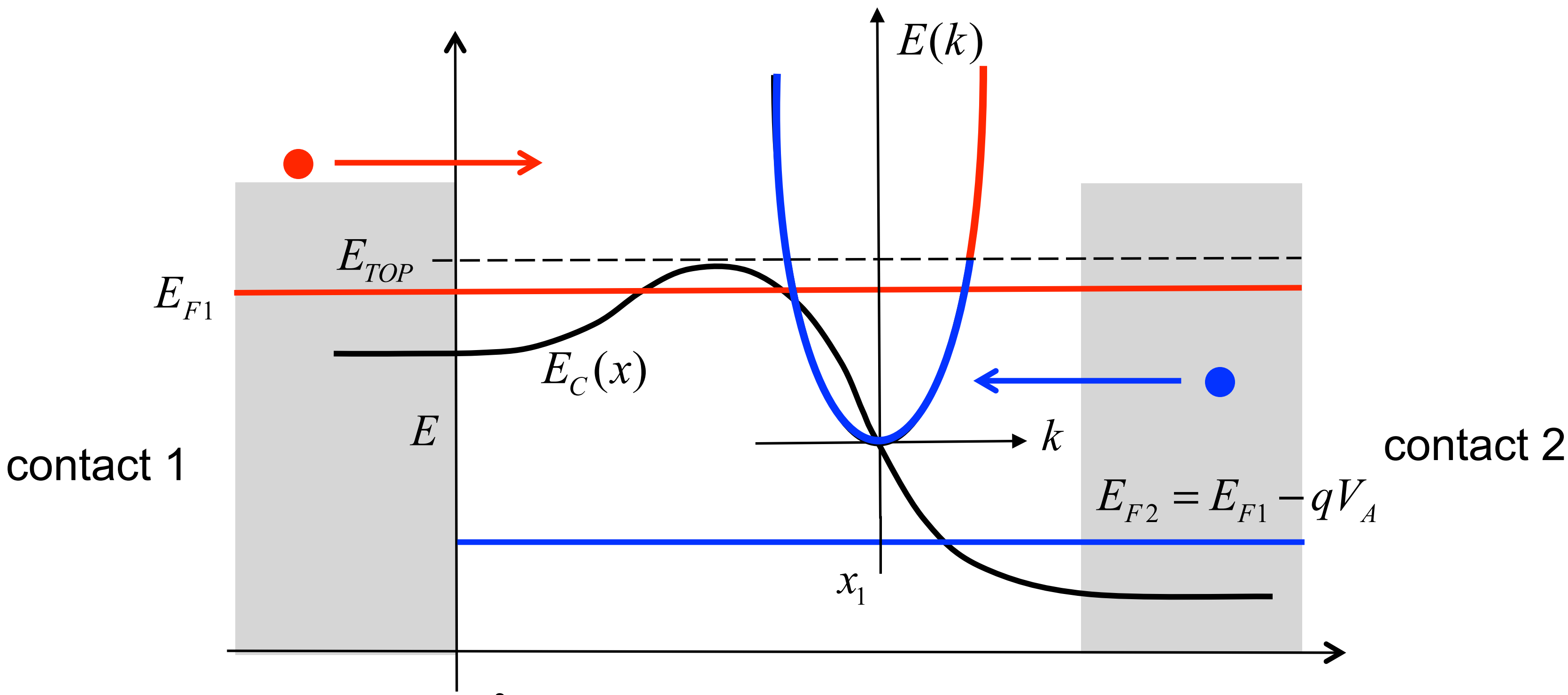
"Local density of states"



$$n(0) = \int D^1(0,E) f_0(E_{F1}) + D^2(0,E) f_0(E_{F2}) dE$$

$$D^1(0,E) = D^2(0,E) = D\ \ (E)/2$$

Solution for *x* > 0

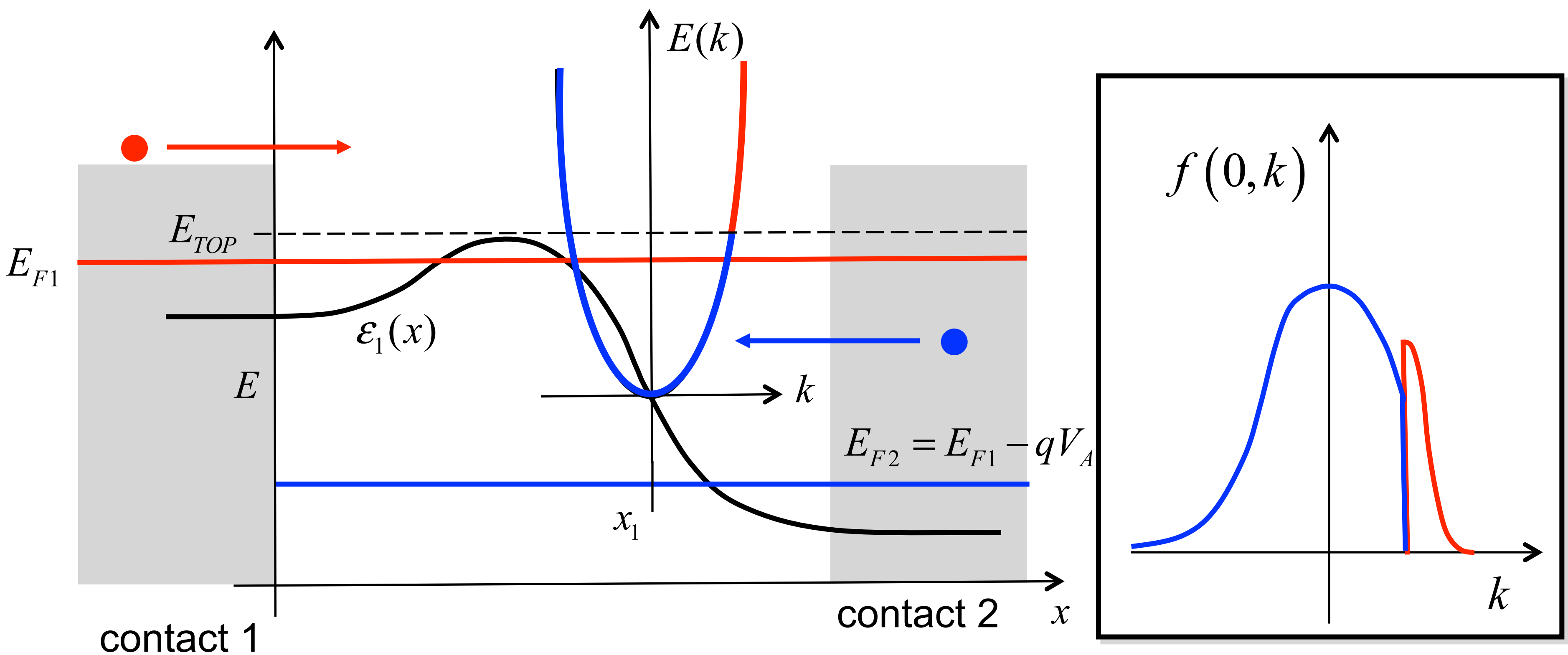


$$n(x_1) = \int D^1(x_1,E) f_0(E_{F1}) + D^2(x_1,E) f_0(E_{F2}) dE$$

"local density of states"

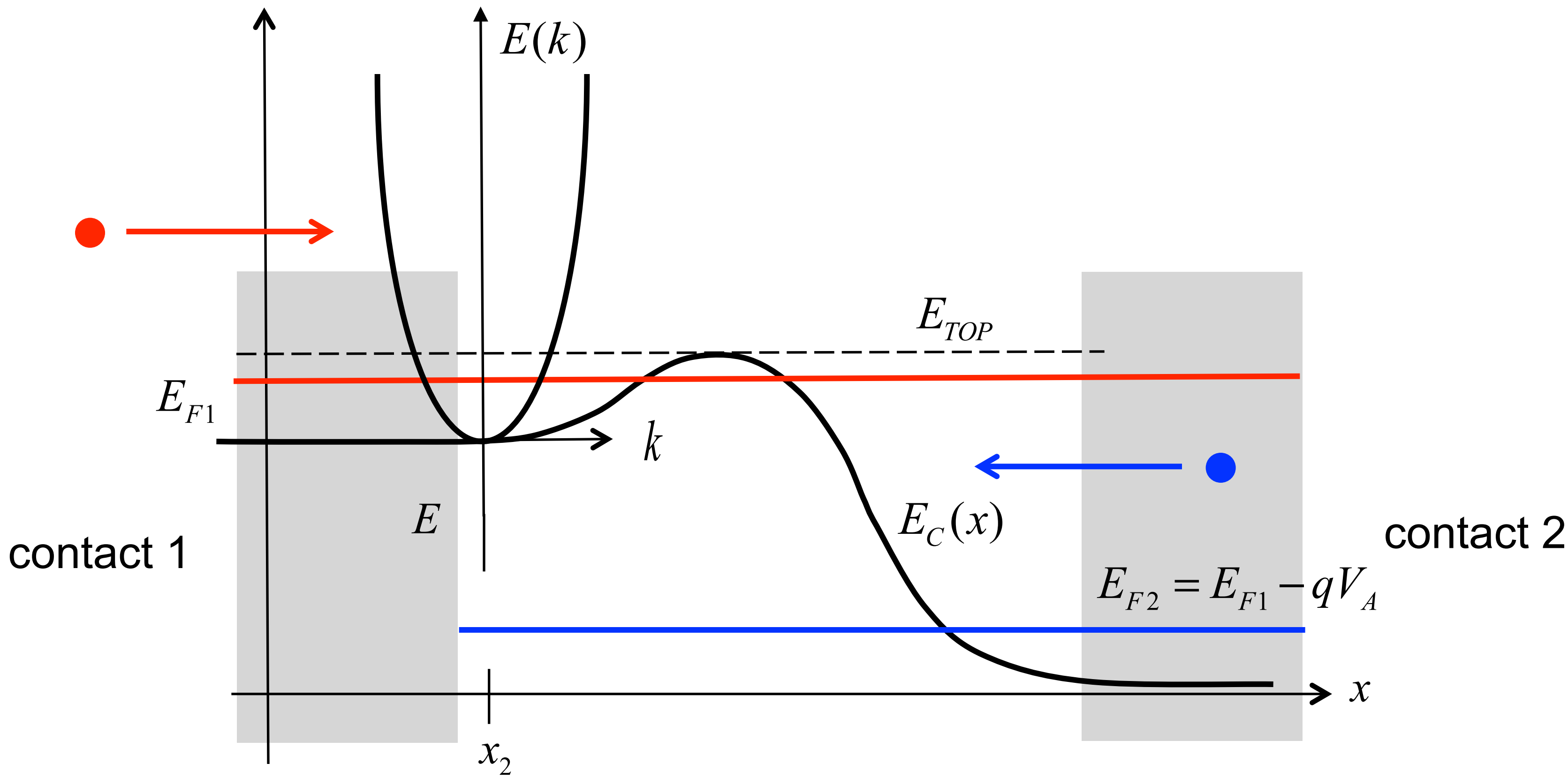
$$D^1(x_1,E), D^2(x_1,E) \neq D\ (E)/2$$

Distribution function

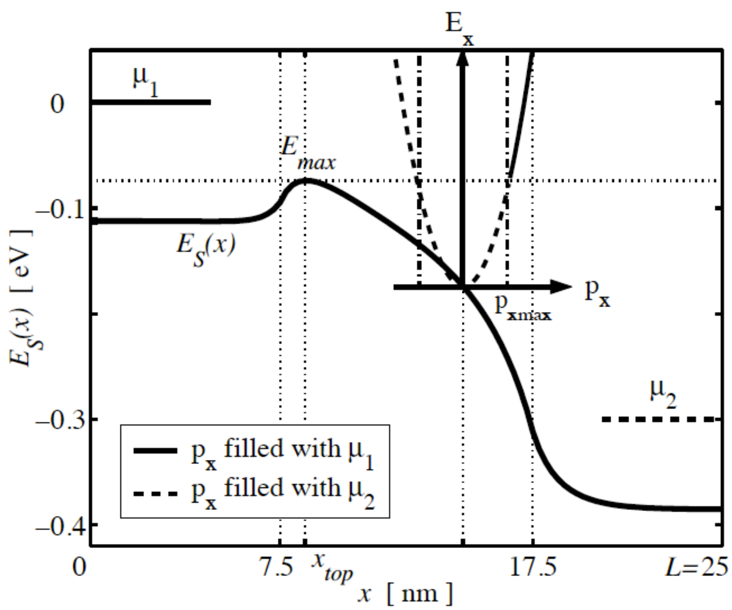


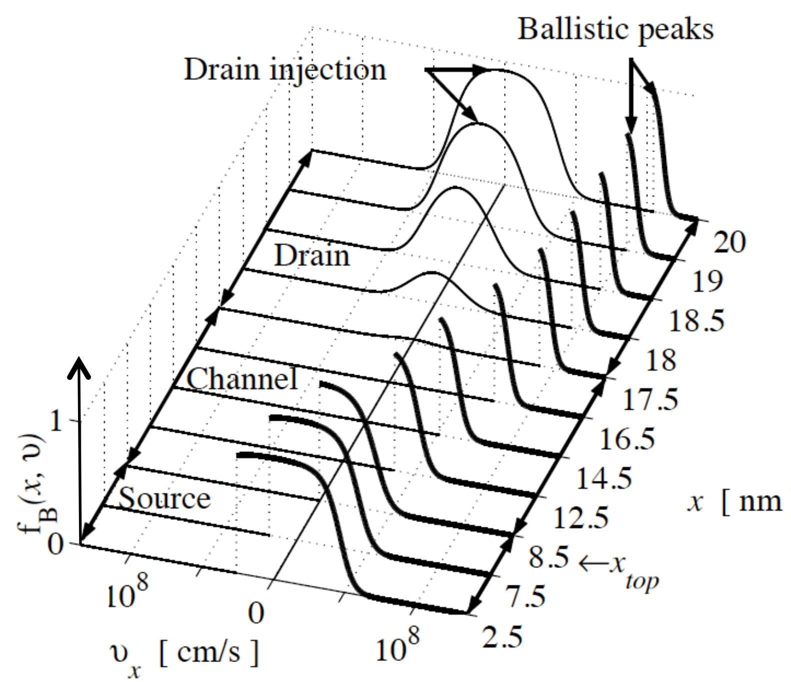
J.-H. Rhew, Zhibin Ren, and Mark Lundstrom, "A Numerical Study of Ballistic Transport in a Nanoscale MOSFET," Solid-State Electronics, **46**,1899, 2002.

Suggested exercise



Distribution function in side a ballistic MOSFET





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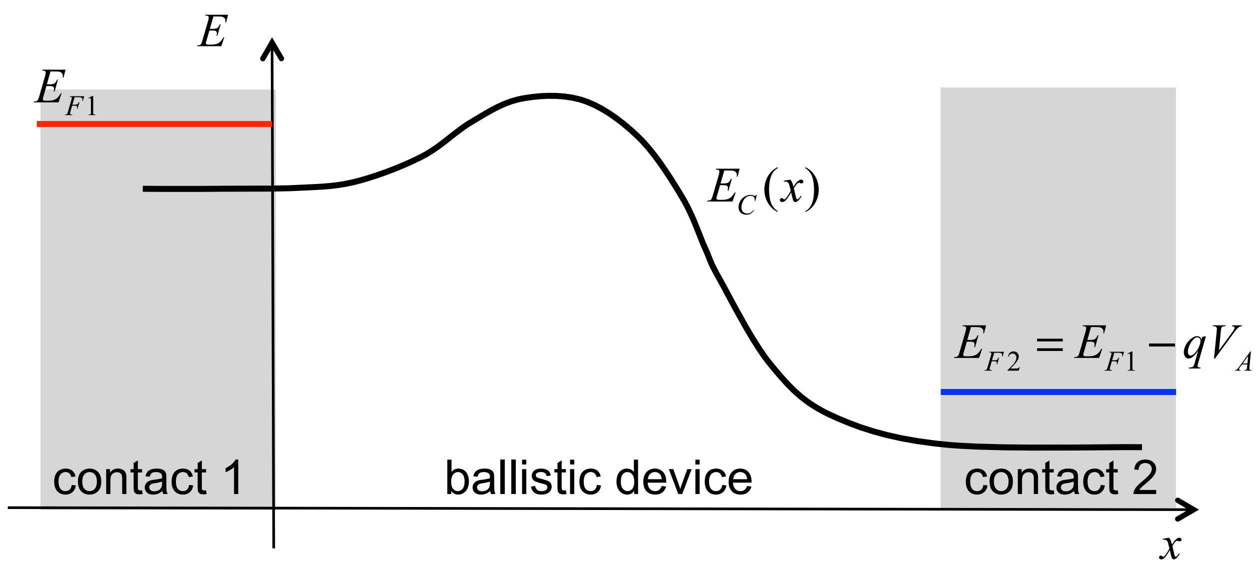
Solution to the ballistic BTE: summary

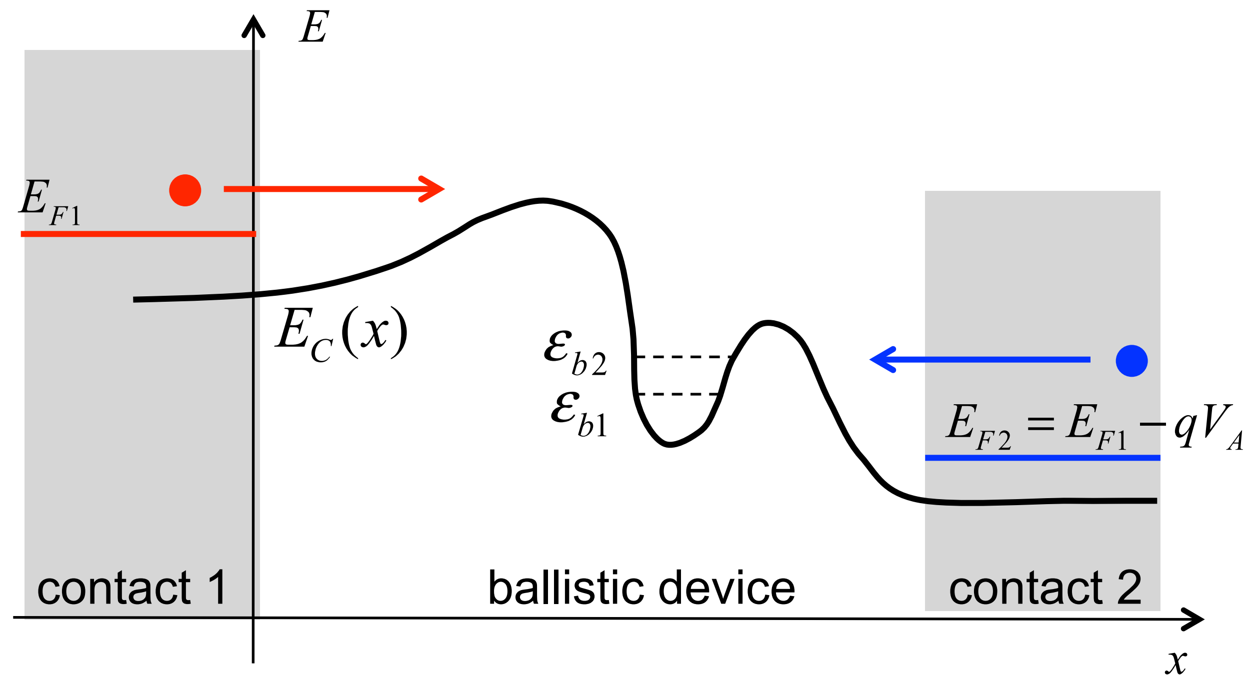


1) states divide into two parts, fillable by each of the contacts

$$n(x) = \int D^1(x,E) f_0(E_{F1}) + D^2(x,E) f_0(E_{F2}) dE$$

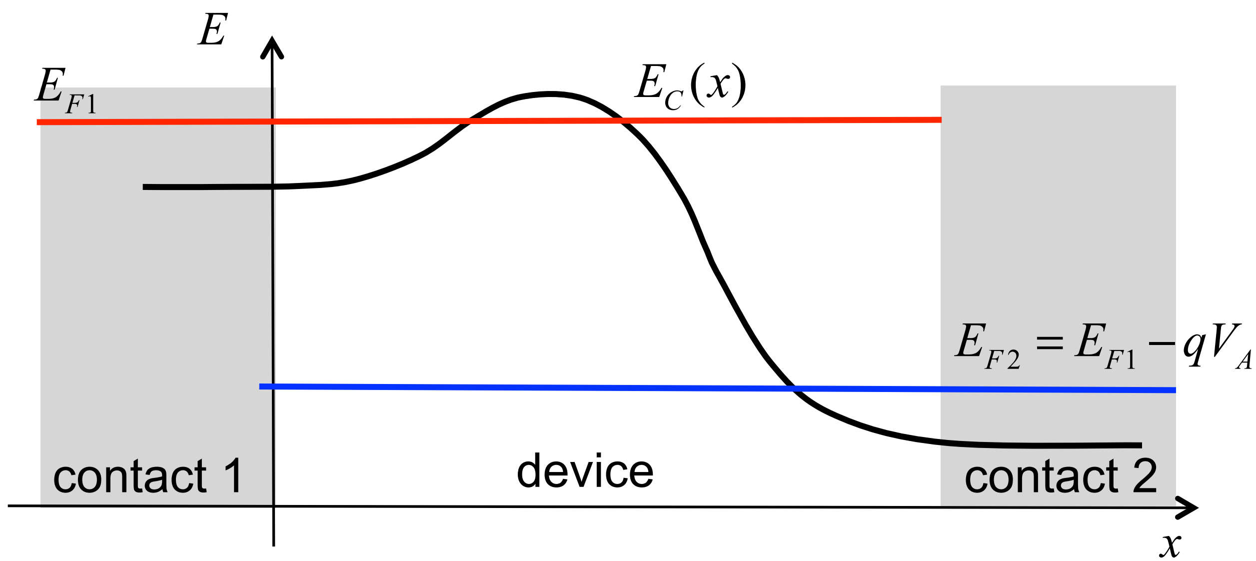
2) but….

The problem with bound states



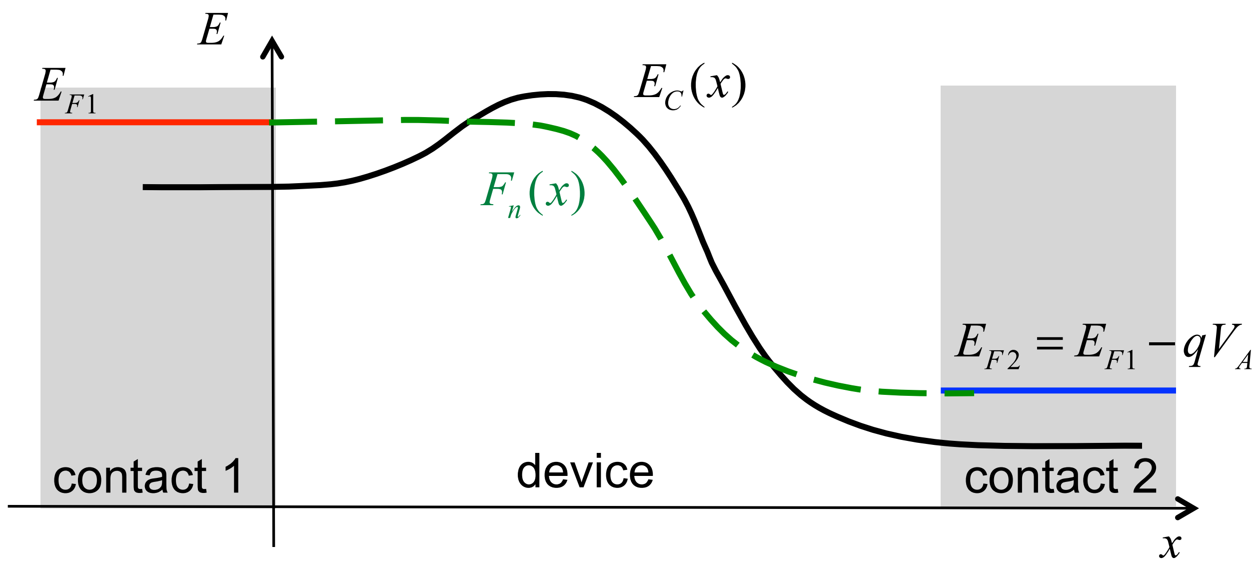
Bound states can occur.
They may be difficult (or impossible to fill from the contacts).
In practice, they could be filled by scattering.

Ballistic transport



Inside the devices, some states are occupied according to the Fermi level of the first contact and some according to the Fermi level of the second contact.

Diffusive transport



$$n(x) = \int D(x,E) f\left[F_n(x)\right] dE$$

$$f(x,E) = \frac{1}{1 + e^{\left[E - F_n(x)\right]/k_B T(x)}}$$

$$D(x,E) = \frac{m^* \sqrt{2m^*\left(E - E_C(x)\right)}}{\pi^2 \hbar^3}$$

References

For examples of how the use of correct boundary conditions can permit the use of diffusion equations in the ballistic and quasi-ballistic regime, see the following references for heat diffusion (e.g. Fourier's Law).

Jesse Maassen and Mark Lundstrom, "Steady-State Heat Transport: Ballistic-to-Diffusive with Fourier's Law," *J. Applied Phys*., **117**, 035104, 2015.

Jan Kaiser, Tianli Feng, Jesse Maassen, Xufeng Wang, Xiulin Ruan, and Mark Lundstrom, "Thermal Transport at the Nanoscale: A Fourier's Law vs. Phonon Boltzmann Equation Study," *J. Appl. Phys.*, **121**, 044302, 2017. DOI: 10.1063/1.4974872

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Summary

1) In a ballistic device, each k-state is occupied according to an equilibrium Fermi function.

2) For a particular k-state at a particular location, the Fermi level to use is the Fermi level of the contact from which the k-state was occupied.

3) Each k-state is in equilibrium with one of the contacts, but the overall distribution is a far from equilibrium as possible.

4) The local density-of-states consists of distinct components fillable by one of the contacts.

5) Extensions to 2D and 3D are more difficult.

Questions

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2) General solution
3) Boundary conditions
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