Lecture17

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Goal

- Application to a specific system
  - At the steady-state, the lowest expansion reads

$$\frac{\partial}{\partial x}\frac{1}{c_1} vZdH f_1(x,H)\Upsilon_{1,0,1} = ZdH\hat{S}_0$$

$$vZdH\frac{\partial}{\partial x}\frac{1}{c_1} f_0(x,H)\Upsilon_{0,1,1} = ZdH\hat{S}_1$$

  - Today, we will apply it to a specific system: Elastic scattering + parabolic band structure

Scattering (1)

- General relation
  - For a scattering whose enery transfer is ΔE, the scattring term is given by

$$\hat{S} = -\frac{1}{(2\pi)^2}\iint S\delta\big(\epsilon(k,\phi) + \Delta E - \epsilon(k',\phi')\big)\,\big(1 - f(x,k',\phi')\big)f(x,k,\phi)\; k'dk'd\phi'$$

$$+\frac{1}{(2\pi)^2}\iint S\delta(\epsilon(k,\phi) - \epsilon(k',\phi') - \Delta E)\big(1 - f(x,k,\phi\,)\big)f(x,k',\phi')\; k'dk'd\phi'$$

  - First integral: Out-scattering, from (k,ϕ) to (k',ϕ')
  - Second integral: In-scattering, from (k',ϕ') to (k,ϕ)

Scattering (2)

- Expanded form

$$Z dH \hat{S}_0 = -dHSZ(\epsilon)Z(\epsilon + \Delta E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x, \epsilon + \Delta E)\right) f_0(x, \epsilon)$$
$$+dHSZ(\epsilon)Z(\epsilon - \Delta E)\frac{1}{c_0} f_0(x, \epsilon - \Delta E)\left(\frac{1}{c_0} - f_0(x, \epsilon)\right)$$

$$Z dH \hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon + \Delta E)\frac{1}{c_0}\left(\frac{1}{c_0} - f_0(x, \epsilon + \Delta E)\right) f_1(x, \epsilon)$$
$$-dHSZ(\epsilon)Z(\epsilon - \Delta E)\frac{1}{c_0} f_0(x, \epsilon - \Delta E) f_1(x, \epsilon)$$

Scattering (3)

- Without the Pauli principle

$$ZdH\hat{S}_0 = -dHSZ(\epsilon)Z(\epsilon + \Delta E)\frac{1}{c_0^2}f_0(x,\epsilon)$$

$$+dHSZ(\epsilon)Z(\epsilon - \Delta E)\frac{1}{c_0^2}f_0(x,\epsilon - \Delta E)$$

$$ZdH\hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon + \Delta E)\frac{1}{c_0^2}f_1(x,\epsilon)$$

  – It is noted that the Pauli principle is necessary in many practical cases.

Elastic scattering

- Let us assume that $\Delta E \to 0$.
  - In this case,

$$ZdH\hat{S}_0 = 0$$

$$ZdH\hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon)\frac{1}{c_0^2}f_1(x,\epsilon)$$

  - In terms of the relaxation time, τ,

$$ZdH\hat{S}_1 = -dHSZ(\epsilon)Z(\epsilon)\frac{1}{c_0^2}f_1(x,\epsilon) = ZdH\left(-\frac{f_1}{\tau}\right)$$

where $\frac{1}{\tau} = SZ\frac{1}{c_0^2}$. In general, it can be a function of the energy.

Elastic scattering only

- Simplified equations
  - Using the relaxation time approximation,

$$\frac{\partial}{\partial x}\frac{1}{c_1}vZdHf_1(x,H)\Upsilon_{1,0,1} = 0$$

$$vZdH\frac{\partial}{\partial x}\frac{1}{c_1}f_0(x,H)\Upsilon_{0,1,1} = ZdH\left(-\frac{f_1(x,H)}{\tau}\right)$$

  - The second equation reveals that

$$-\tau v\frac{\partial}{\partial x}\frac{1}{c_1}f_0(x,H)\Upsilon_{0,1,1} = f_1(x,H)$$

  - By using the above equation, f_1 can be elliminated.

Elastic scattering only

- Second-order equation
  - After f_1 is elliminated, the equation for f_0 reads (Many constants are removed out.)

$$\frac{\partial}{\partial x}\left[\tau v^2 Z \frac{\partial}{\partial x} f_0(x, H)\right] = 0$$

Band structure

- Parabolic band structure
  - When we assume $\epsilon = \frac{\hbar^2}{2m}k^2$, $v = \sqrt{\frac{2\epsilon}{m}}$.
  - Since $Z = \frac{1}{(2\pi)^2}\frac{k}{v}$, we have $vZ = \frac{k}{(2\pi)^2} = \frac{1}{(2\pi)^2\hbar}\sqrt{2m\epsilon}$.
  - Then, $\tau v^2 Z = \tau\frac{2\epsilon}{(2\pi)^2}$.
  - Under the constant relaxation time, (Constants are removed again.)

$$\frac{\partial}{\partial x}\left[(H + qV)\frac{\partial}{\partial x}f_0(x, H)\right] = 0$$

Goal

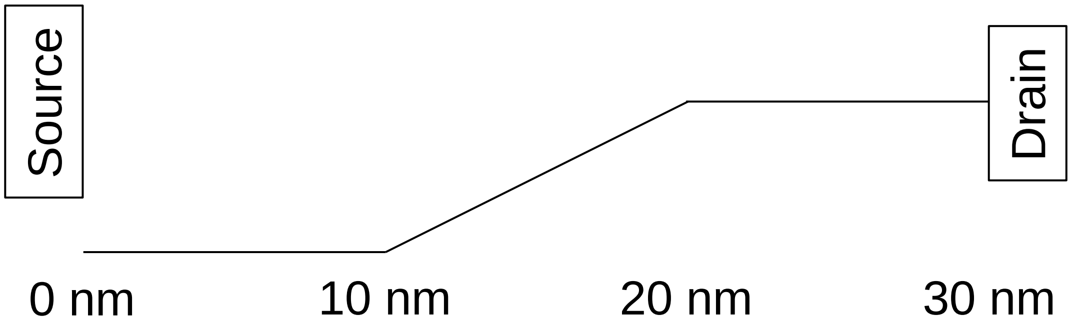
- Implementation
  - For a parabolic band system only with an elastic scattering, the Boltzmann transport equation can be written as

$$\frac{\partial}{\partial x}\left[(H+qV)\frac{\partial}{\partial x}f_0(x,H)\right]=0$$

  - Today, we will solve the above equation.

Structure

- Consider a 30-nm-long structure.
  - From 0 nm to 10 nm, V vanishes.
  - From 10 nm to 20 nm, V increases linearly.
  - From 20 nm to 30 nm, $V = V_D > 0$.
  - The potential profile looks like:



Boundary condition

- We must specify f_0 at both ends.
  - At 0 nm, we assume that

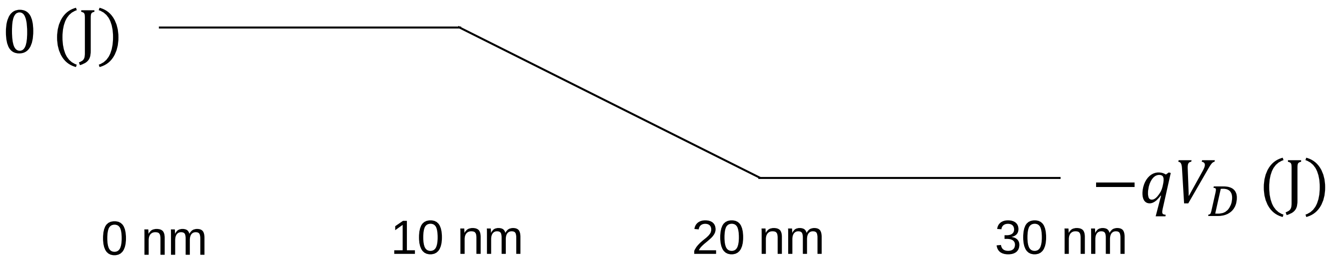
$$f_0(0, H) = \sqrt{2\pi}\frac{1}{1 + \exp\left(\frac{H}{k_B T}\right)}$$

  - At 30 nm, where $V = V_D > 0$, we assume that

$$f_0(30\mathrm{nm}, H) = \sqrt{2\pi}\frac{1}{1 + \exp\left(\frac{H + qV_D}{k_B T}\right)}$$

Cases

- When H is smaller than $-qV_D$,
  - There is no available state at all.
- When H is larger than $-qV_D$, but smaller than 0,
  - No connection to the source terminal
- Therefore, we will consider only $H > 0$.
- Energy diagram



Discretization

- Integrated around $x = x_i$
  - Now we have

$$(H + qV_{i+0.5})\frac{f_0(x_{i+1}, H) - f_0(x_i, H)}{\Delta x} - (H + qV_{i-0.5})\frac{f_0(x_i, H) - f_0(x_{i-1}, H)}{\Delta x} = 0$$

  - Of course, Δx can be easily removed out.
  - Coefficient for $f_0(x_{i+1}, H)$: $H + qV_{i+0.5}$
  - Coefficient for $f_0(x_i, H)$: $-2H - qV_{i+0.5} - qV_{i-0.5}$
  - Coefficient for $f_0(x_{i-1}, H)$: $H + qV_{i-0.5}$

MATLAB example (1)

- In this example, 300 intervals are introduced.
  - Constants are defined.

```
q = 1.602192e-19; % Elementary charge, C
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
```

  - First, set H and V_D.

```
H = 0.1; % (eV)
VD = 0.001; % (V)
```

  - Next, set the number of points.

```
N = 301;
interface1 = 101;
interface2 = 201;
```

MATLAB example (2)

- Preparation of some quantities
  - The boundary values are calculated.

```
fs = sqrt(2*pi)/(1 + exp(q*H/(k_B*T)));
fd = sqrt(2*pi)/(1 + exp(q*(H+VD)/(k_B*T)));
```

  - For that purpose, V is prepared.

```
V = zeros(N,1);
V(interface1:interface2,1) = [0:1/(interface2-interface1):1]*VD;
V(interface2:N,1) = VD;
```

MATLAB example (3)

- Then, the matrix is constructed.
  - Like the Poisson equation,

```
A = zeros(N,N);
A(1,1) = 1.0;
for ii=2:N-1
   c1 = H + 0.5*(V(ii,1)+V(ii-1,1));
   c2 = H + 0.5*(V(ii+1,1)+V(ii,1));
   A(ii,ii-1) = c1; A(ii,ii) = -c1-c2; A(ii,ii+1) = c2;
end
A(N,N) = 1.0;
```

MATLAB example (4)

- The boundary condition is imposed.
  - For that purpose, V is prepared.

```
b = zeros(N,1);
b(1,1) = fs;
b(N,1) = fd;
```

  - Now solve it.

```
f0 = A \ b;
```