# ECE-656: Fall 2011

# Lecture 29:

# The BTE Revisited:
equilibrium and ballistic

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# outline

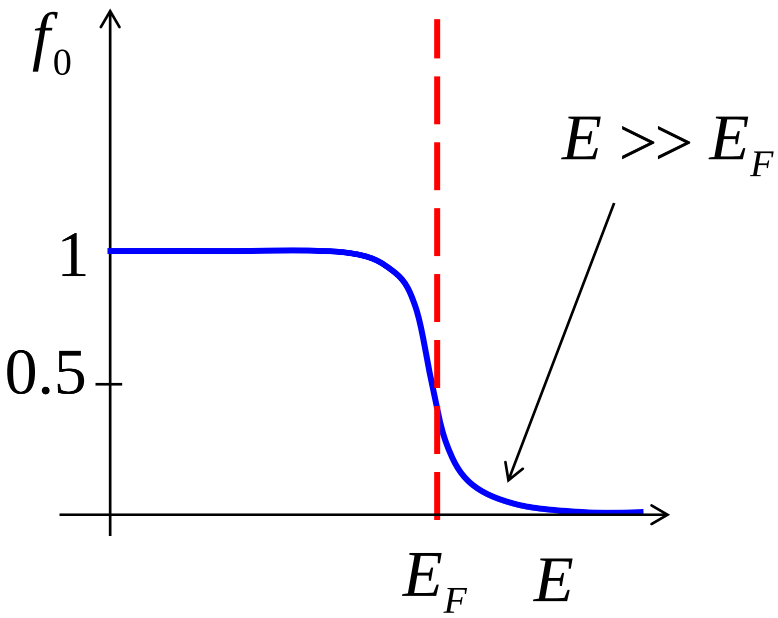
1) **Quick review**
2) Equilibrium BTE
3) Ballistic BTE
4) Discussion
5) Summary

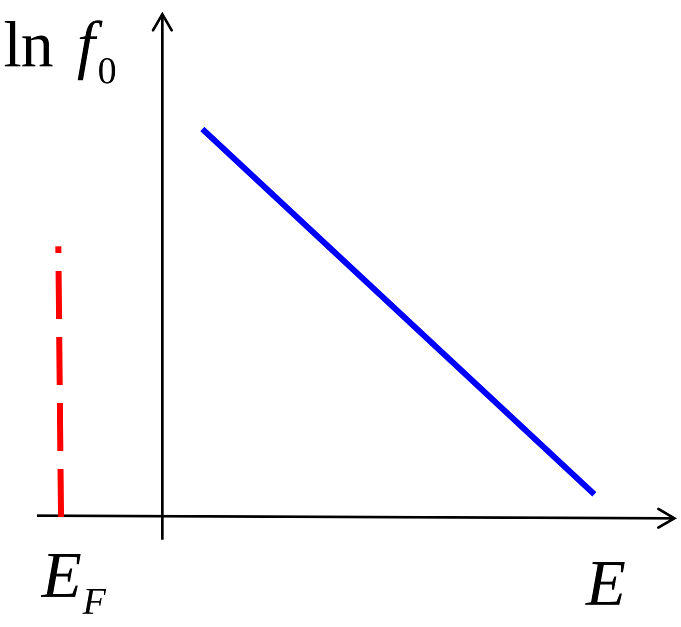
(Reference: Chapter 3, Lundstrom, FCT)

# equilibrium distribution function

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T_L}}$$

$$f_0 \approx e^{-(E - E_F)/k_B T_L} << 1$$




(nondegenerate)

# chemical potential and Fermi level

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T_L}}$$

We will use $E_F$

$$f_0 = \frac{1}{1 + e^{(E - \mu)/k_B T_L}}$$

$\mu$ is the chemical (or electrochemical) potential.

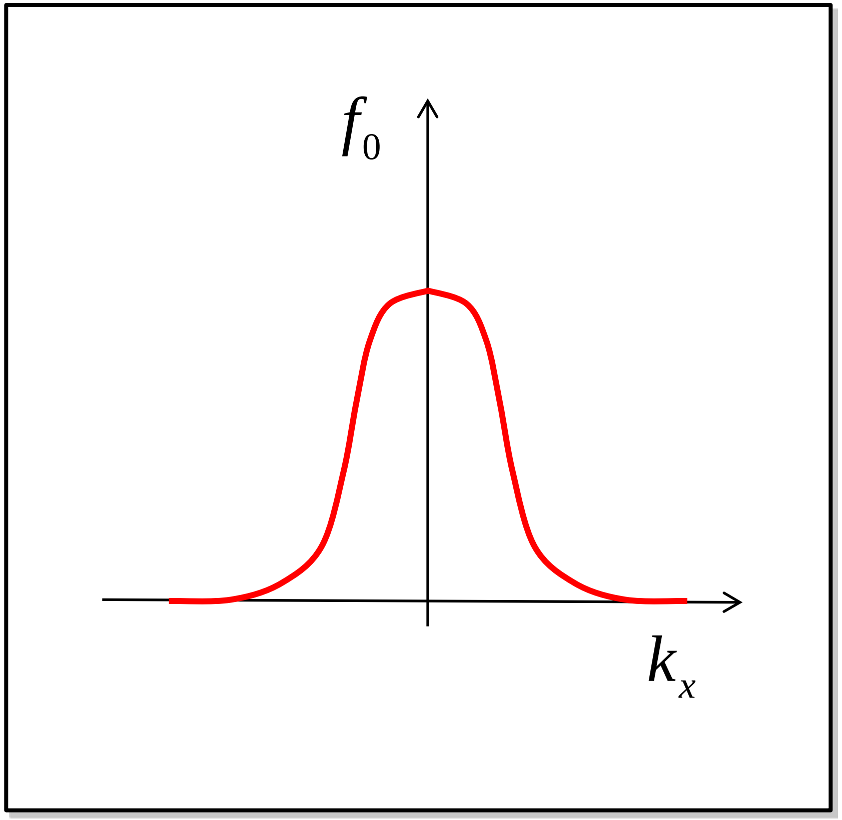
$\mu(T = 0)$ is the Fermi level

# $f_0$ in $k$-space

$$f_0 \approx e^{(E_F - E)/k_B T_L}$$

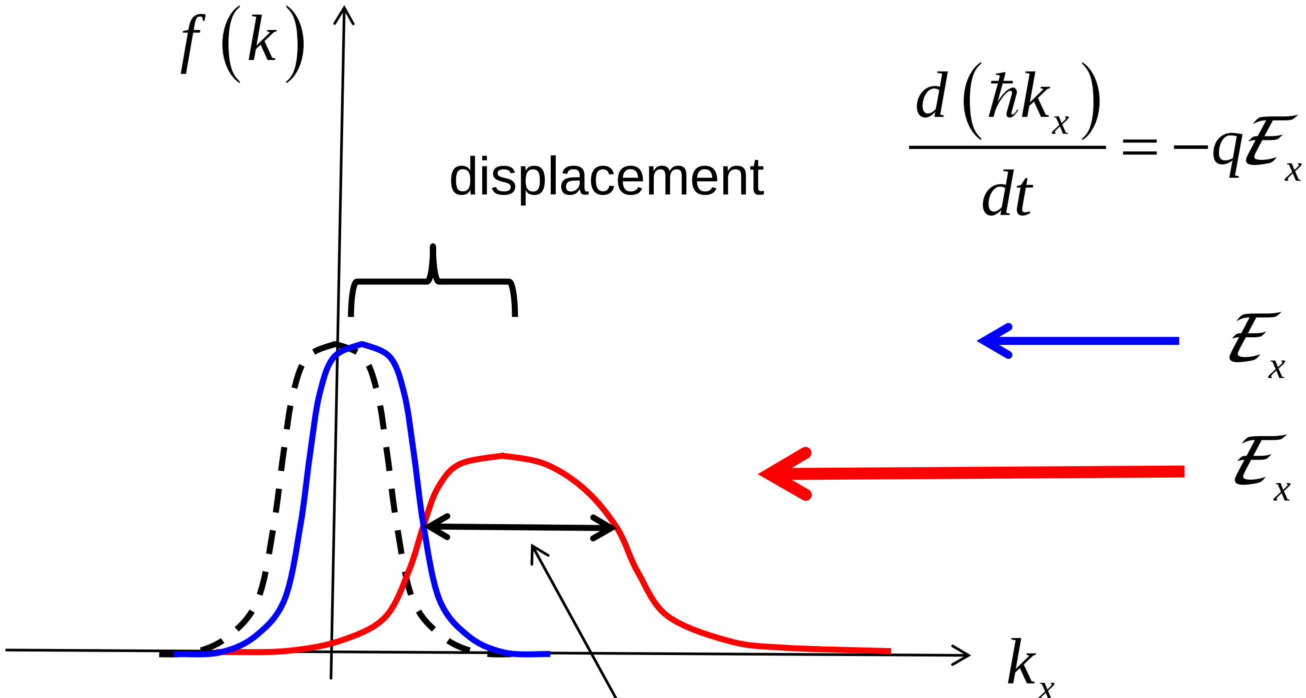
$$E = E_C + E(k) \approx E_C + \frac{\hbar^2 k^2}{2m^*}$$

$$f_0 \approx e^{(E_F - E_C)/k_B T_L} e^{-\hbar^2 k^2 / 2m^* k_B T_L}$$




Maxwellian distribution
(spread is related to $T_L$ )

# *f* out of equilibrium




$$\frac{d(\hbar k_x)}{dt} = -q\mathcal{E}_x$$

spread is related to the electron temperature, $T_e > T_L$

To find *f* out of equilibrium, solve the BTE.

# BTE

$$f\left(\vec{r},\vec{p},t\right)$$

$$\frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_{r}f+\vec{F}_{e}\bullet\nabla_{p}f=\hat{C}f$$

$$\hat{C}f\left(\vec{r},\vec{p},t\right)=\sum_{p'}S\left(\vec{p}',\vec{p}\right)f\left(\vec{p}'\right)\left[1-f\left(\vec{p}\right)\right]$$

$$-\sum_{p'}S\left(\vec{p},\vec{p}'\right)f\left(\vec{p}\right)\left[1-f\left(\vec{p}'\right)\right]$$

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# BTE in equilibrium

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

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

-equilibrium

-ballistic transport

consider equilibrium first and solve:

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

# detailed balance

$$\hat{C}f = 0$$

$$\hat{C}f = \sum_{p'} S(\vec{p}\,', \vec{p})\, f(\vec{p}\,')\left[1 - f(\vec{p})\right] - \sum_{p'} S(\vec{p}, \vec{p}\,')\, f(\vec{p})\left[1 - f(\vec{p}\,')\right] = 0$$

$$S(\vec{p}\,', \vec{p})\, f_0(\vec{p}\,')\left[1 - f_0(\vec{p})\right] = S(\vec{p}, \vec{p}\,')\, f_0(\vec{p})\left[1 - f_0(\vec{p}\,')\right]$$

(holds for **any** pair of p and p')

# BTE in equilibrium

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

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!*

# equilibrium distribution function

from EE-606, we know:

$$f_0 = \frac{1}{1+e^{(E-E_F)/k_B T_L}} = \frac{1}{1+e^{\Theta}} \qquad \Theta = \left[E_C(\vec{r}) + E(\vec{k}) - E_F\right] / k_B T_L$$

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

equilibrium BTE

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

$$\vec{\upsilon} \bullet \left\{ \frac{\nabla_r E_C - \nabla E_F}{k_B T_L} + \frac{(E - E_F)}{k_B} \nabla_r \left( \frac{1}{T_L} \right) \right\} + \vec{F}_e \bullet \frac{\vec{\upsilon}}{k_B T_L} = 0$$

(The terms $\frac{\partial f_0}{\partial \Theta}$, $\nabla_r E_C$, and $\vec{F}_e \bullet$ are crossed out with red X marks.)

# equilibrium

$$\vec{\upsilon} \bullet \left\{ -\nabla E_F + \frac{\left(E - E_F\right)}{k_B T_L} \left( -\frac{\nabla_r T_L}{T_L} \right) \right\} = 0$$

to satisfy this equation for **any** energy, $E_{TOT}$, $\nabla E_{\mathrm{F}} = \nabla T = 0$

***the Fermi level and temperature are constant in equilibrium*.**

# but…

*T.E. Humphrey and H. Linke argue that in a nanostructured material with one energy channel, it is possible to have Fermi level and temperature gradients in equilibrium.*

*Phys. Rev. Lett.,* ***94****, 096601, 11 March 2005.*

# what determines $f_0$, the equilibrium $f$ ?

$$\upsilon \bullet \nabla_r f_0 + \mathbf{F}_e \bullet \nabla_p f_0 = \hat{C} f_0 = 0$$

satisfied by any function of total energy

must ensure detailed balance in equilibrium.

only satisfied by:

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T_L}}$$

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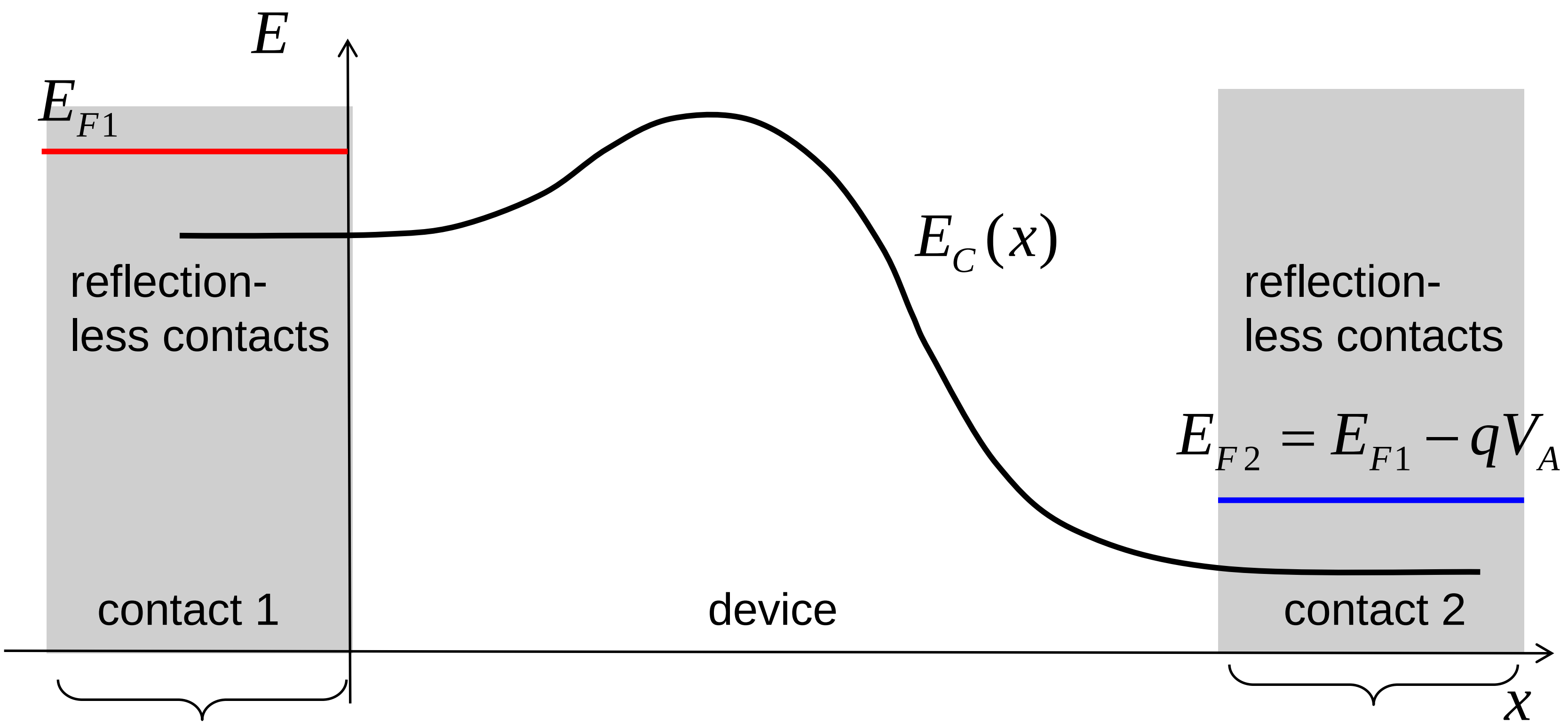
# generic ballistic device




thermal equilibrium reservoir

**ballistic**

thermal equilibrium reservoir

$$f(E) = f_0(E_{F1})$$

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

$$f(E) = f_0(E_{F2})$$

# solution for a ballistic device

***Steady-state ballistic BTE:***

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

***Solution:***

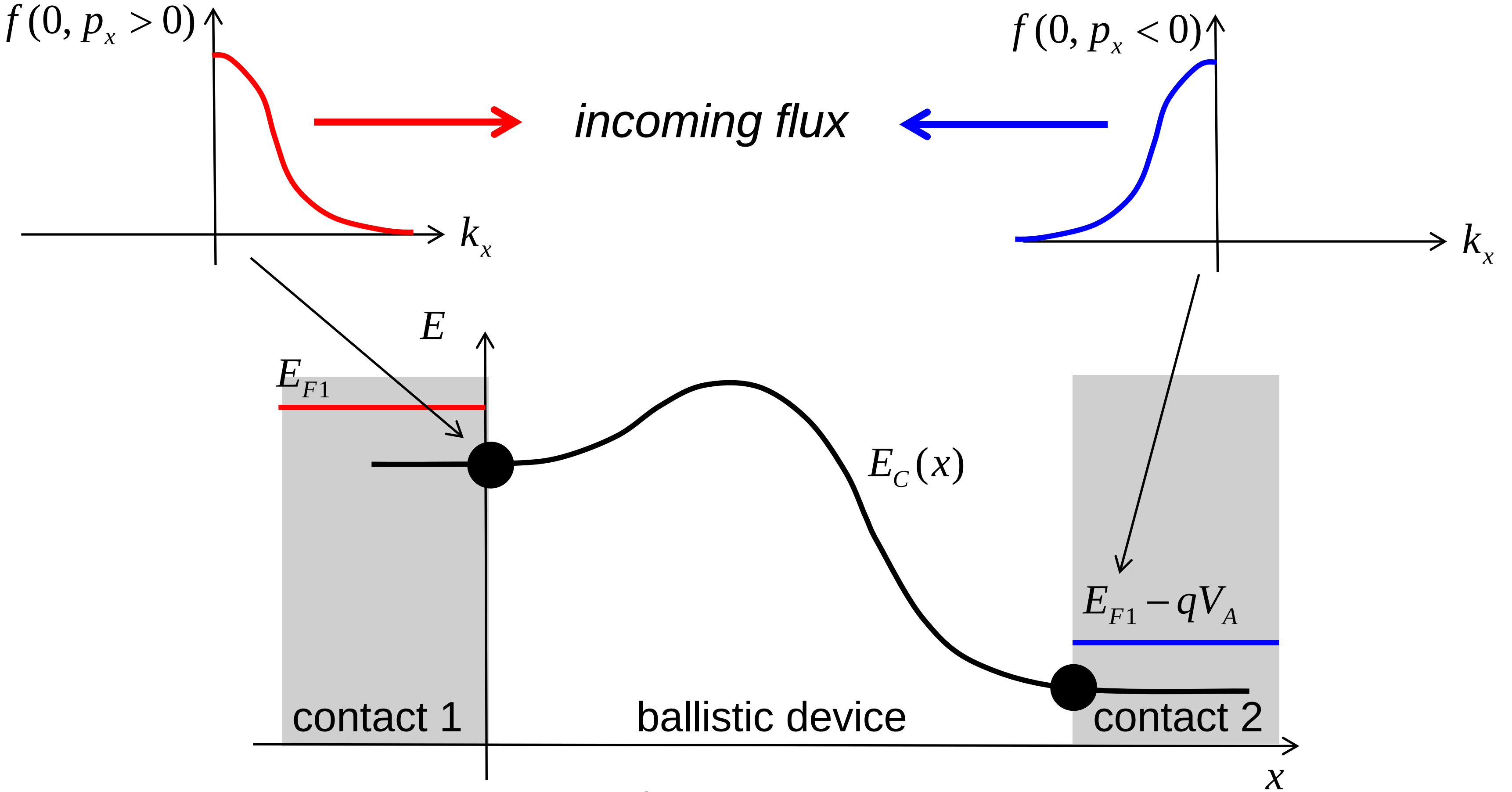
$$f(x, p_x) = g\left(E\right) = g\left[E_C(x) + E(k_x)\right]$$

***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.

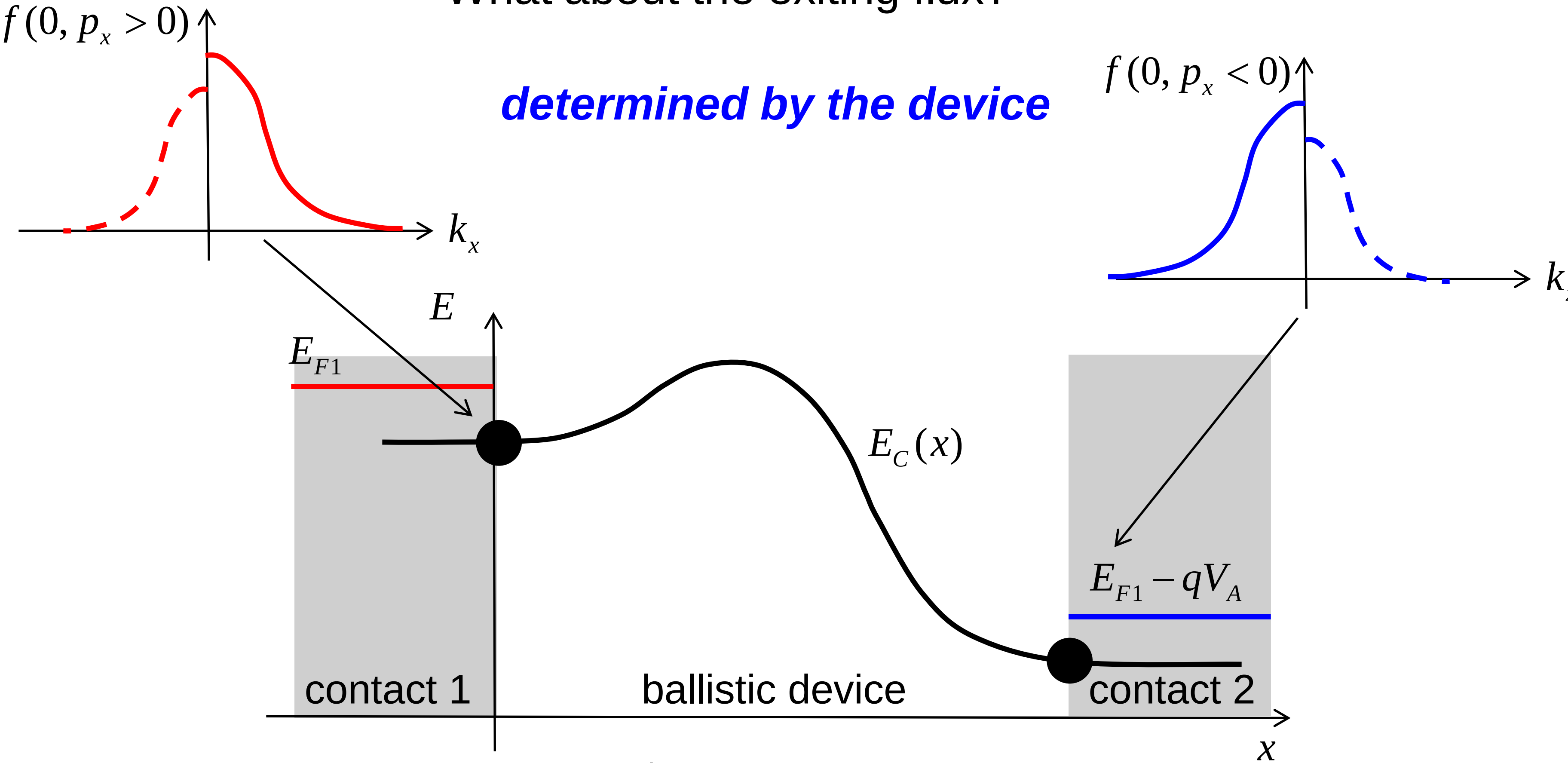


# boundary conditions for the BTE

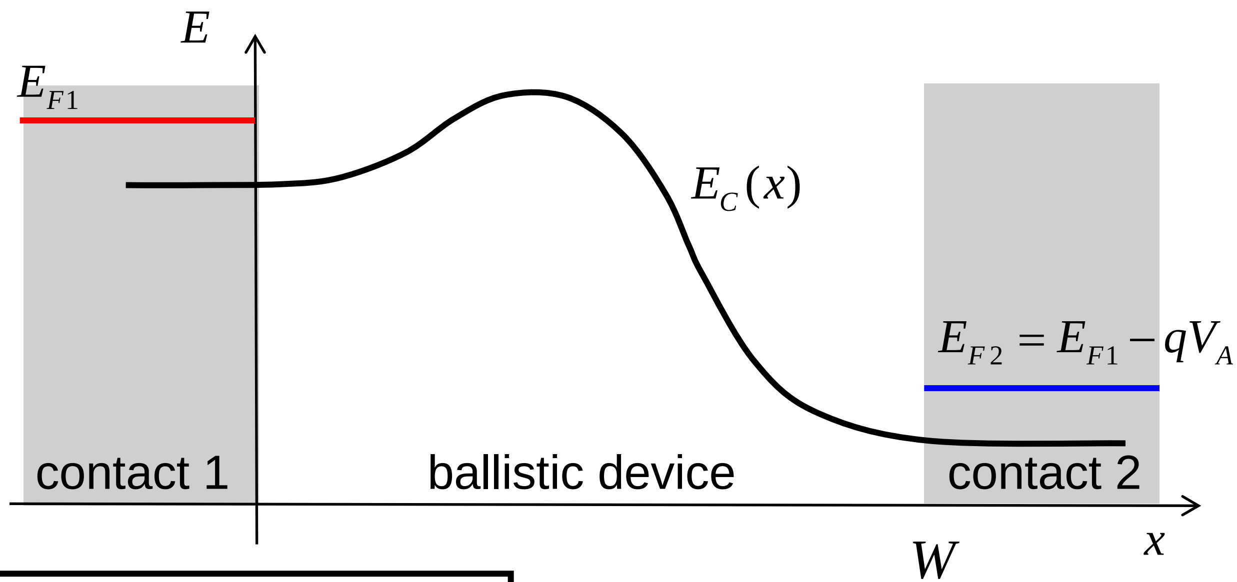
**Solution:** Specify incoming flux.

What about the exiting flux?

***determined by the device***



# solution to the s.s. ballistic BTE




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

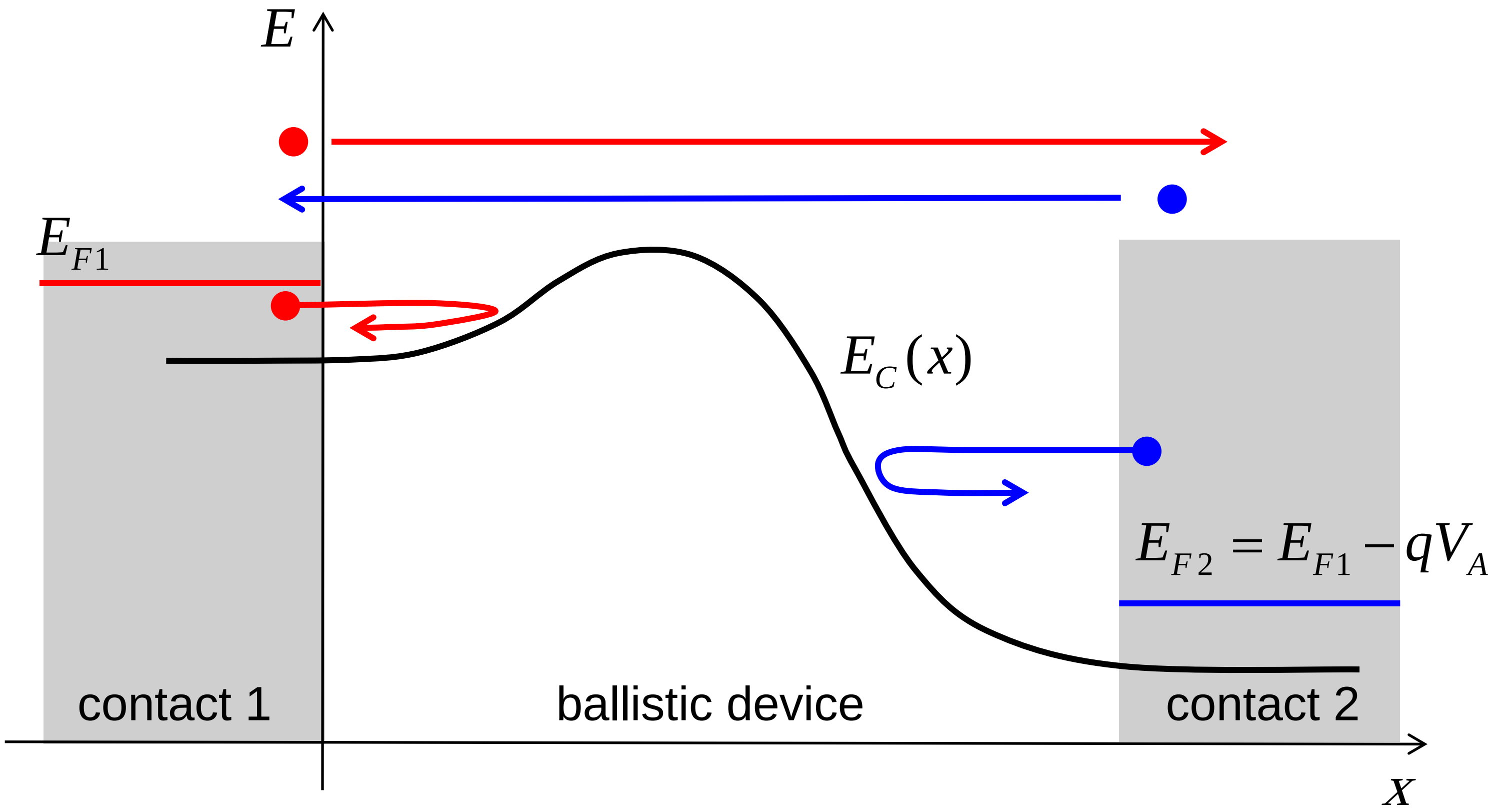
$$f(0, p_x > 0) = \frac{1}{1 + e^{(E - E_{F1})/k_B T_L}}$$

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

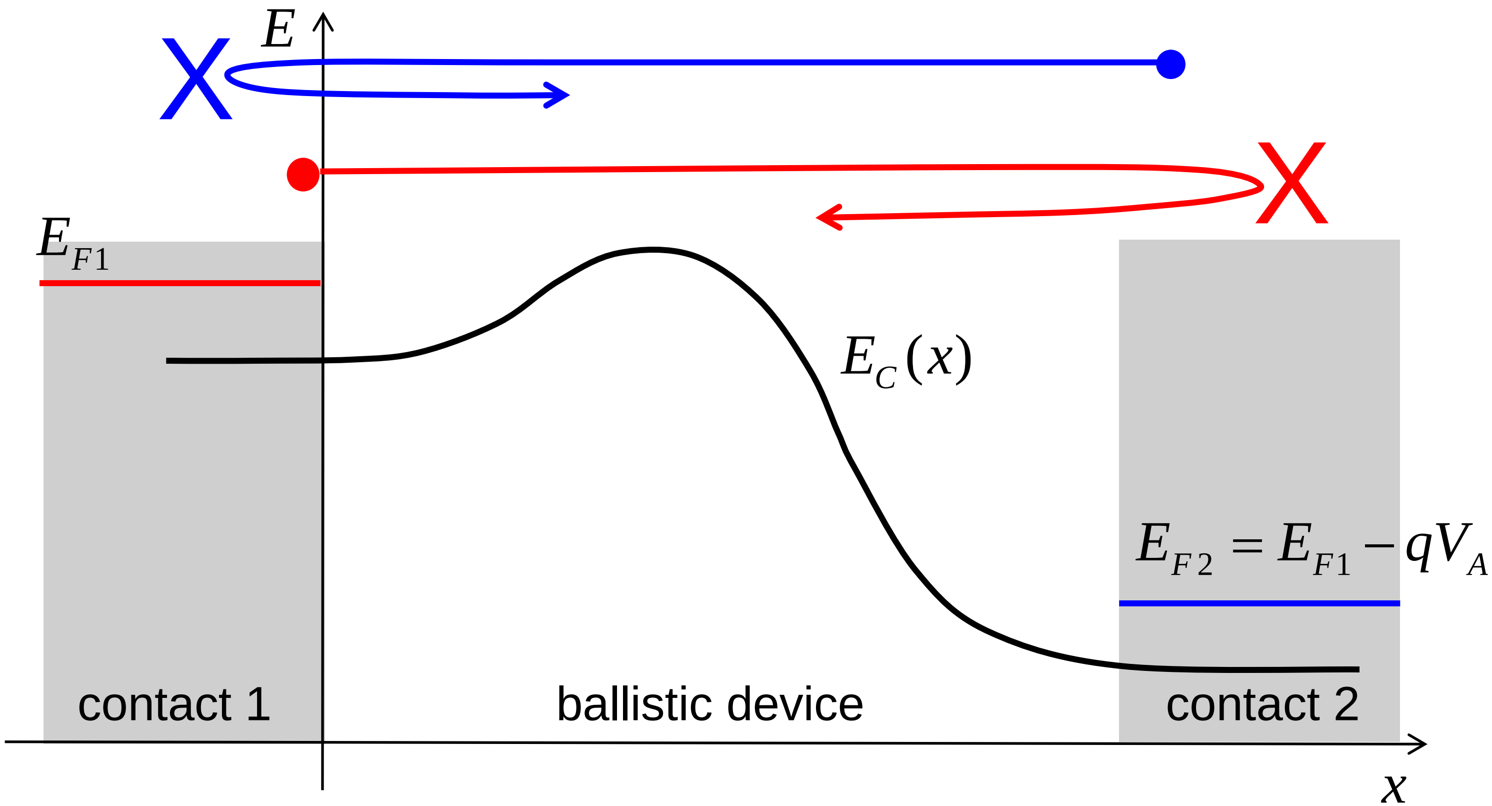
$$f(x, p_x) = g\left[E_C(x) + E(k_x)\right]$$

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

# 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

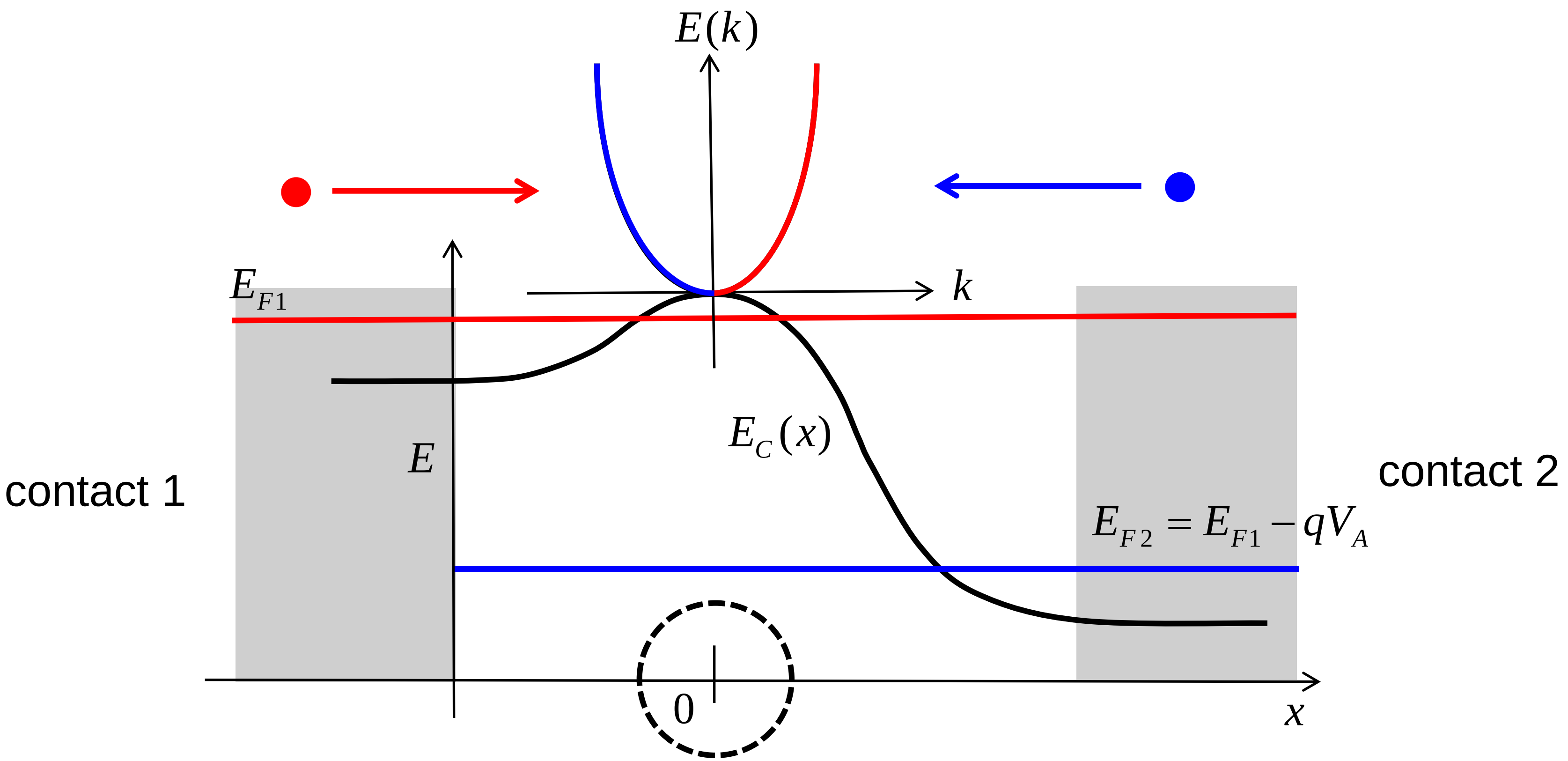
Within a ballistic device, the probability that a *k*-state is occupied is given by an equilibrium Fermi function.

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

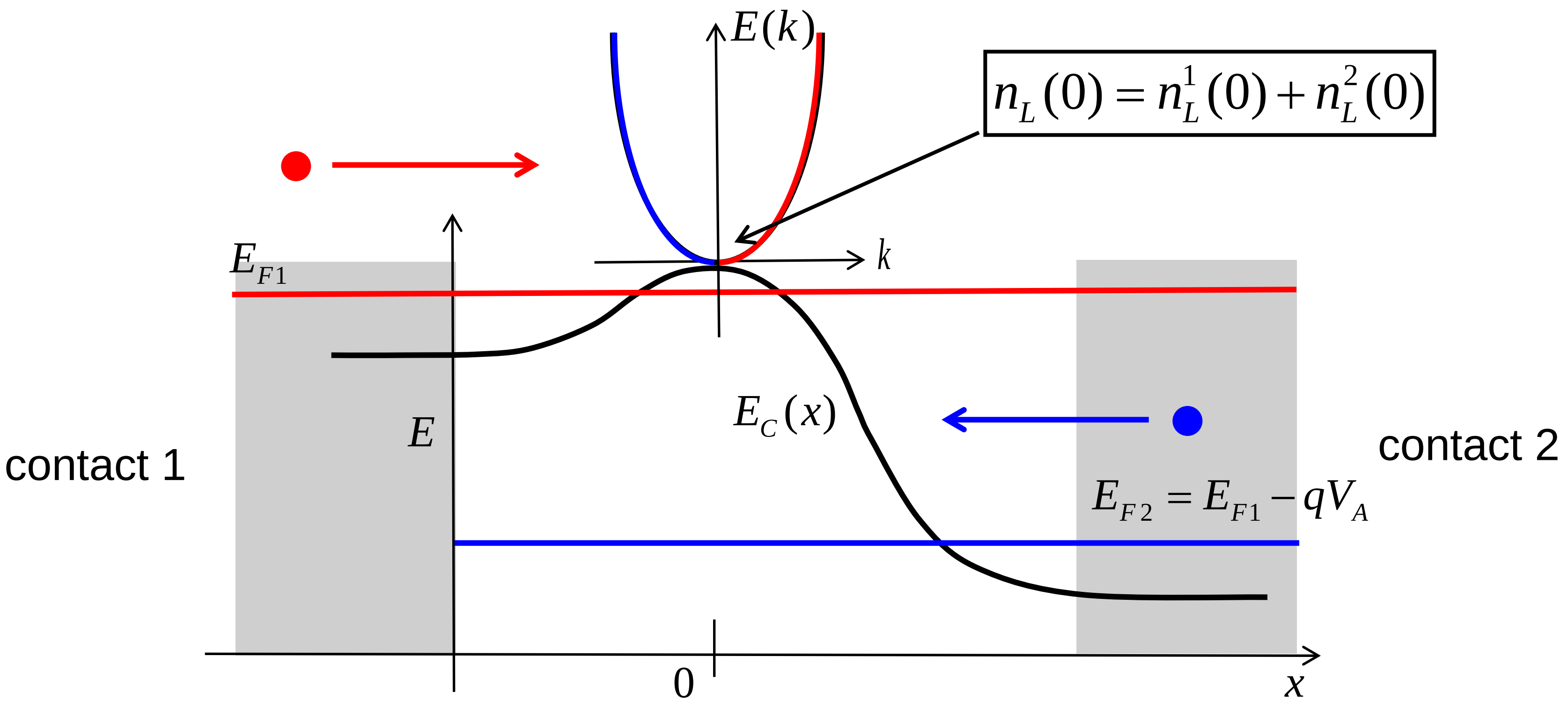
Within a ballistic device, each *k*-state is in **equilibrium** with one contact or the other.

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

# example



# example



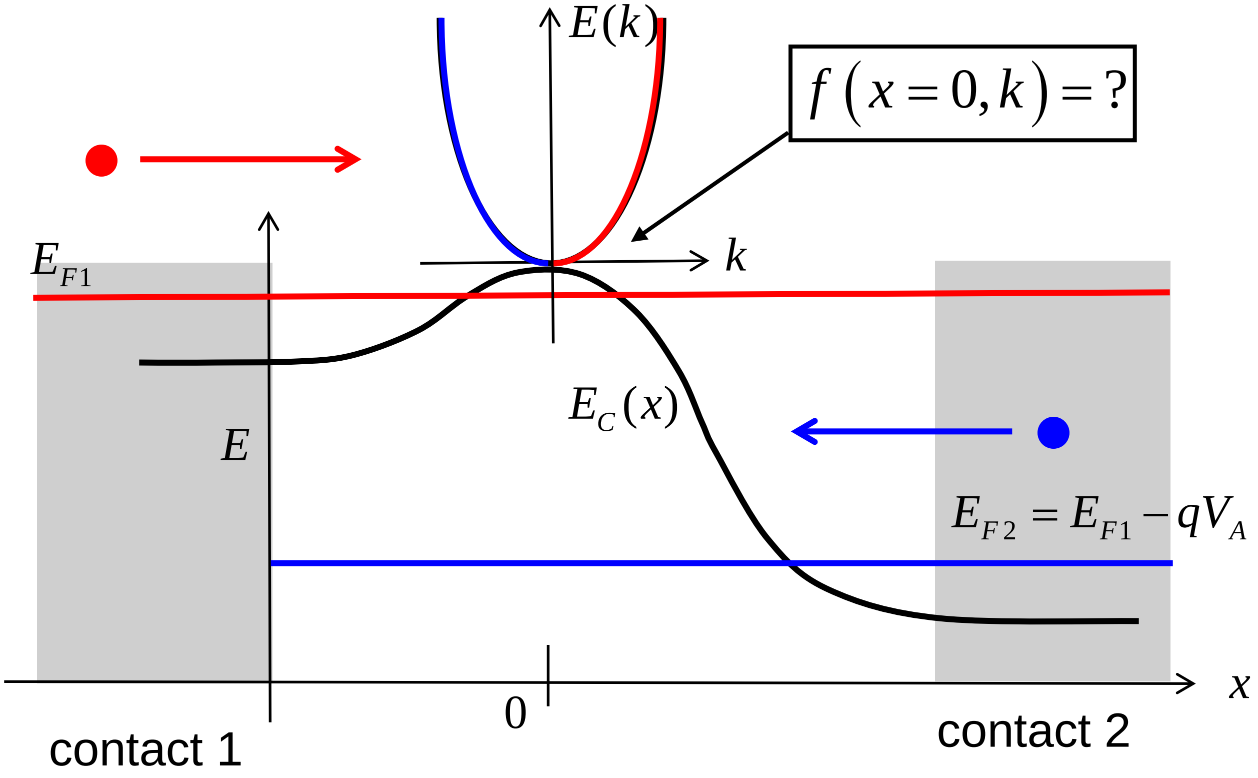

$$n_L^1(0) = n_L^+(0) = \frac{1}{L}\sum_{k_x>0} f_0(E_{F1})$$

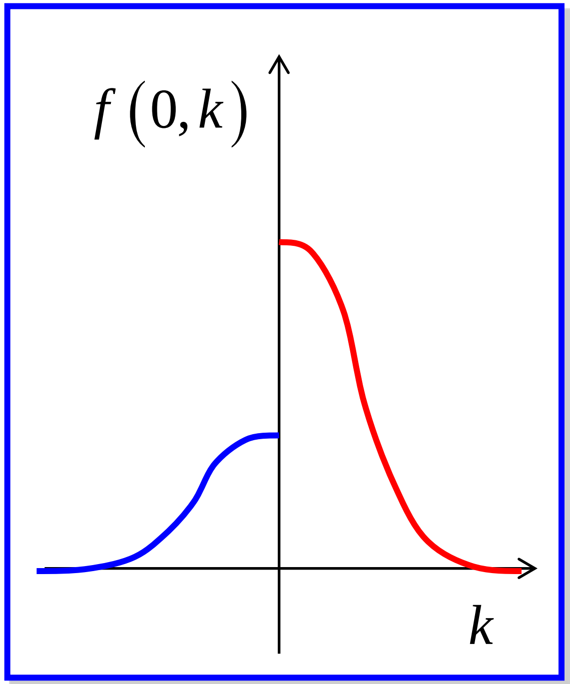
$$n_L^1(0) = \int D_{1D}^1(0,E) f_0(E_{F1}) dE$$

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

$$n_L^2(0) = \int D_{1D}^2(0,E) f_0(E_{F2}) dE$$

# example

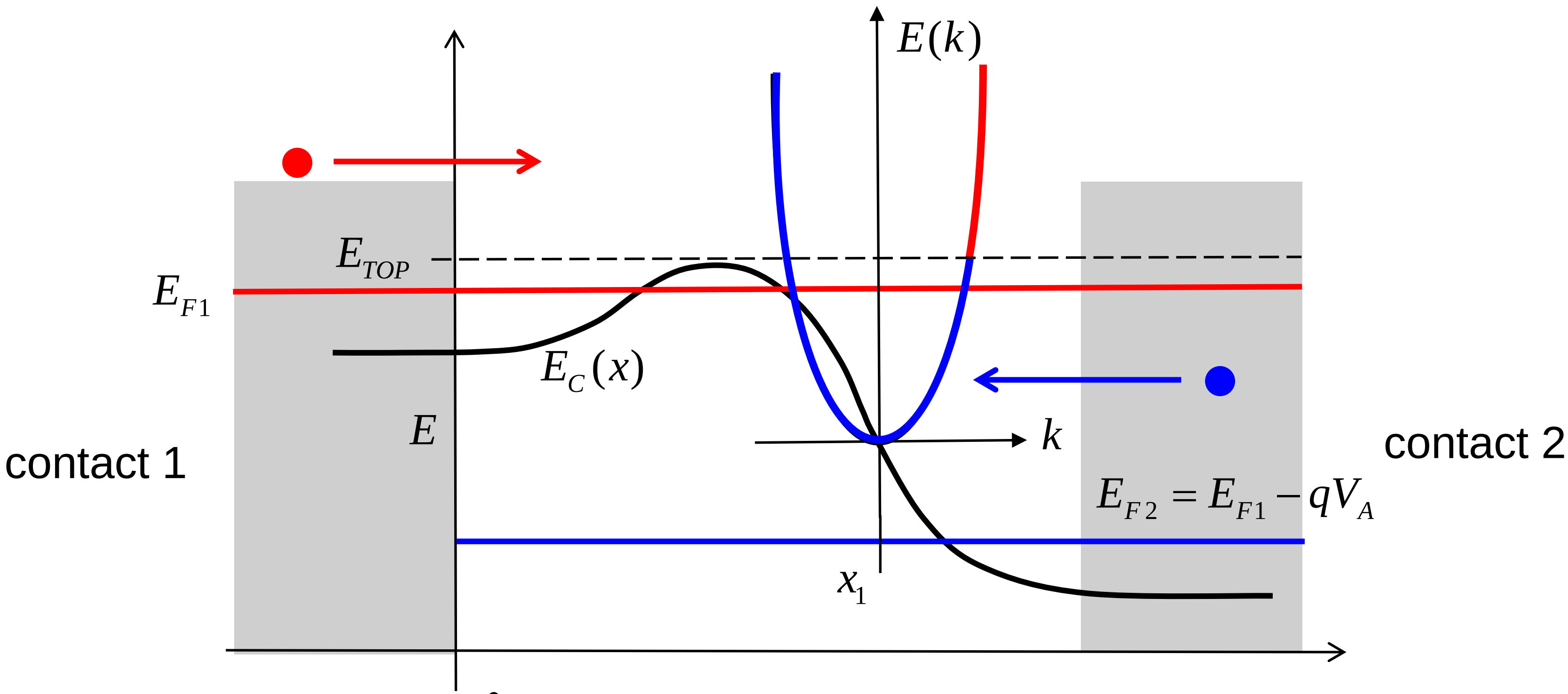



$$n_L(0) = \frac{1}{L}\sum_{k_x>0} f_0(E_{F1}) + \frac{1}{L}\sum_{k_x<0} f_0(E_{F2}) = \int D_{1D}^1(0,E) f_0(E_{F1}) + D_{1D}^2(0,E) f_0(E_{F2}) d$$

$$D_{1D}^1(0,E) = D_{1D}^2(0,E) = D_{1D}(E)/2$$

# another example

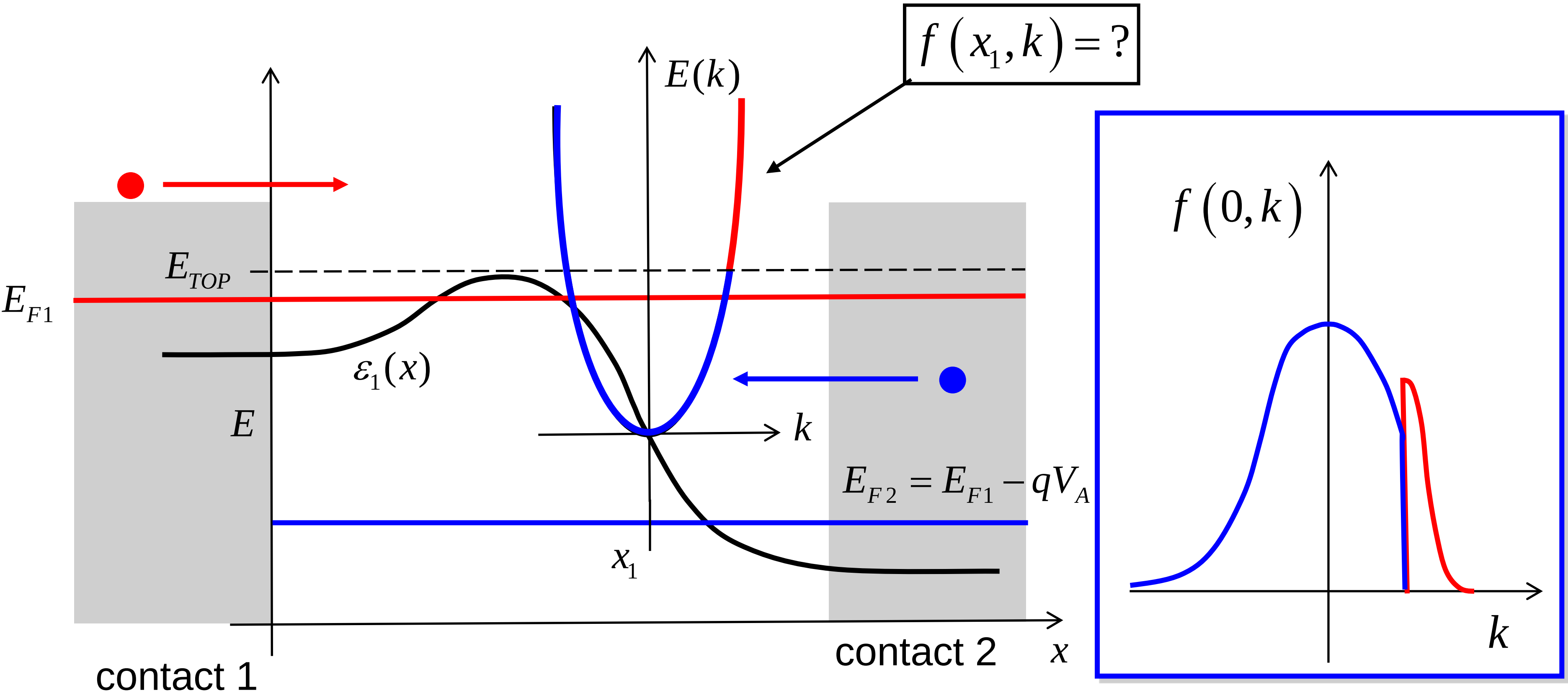



$$n_L(x_1) = \int D_{1D}^1(x_1, E) f_0(E_{F1}) + D_{1D}^2(x_1, E) f_0(E_{F2}) dE$$

***"local density of states"***

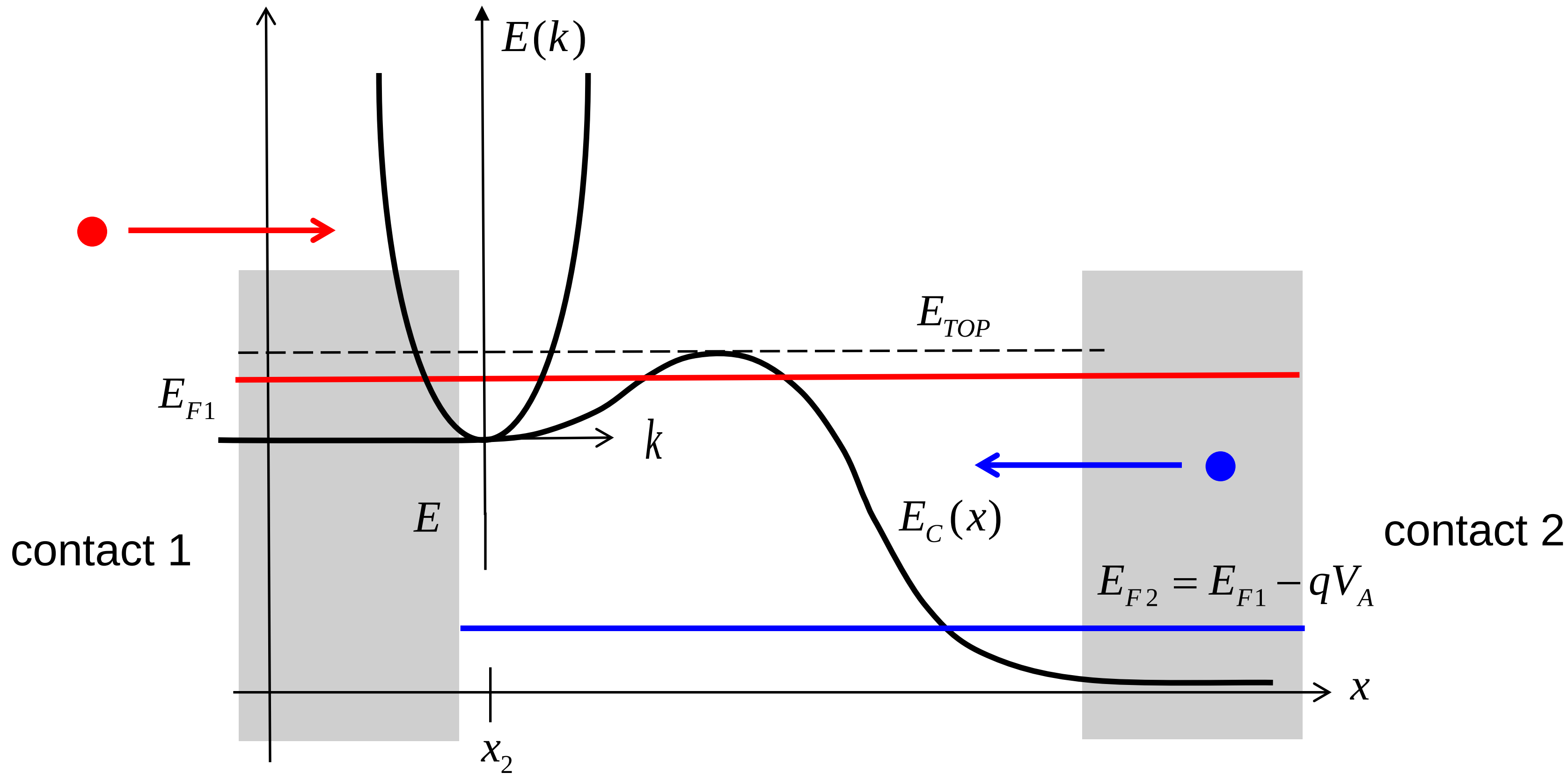
$$D_{1D}^1(x_1, E), D_{1D}^2(x_1, E) \neq D_{1D}(E)/2$$

# distribution function

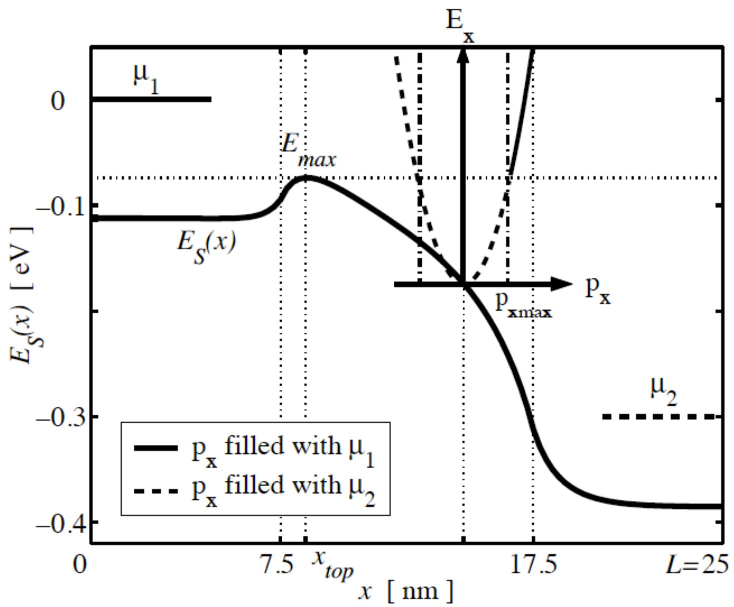


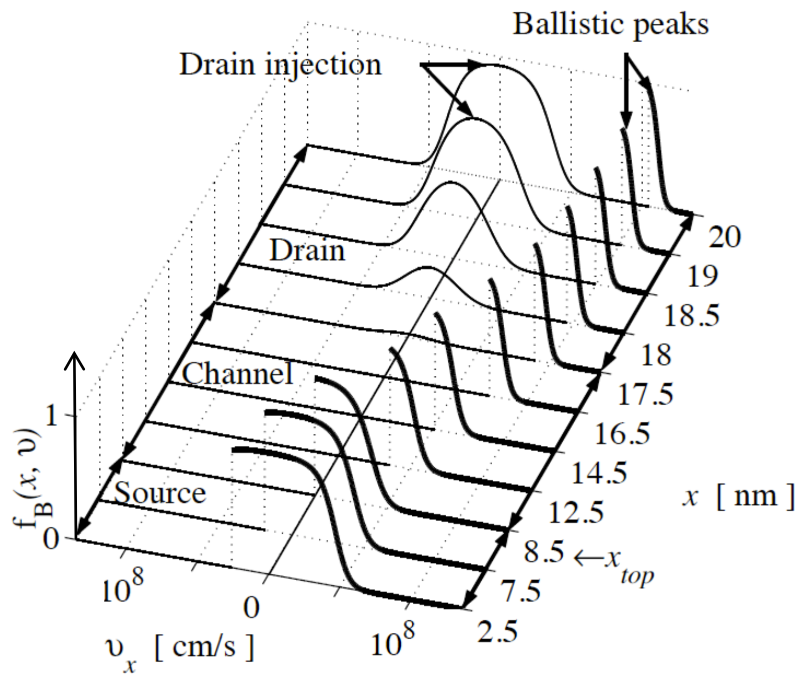

J.-H. Rhew, Zhibin Ren, and Mark Lundstrom, “A Numerical Study of Ballistic Transport in a Nanoscale MOSFET,” Solid-State Electronics, **46**,1899, 2002.

# suggested exercise



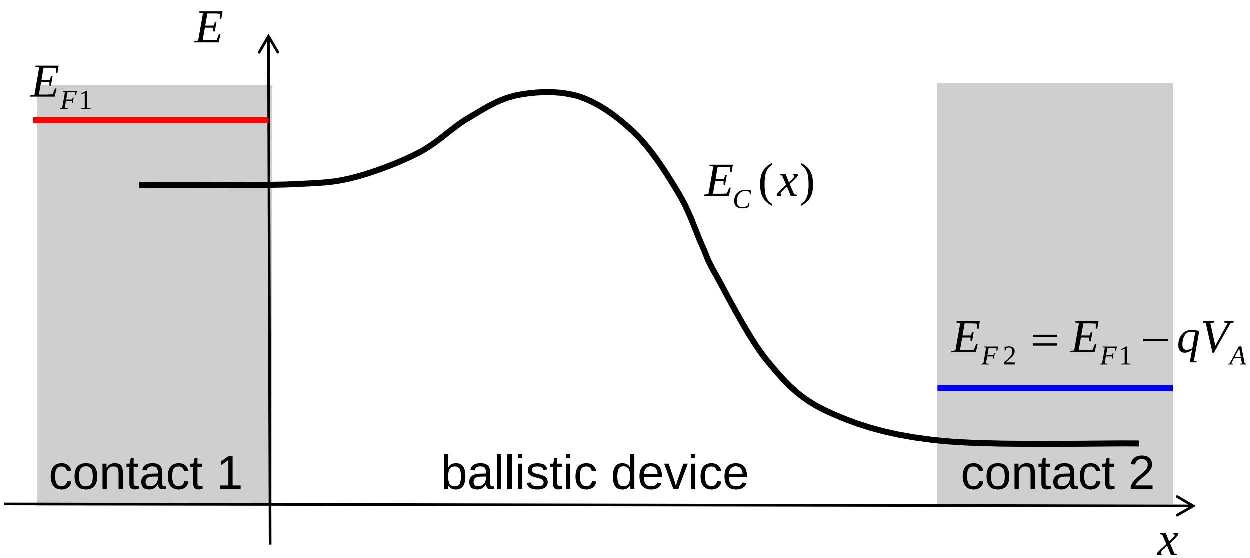
# distribution function




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

# solution to the ballistic BTE: summary

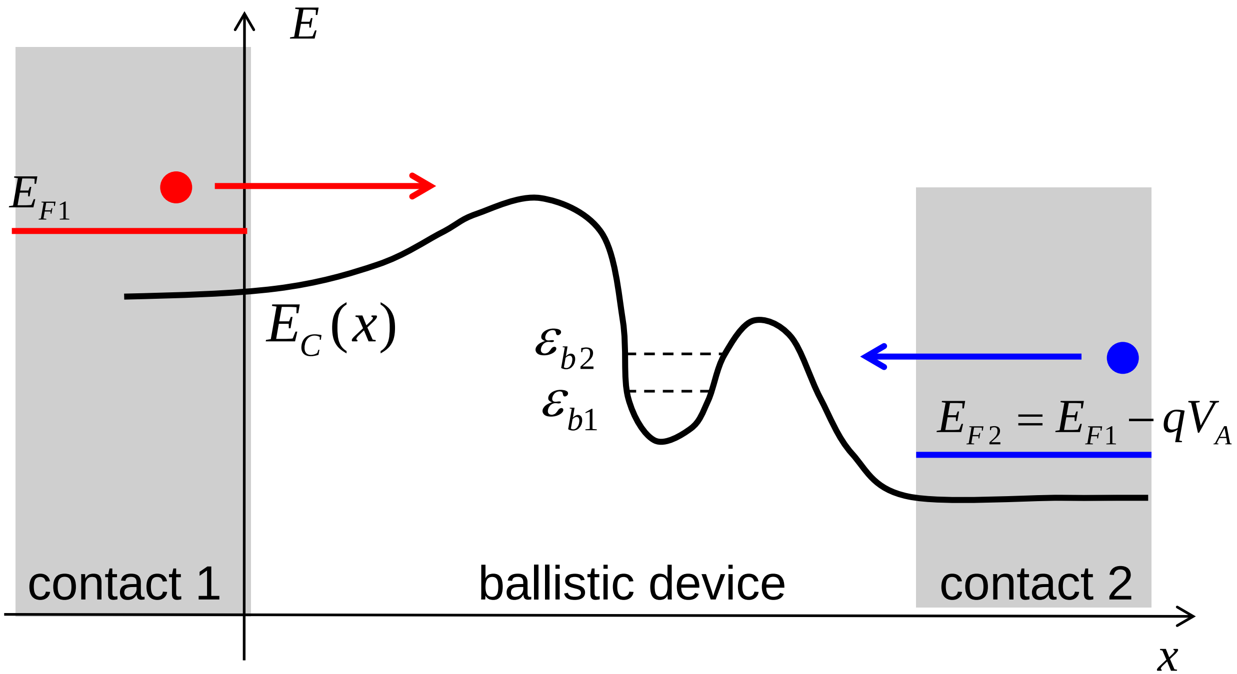



1) states divide into two parts, fillable by each of the contacts

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

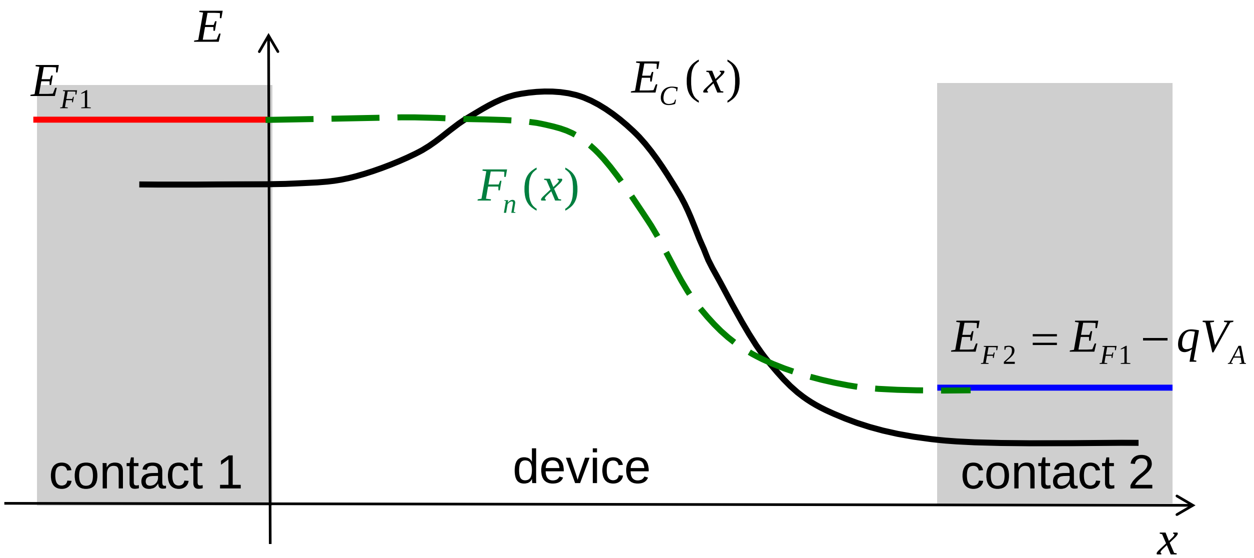
2) but….

# 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.

# diffusive transport




$$n_L(x) = \int D_{1D}(x,E) f\left[F_n\left(x\right)\right] dE$$

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

$$D_{1D}(x,E) = \frac{1}{\pi\hbar}\sqrt{2m^* / \left(E - E_C(x)\right)}$$

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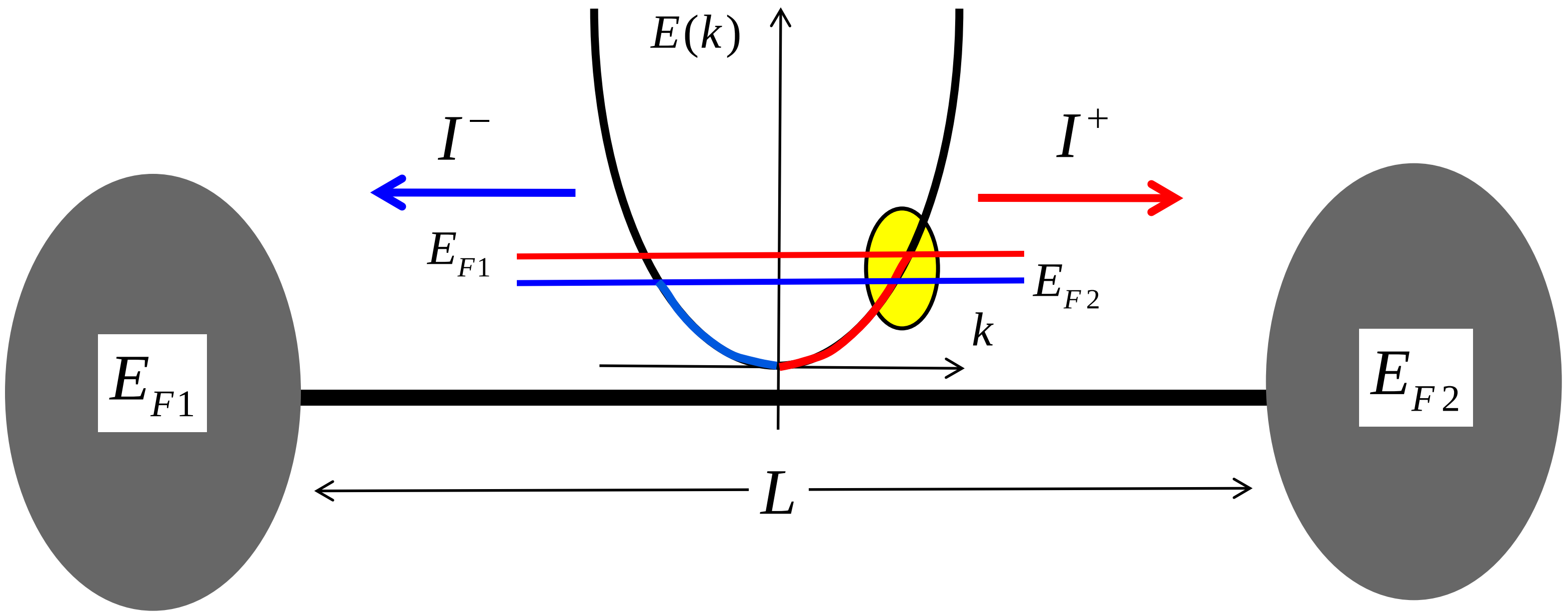
# connection to Landauer




$$I^- = \frac{1}{L}\sum_{k<0} q\upsilon_x f_0(E_{F2})$$

$$I = I^+ - I^-$$

$$I^+ = \frac{1}{L}\sum_{k>0} q\upsilon_x f_0(E_{F1})$$

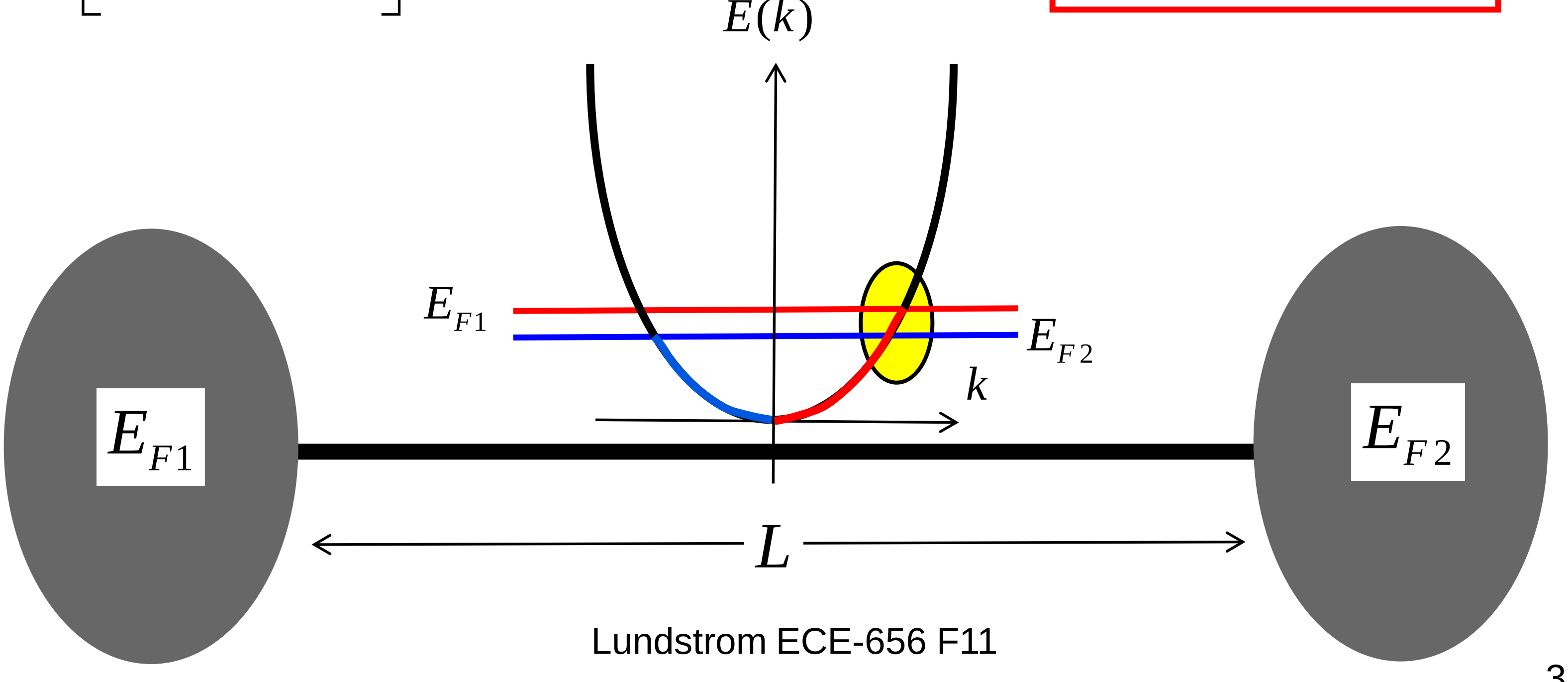
# current

$$I = q\left[\frac{D_{1D}(E_F)}{2}(E_{F1} - E_{F2})\right]\upsilon_F$$

$$M(E_F) = \frac{h}{4} D_{1D}(E_F)\upsilon_F$$

$$I = q^2\left[\frac{D_{1D}(E_F)}{2}\upsilon_F\right]V$$

$$I = \frac{2q^2}{h} M(E_F) V$$



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# summary

1) Any function of total energy satisfies the equilibrium or ballistic BTE.

2) Equilibrium requires that both the Fermi level and temperature be independent of position (except for a single energy channel).

3) It is easy to solve the ballistic BTE in near or far from equilibrium by filling states from the appropriate contact.

# questions?

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