ECE-656: Fall 2009

Lecture 13:
Solving the BTE: equilibrium and ballistic

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outline

1) Quick review

2) Equilibrium BTE

3) Ballistic BTE

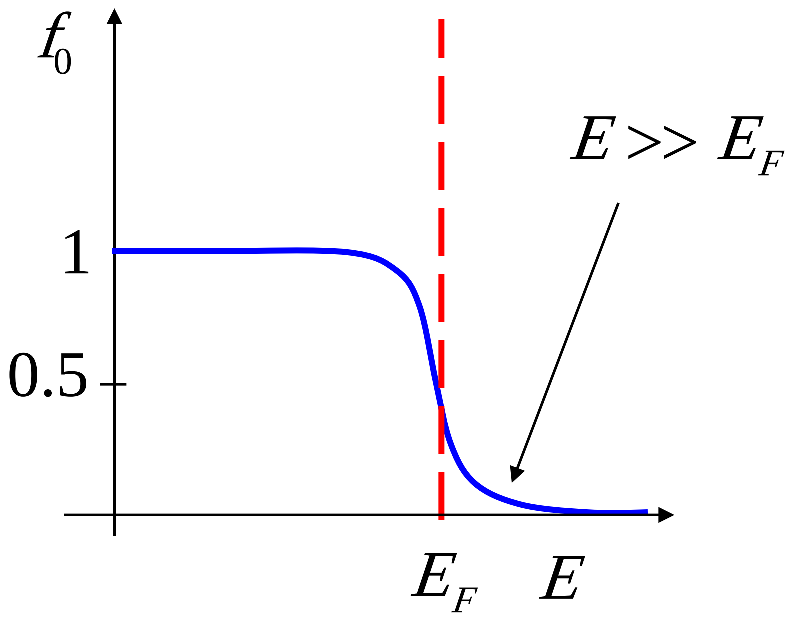
4) Discussion

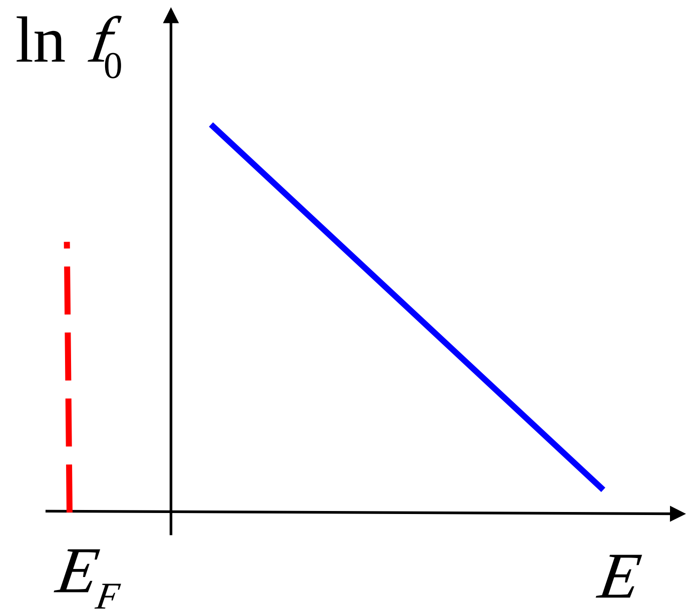
5) Summary

equilibrium distribution function

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

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





(nondegenerate)

chemical potential and Fermi level

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

We will use E_F

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

μ is the chemical (or electrochemical) potential.

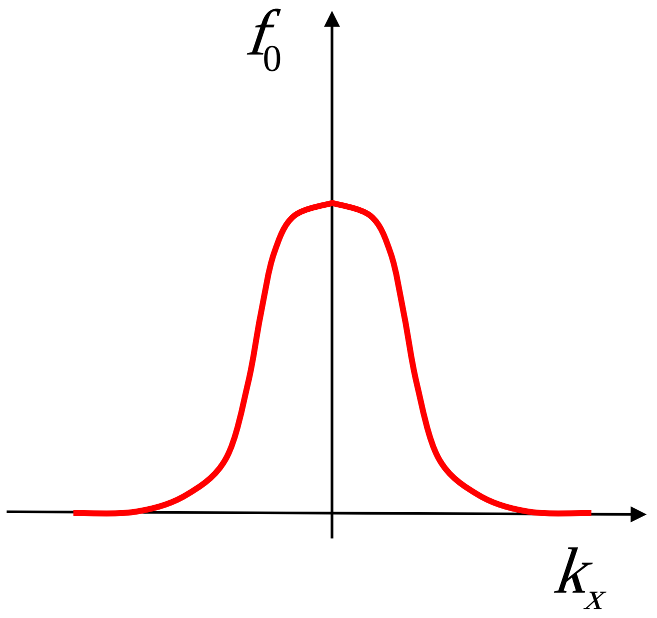
$\mu(T = 0)$ is the Fermi level

f_0 in k-space

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

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

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



Maxwellian distribution
(spread is related to *T*)

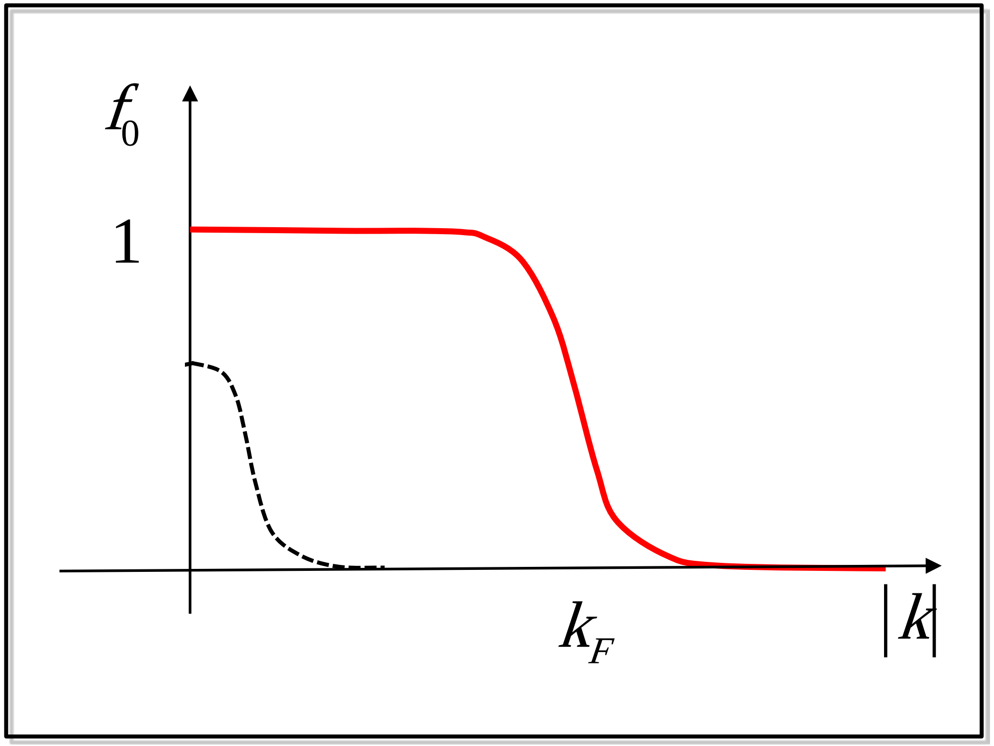
f_0 in k-space (ii)

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

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

$$E_F = E_C + \frac{\hbar^2 k_F^2}{2 m^*}$$

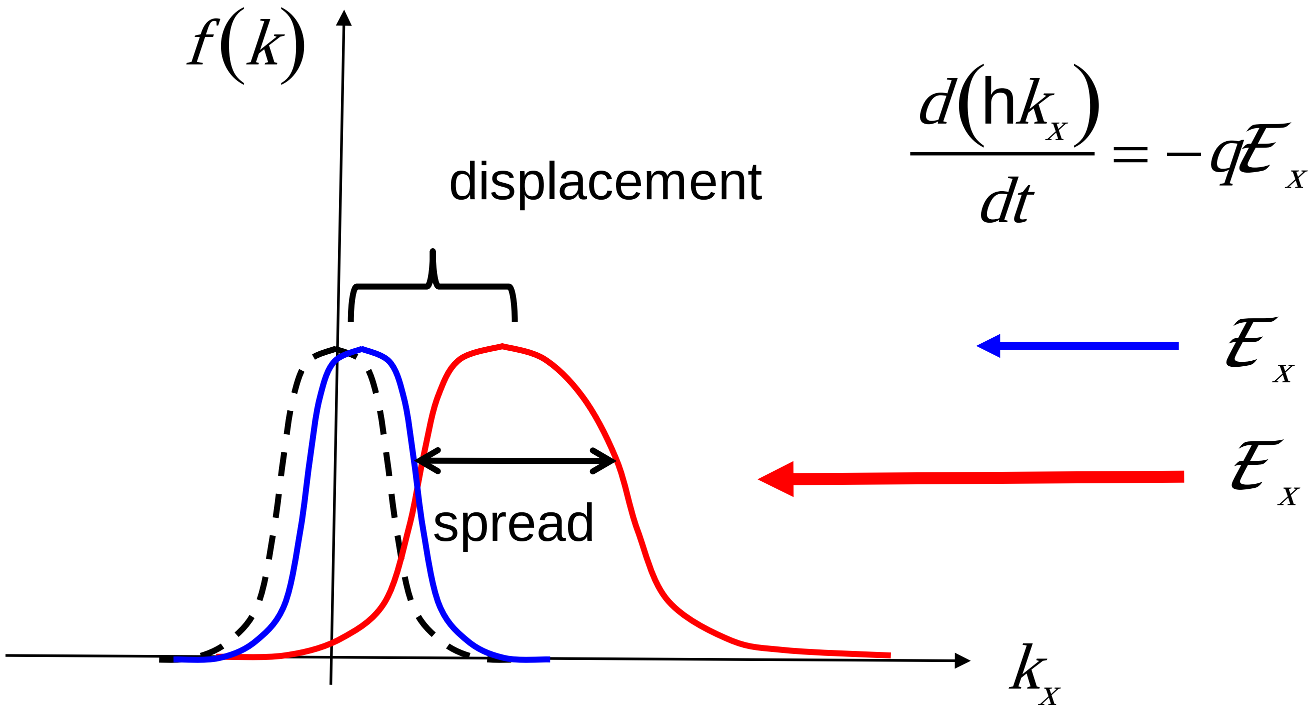
$$f_0 = \frac{1}{1 + e^{\hbar^2 \left(k^2 - k_F^2\right)/2 m^* k_B T}}$$



Fermi-Dirac distribution

f out of equilibrium

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



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

BTE

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

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

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

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

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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:

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

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

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

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

Any function of total energy satisfies the equilibrium BTE!

equilibrium distribution function

from EE-606, we know:

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

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

equilibrium BTE

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

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

equilibrium

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

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, 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:

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

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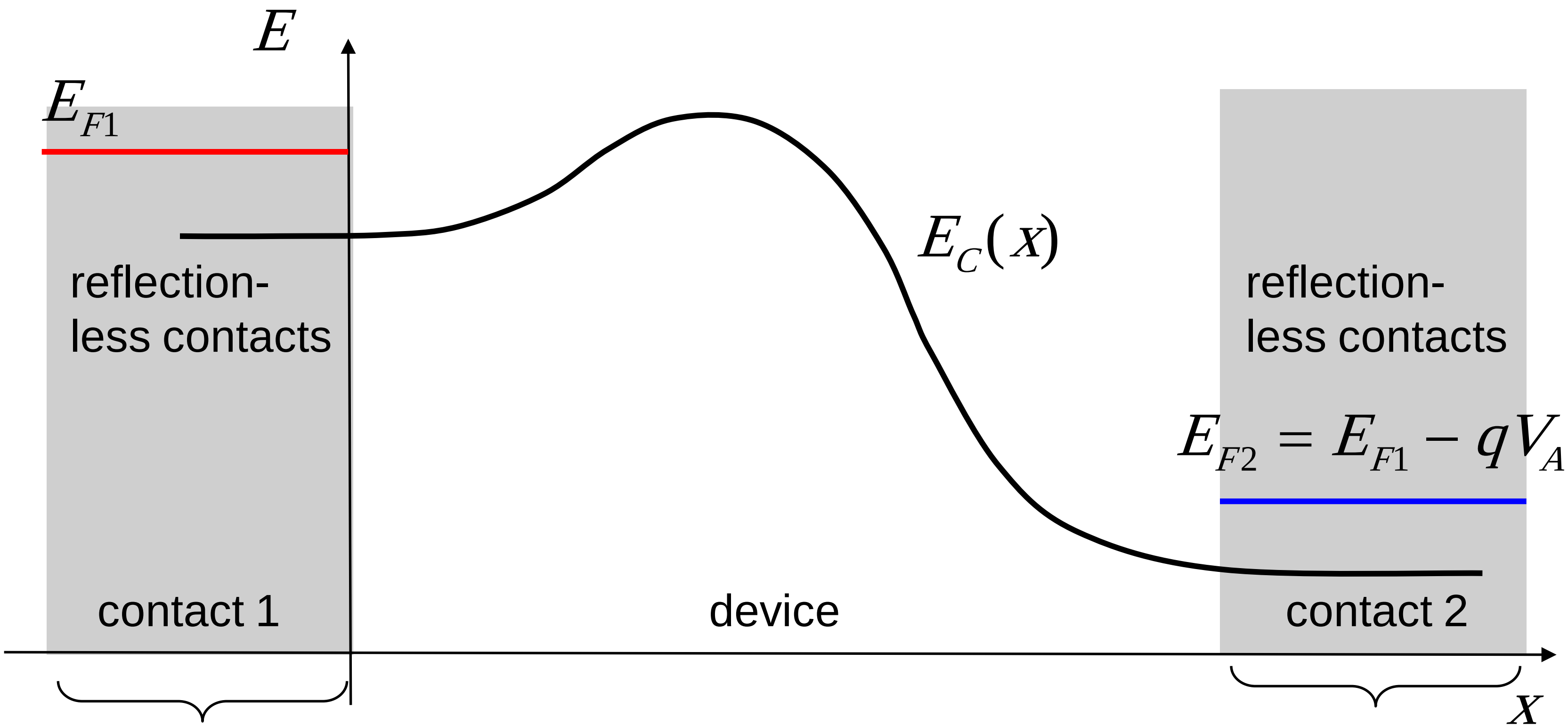
generic ballistic device



thermal equilibrium reservoir

$$f(E) = f_0(E_F)$$

ballistic

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

thermal equilibrium reservoir

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

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:

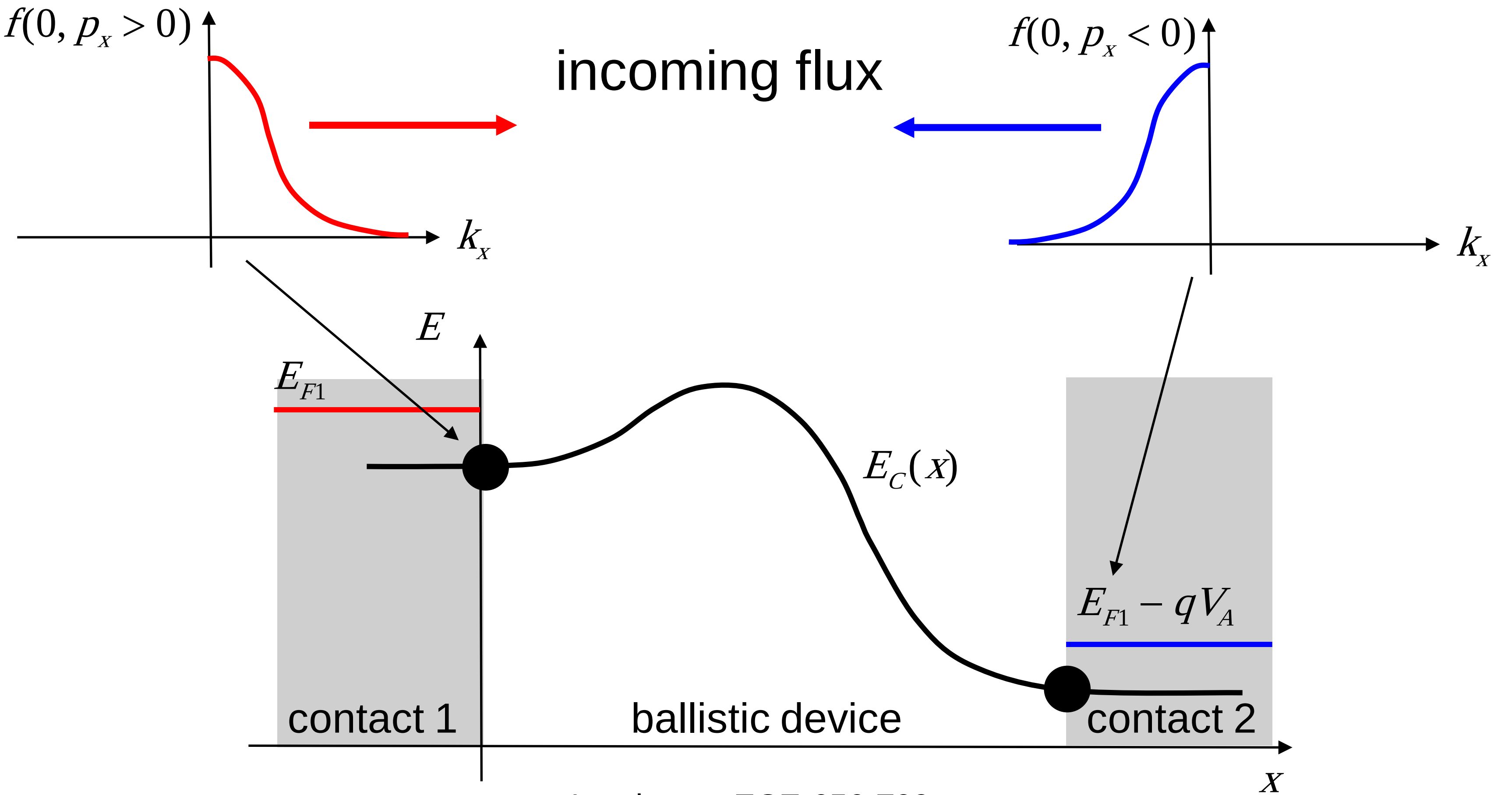
$$f(x, p_x) = g(E) = g\left[E_C(x) + E(\hbar k_x)\right]$$

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.

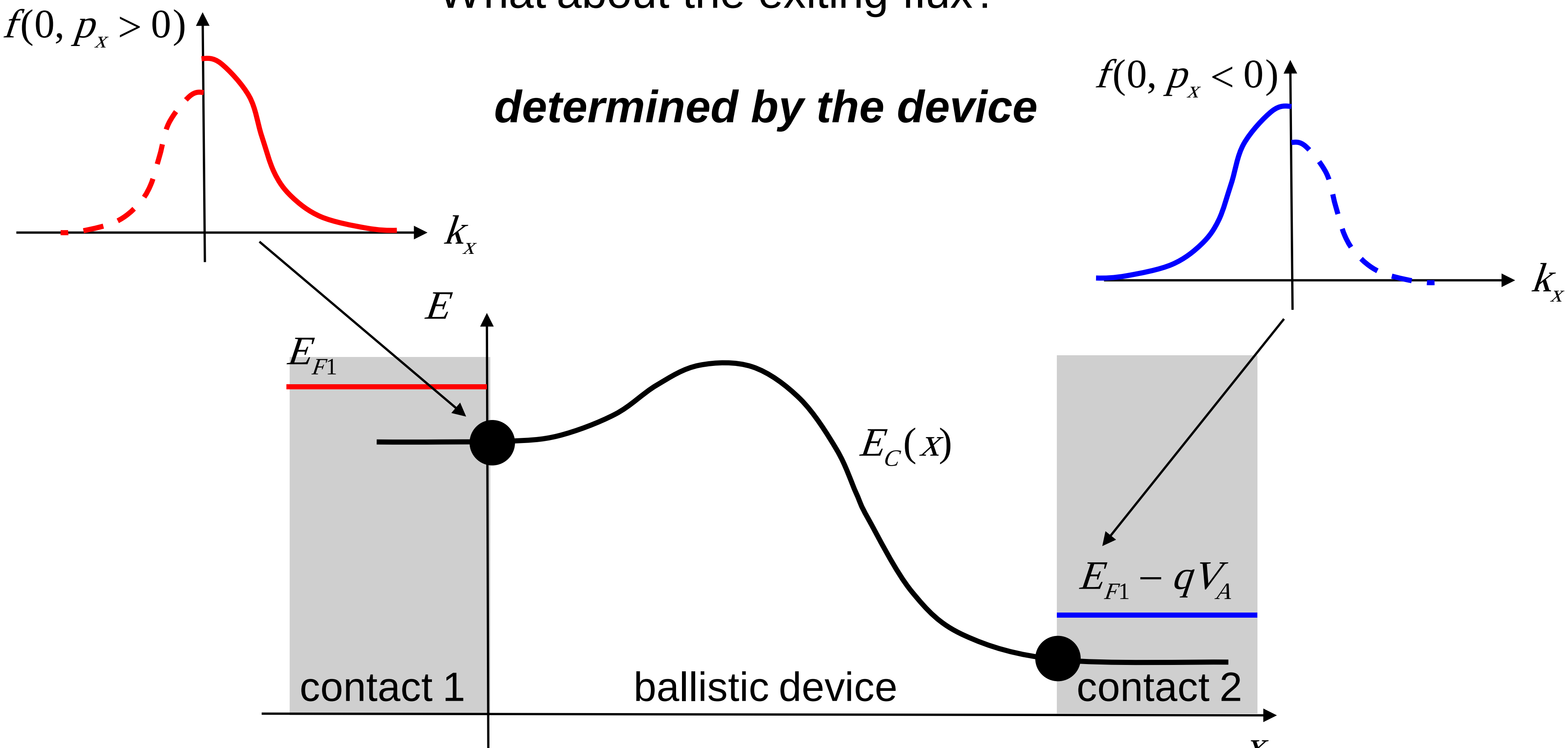


boundary conditions for the BTE

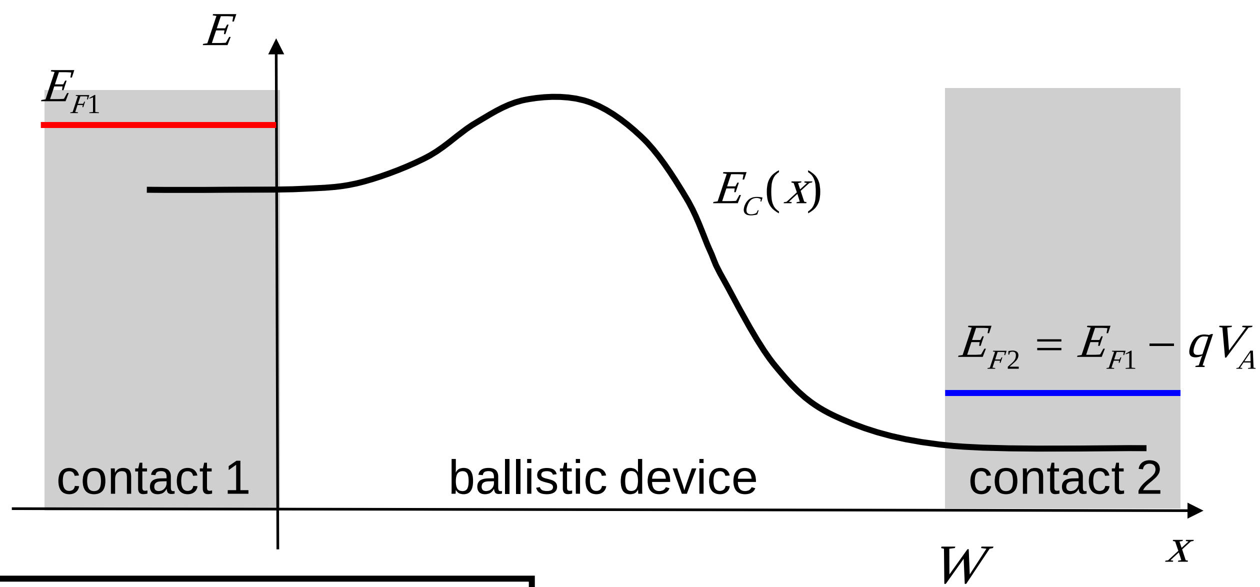
Solution: Specify incoming flux.

What about the exiting flux?

determined by the device



solution to the s.s. ballistic BTE



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

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

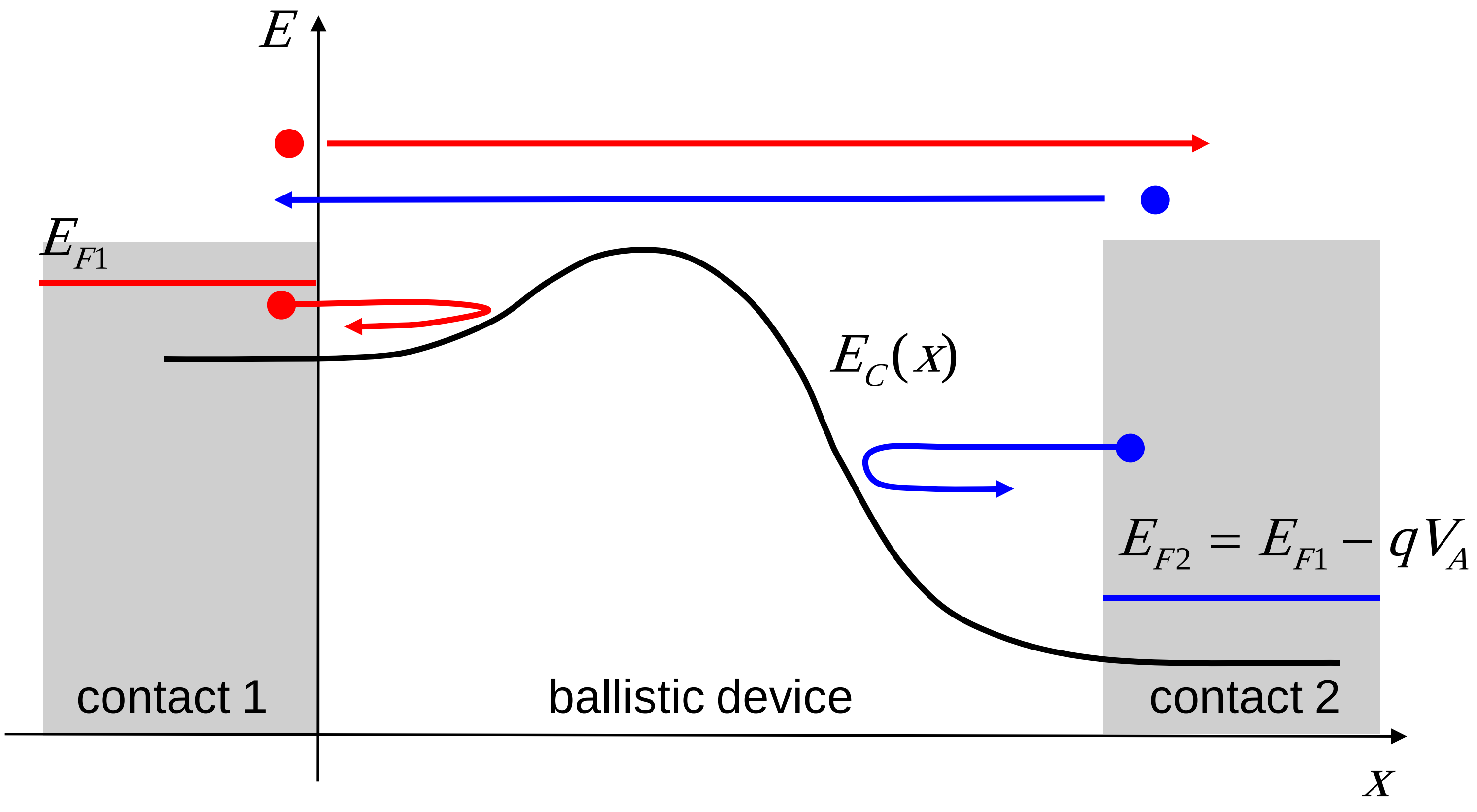
$$f(W, p_x < 0) = \frac{1}{1 + e^{(E - E_{F2})/k_B T}}$$

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

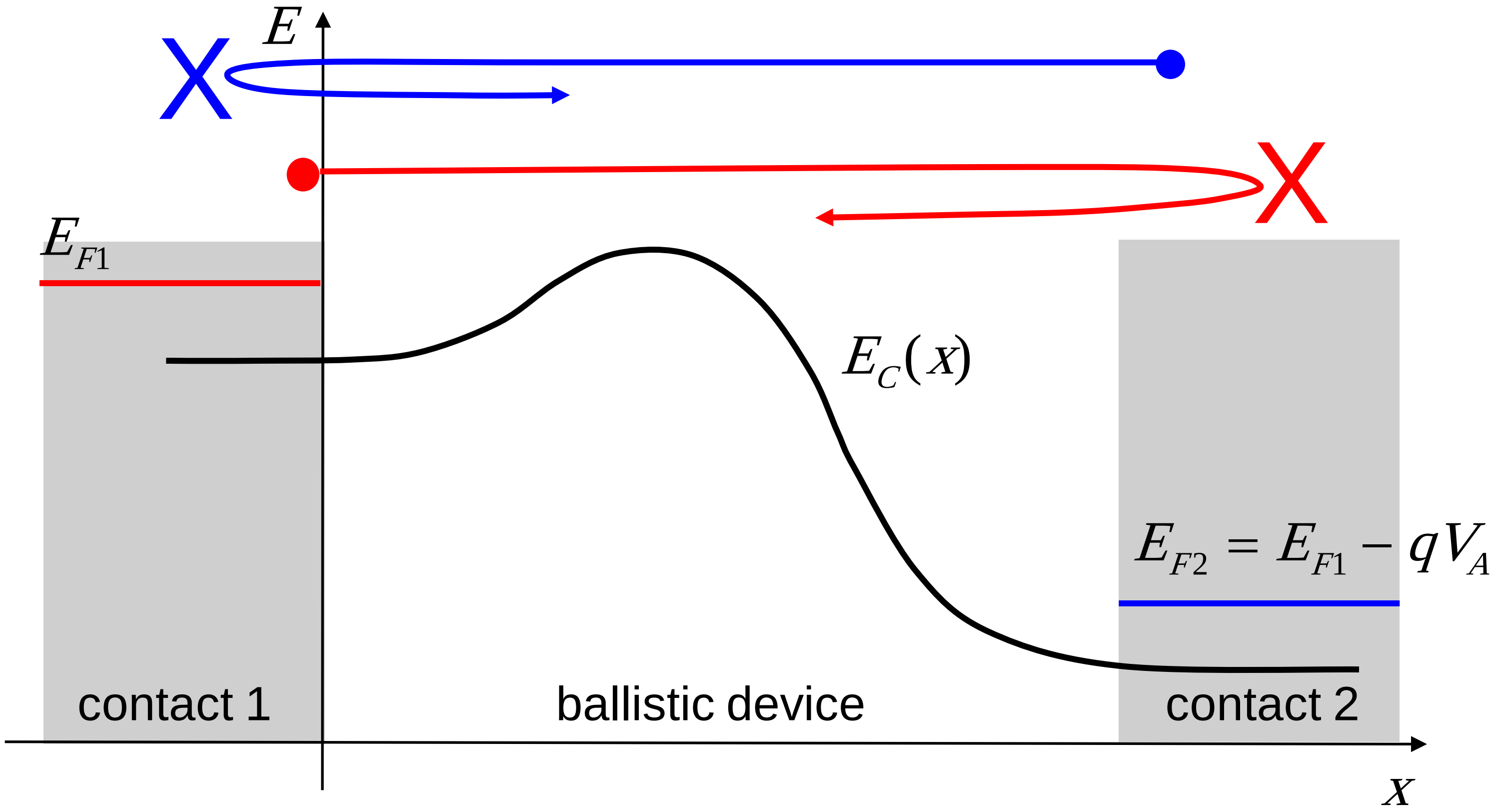
$$f(x,p_x) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

but what Fermi level do we use?

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

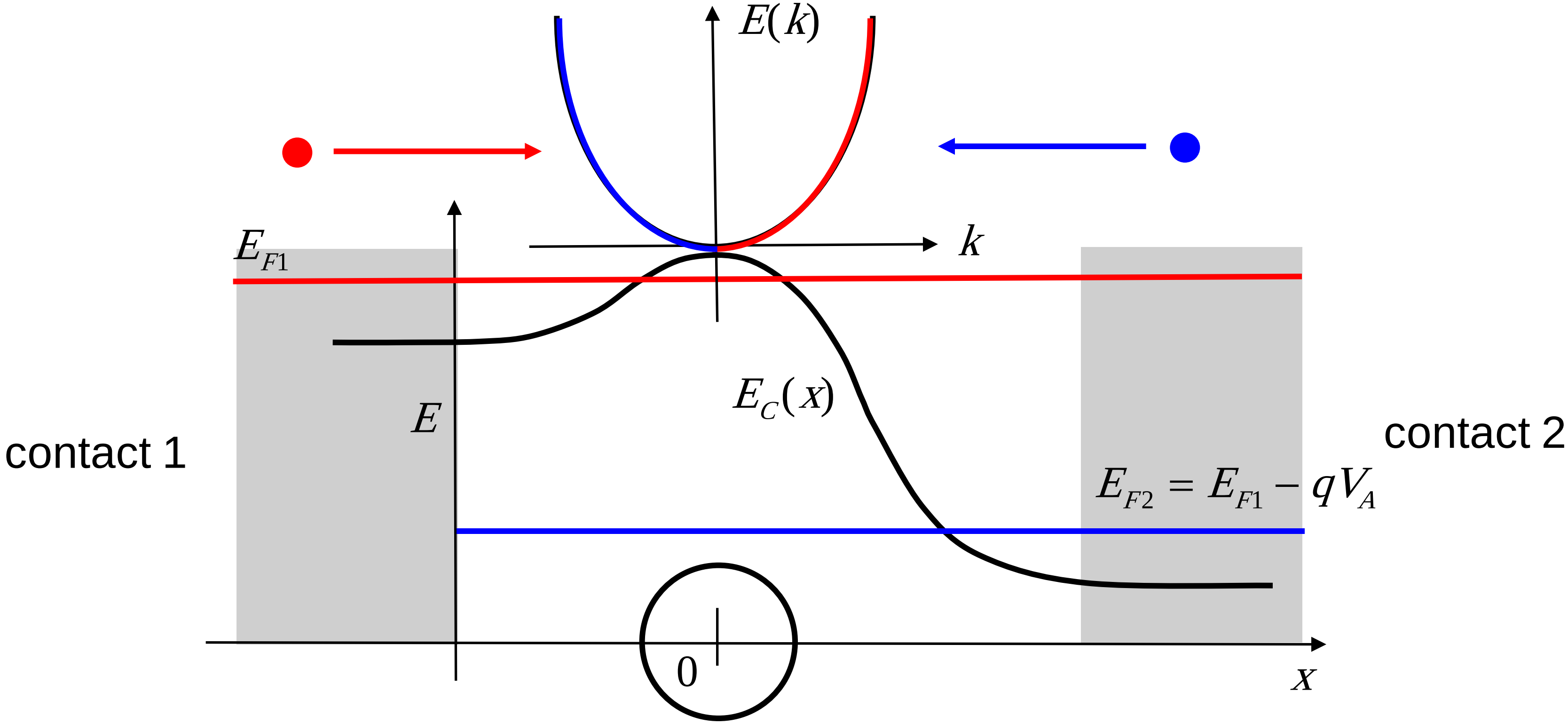
Within a ballistic device, the probability that a *k*-state is occupied is given by an equilibrium Fermi function.

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

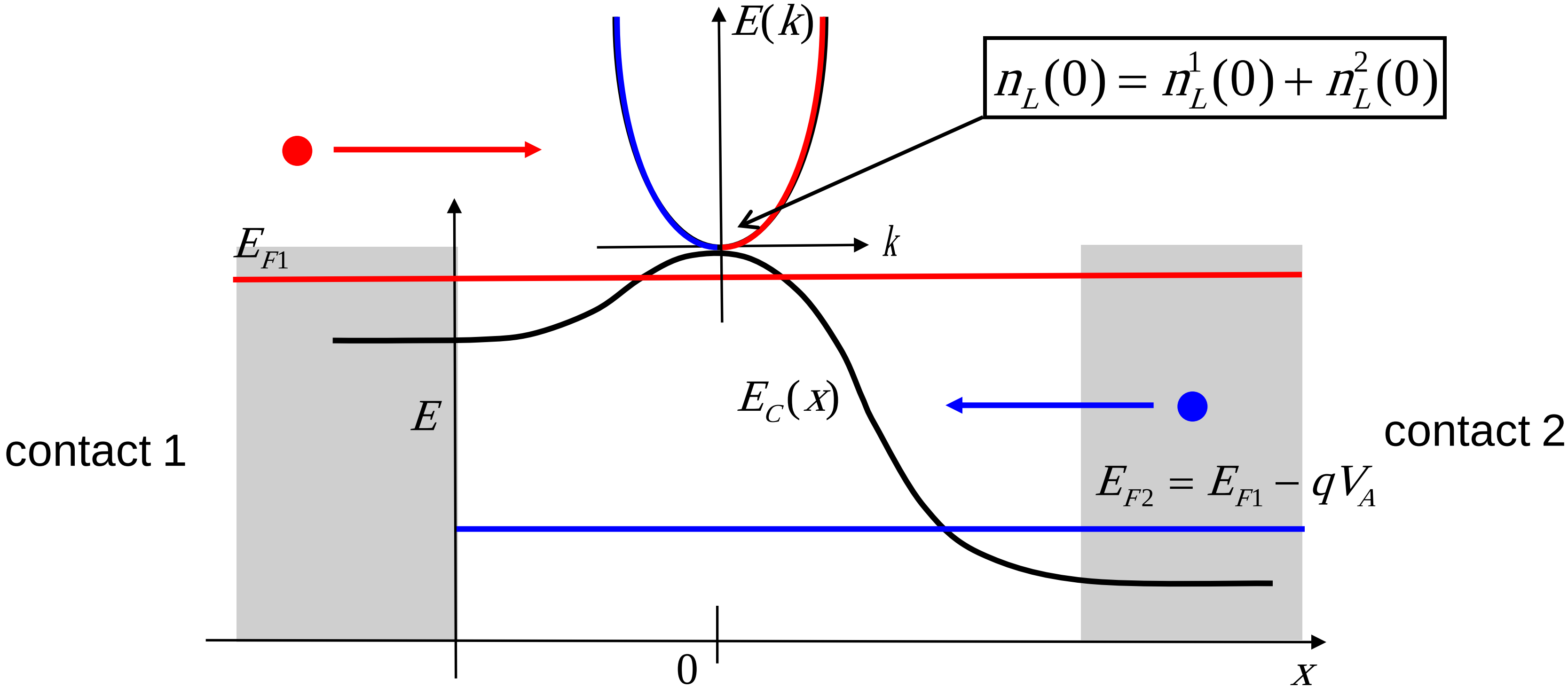
Within a ballistic device, each *k*-state is in **equilibrium** with one contact or the other.

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

example



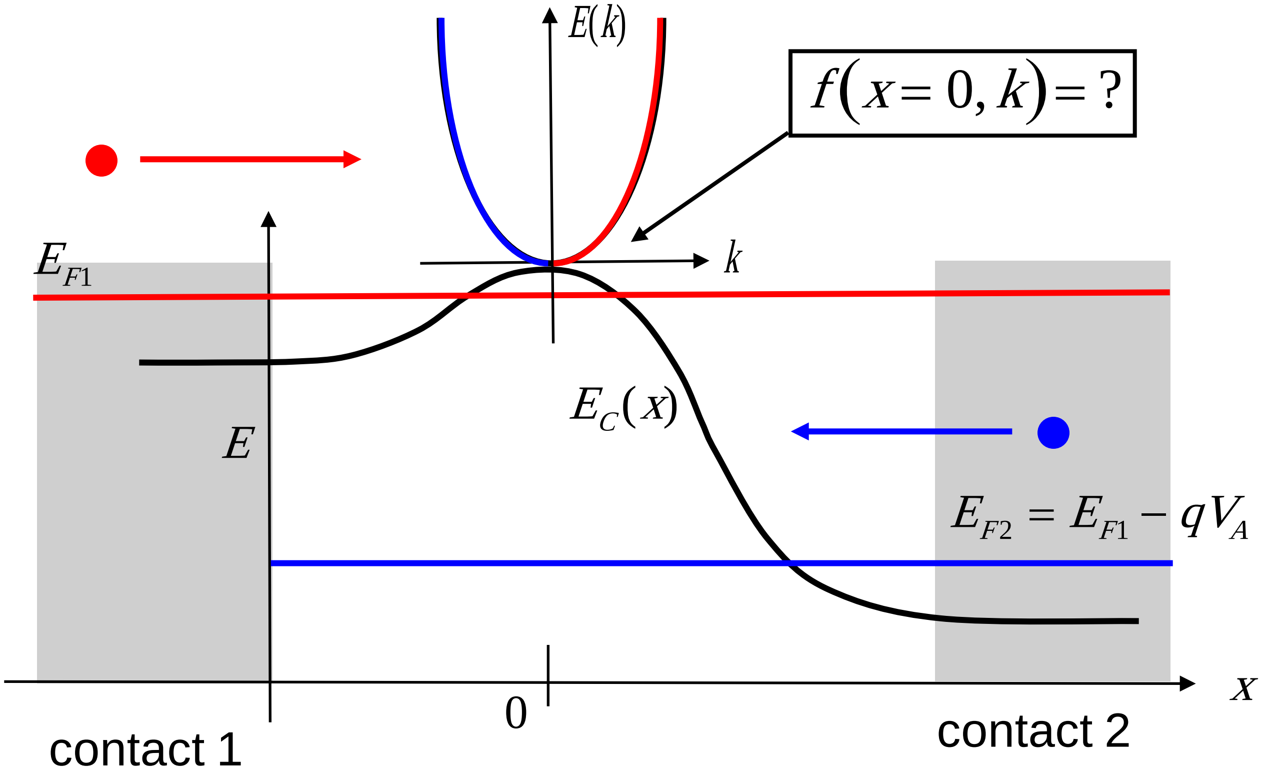
example

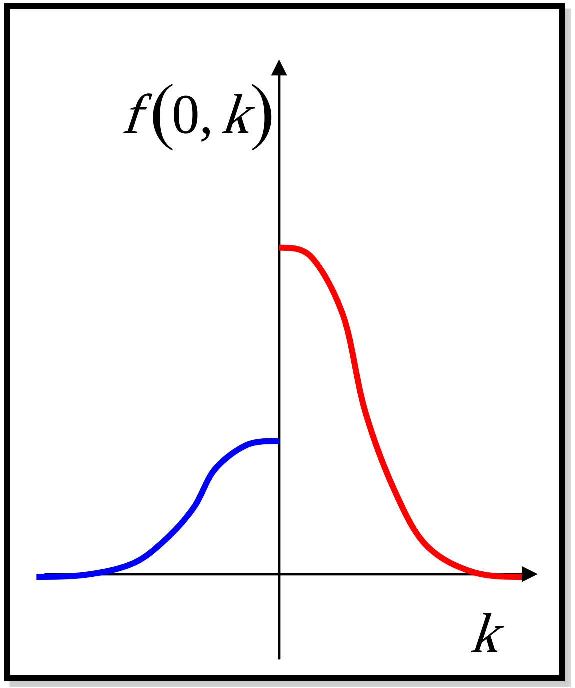


$$n_L^1(0) = n_L^+(0) = \frac{1}{L}\sum_{k_x>0} f_0(E_{F1}) \qquad n_L^1(0) = \int D_{1D}^1(0,E)\, f_0(E_{F1})\, dE$$

$$n_L^2(0) = n_L^-(0) = \frac{1}{L}\sum_{k_x<0} f_0(E_{F2}) \qquad n_L^2(0) = \int D_{1D}^2(0,E)\, f_0(E_{F2})\, dE$$

example

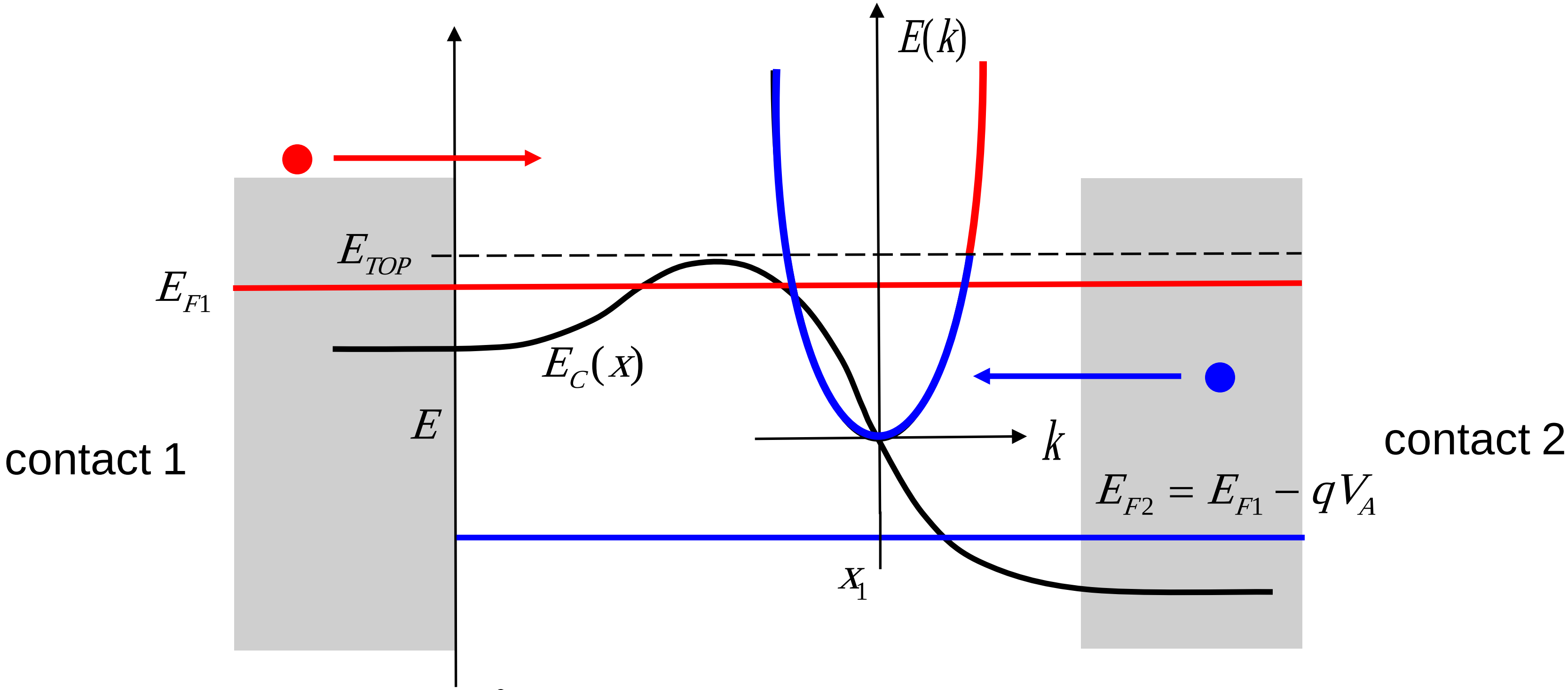




$$n_L(0)=\frac{1}{L}\sum_{k_x>0} f_0(E_{F1})+\frac{1}{L}\sum_{k_x<0} f_0(E_{F2})=\int D_{1D}^{1}(0,E)\,f_0(E_{F1})+D_{1D}^{2}(0,E)\,f_0(E_{F2})\,dE$$

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

another example

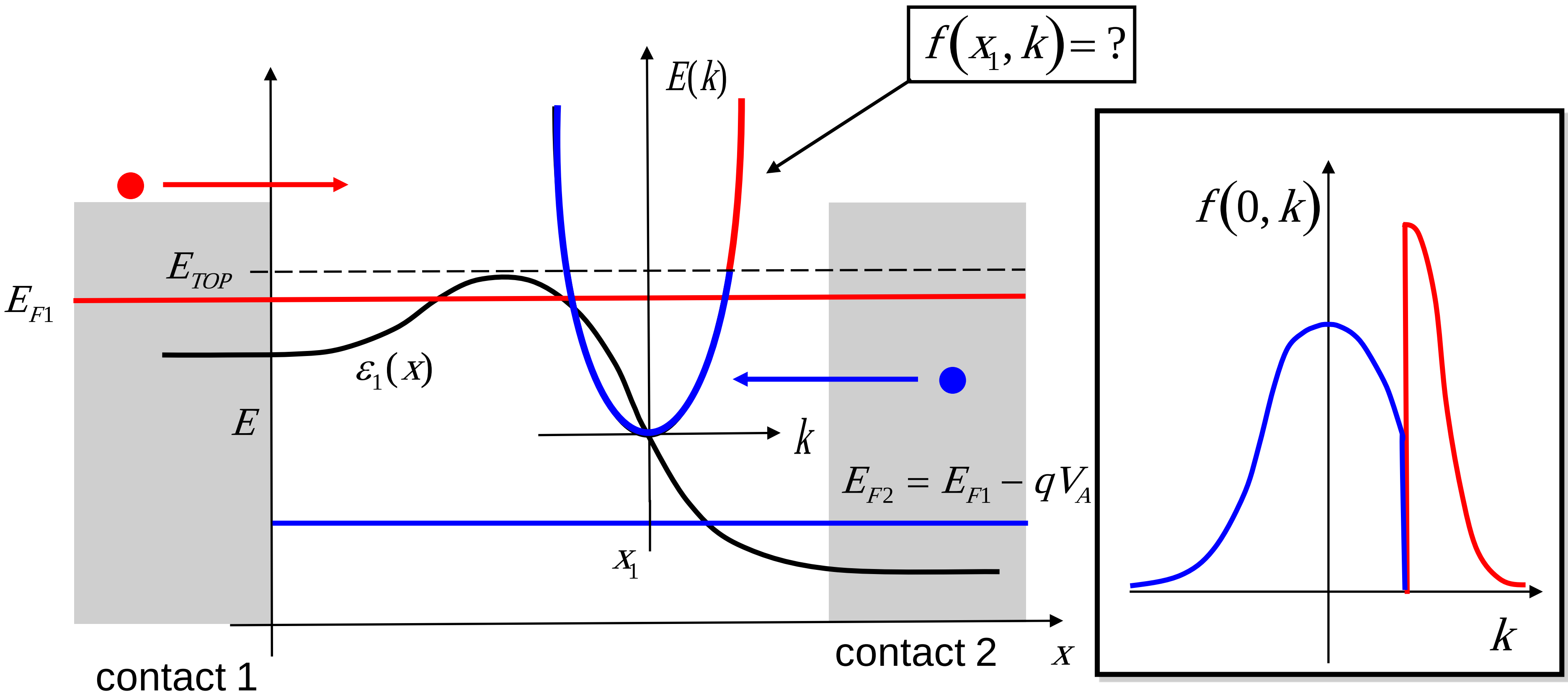


$$n_L(x_1) = \int D^1_{1D}(x_1, E)\, f_0(E_{F1}) + D^2_{1D}(x_1, E)\, f_0(E_{F2})\, dE$$

"local density of states"

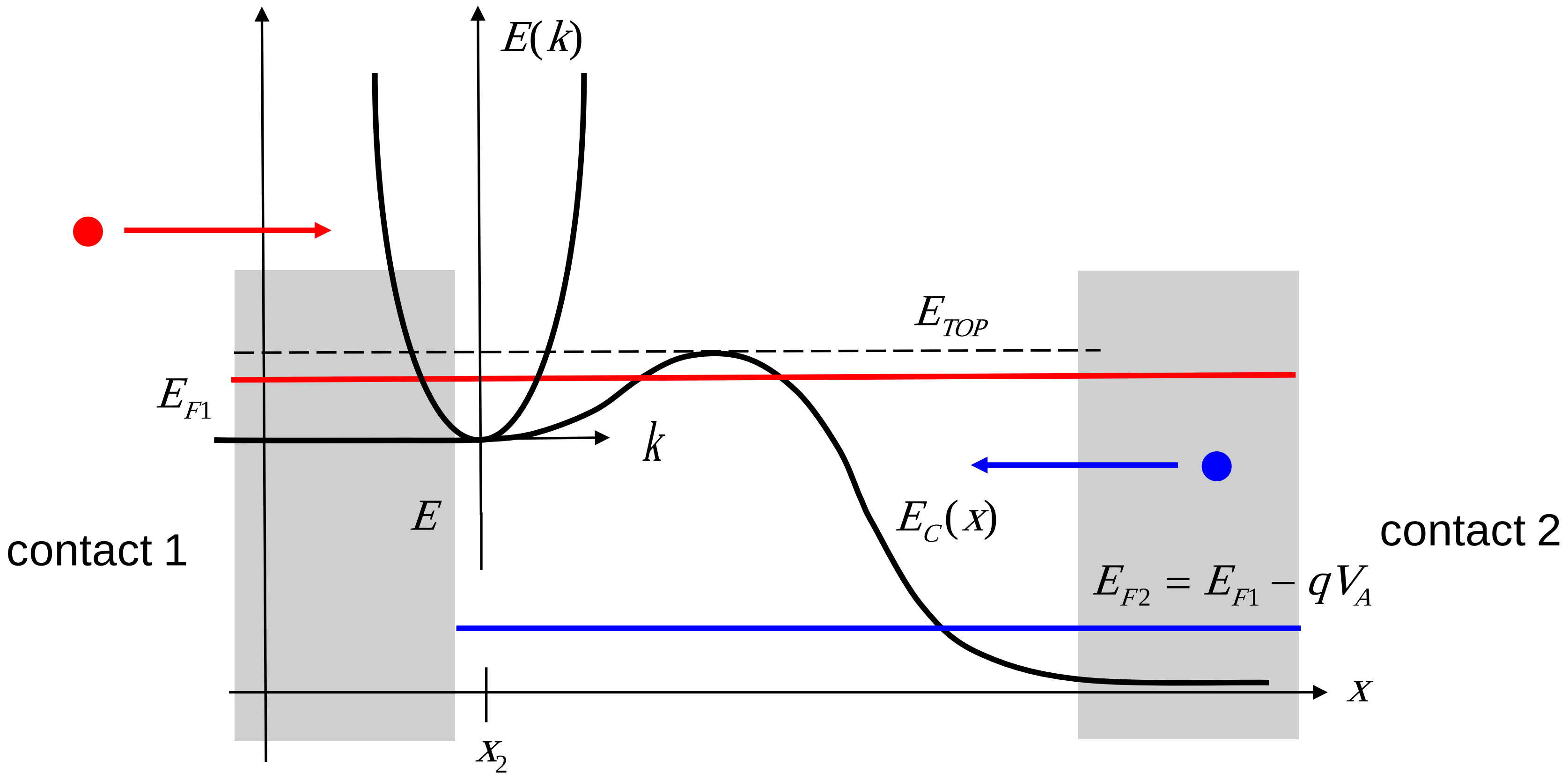
$$D^1_{1D}(x_1, E), D^2_{1D}(x_1, E) \neq D_{1D}(E)/2$$

distribution function

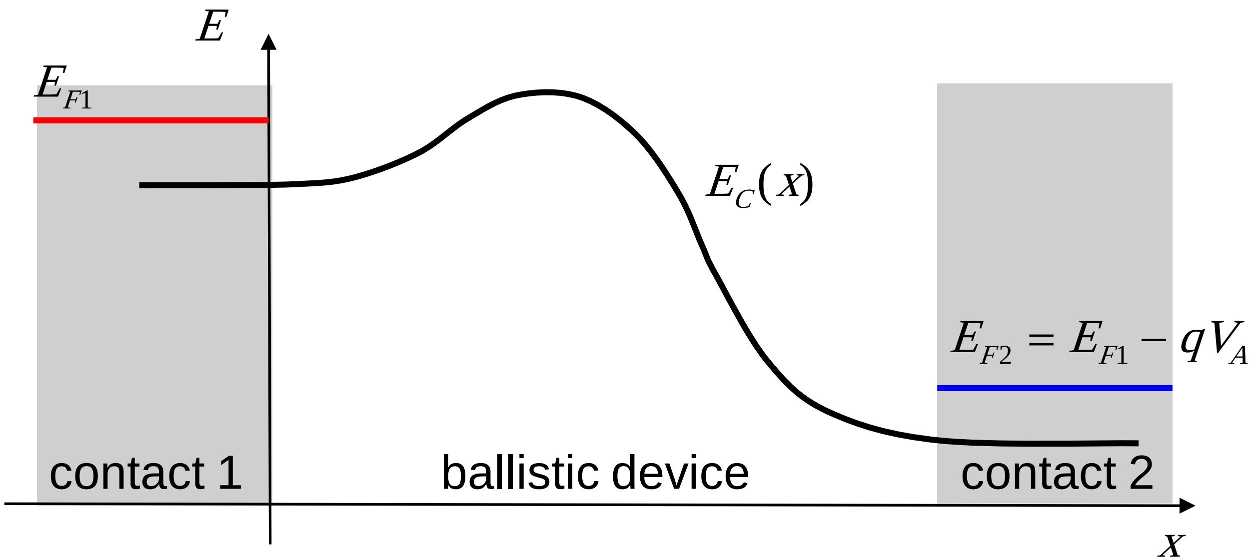


J.-H. Rhew, Zhibin Ren, and Mark Lundstrom, "A Numerical Study of Ballistic Transport in a Nanoscale MOSFET," Solid-State Electronics, **46**,1899, 2002.

suggested exercise



solution to the ballistic BTE: summary

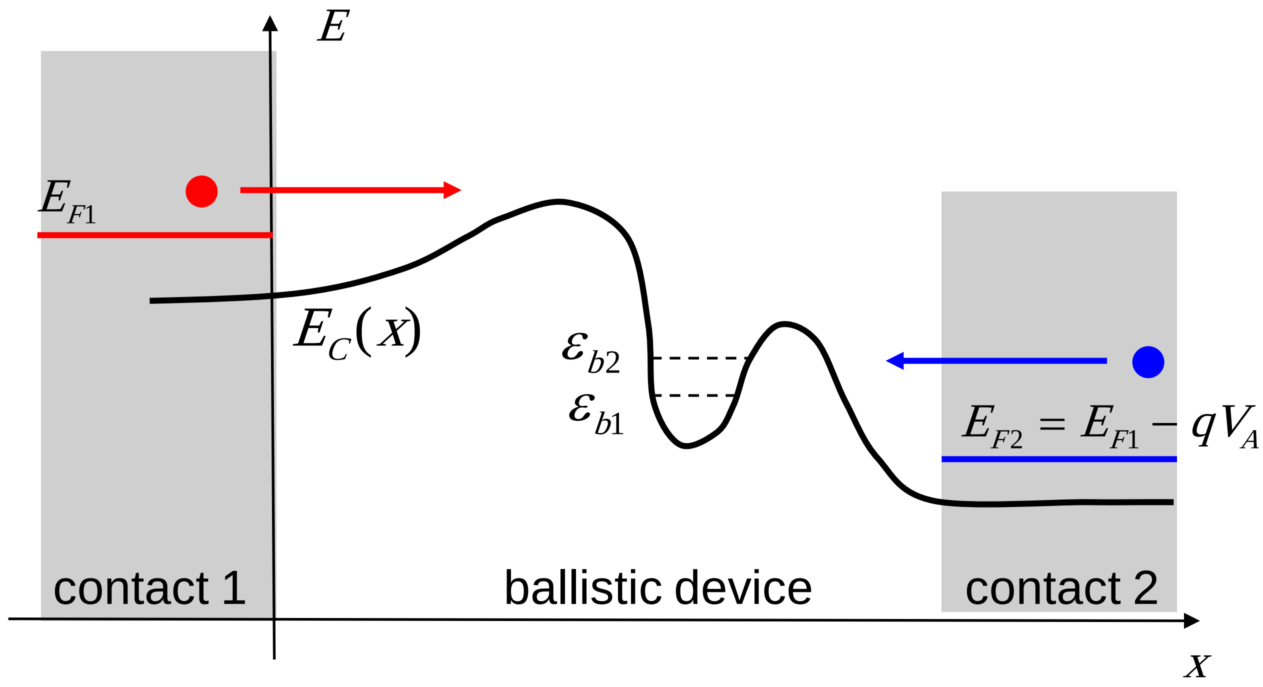


1) states divide into two parts, fillable by each of the contacts

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

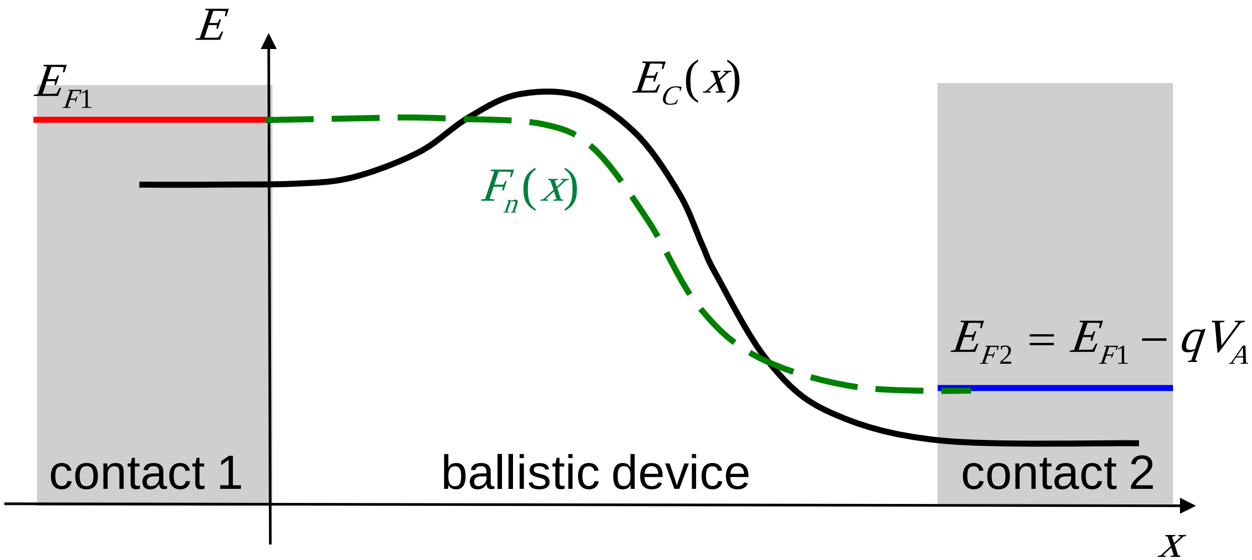
2) but….

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



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

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

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

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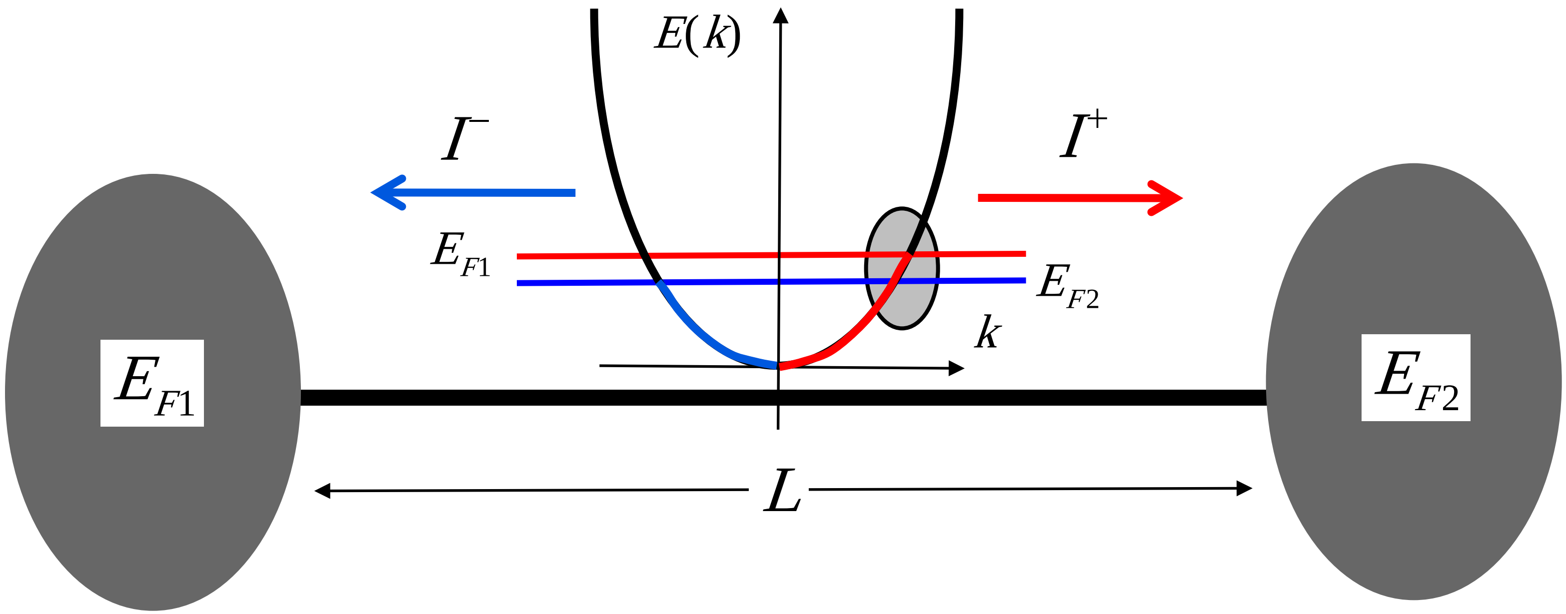
from Lecture 7



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

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

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

current

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

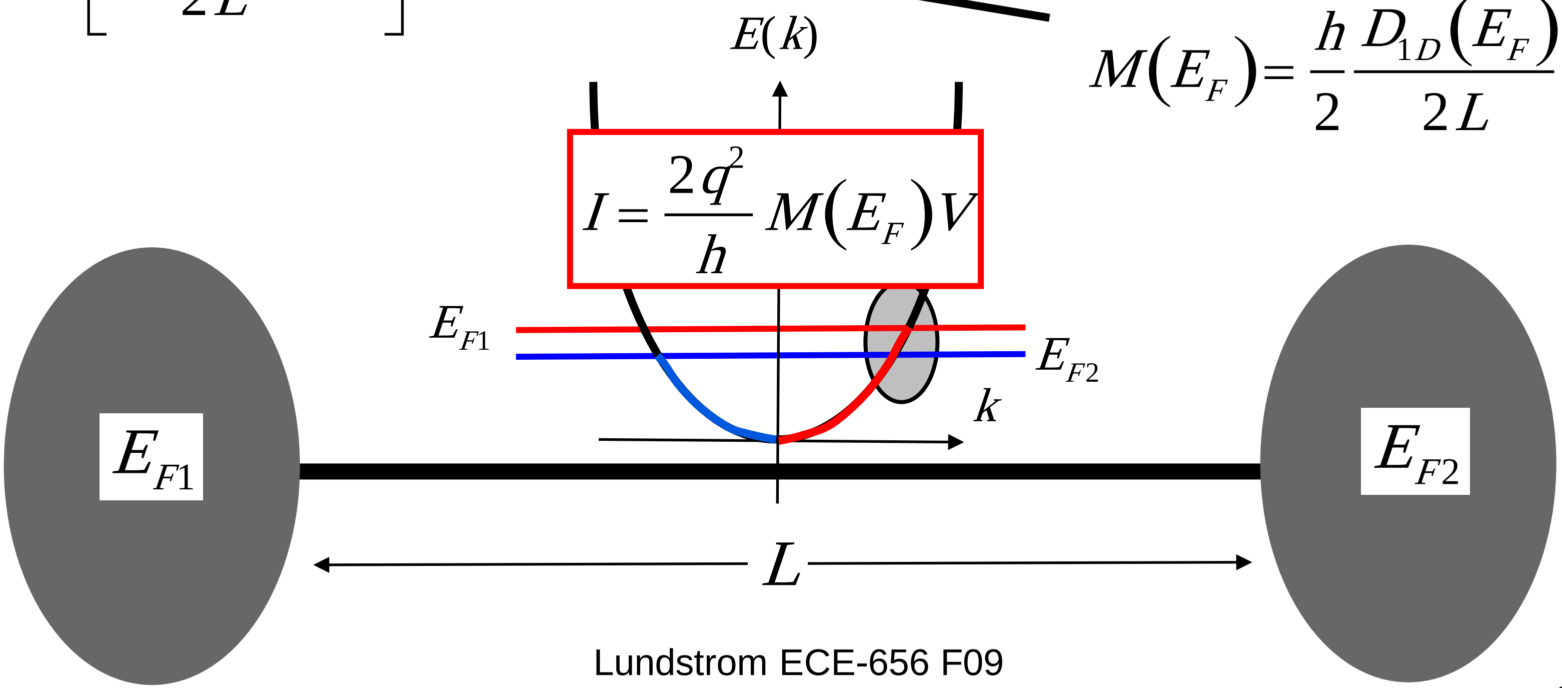
$$I = q^2\left[\frac{D_{1D}(E_F)}{2L}\upsilon_F\right]V$$

$$M(E_F) = \gamma(E_F)\pi\frac{D_{1D}(E_F)}{2}$$

$$\gamma(E_F) = \frac{\mathrm{h}}{\tau} = \frac{\mathrm{h}}{L/\upsilon_F}$$

$$M(E_F) = \frac{h}{2}\frac{D_{1D}(E_F)}{2L}\upsilon_F$$

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



questions

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