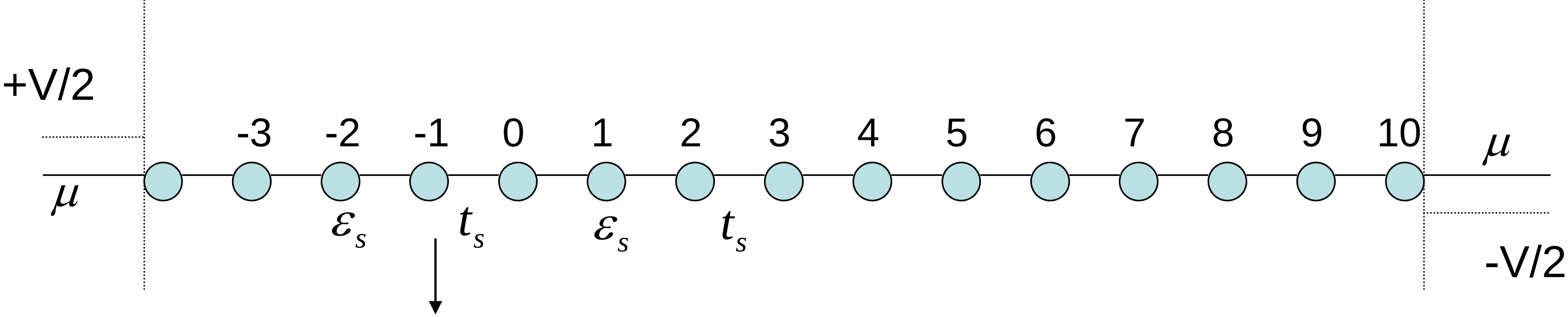
Infinite Chain of atoms with only one s-electron per atom:



$$\begin{cases} t_s\psi_{p-1} + (\varepsilon_s - E)\psi_p + t_s\psi_{p+1} = 0 \\ \Rightarrow \psi_p \propto e^{ikp} \text{ and } \mathrm{E} - \varepsilon_s = t_s(e^{ik} + e^{-ik}) = 2t_s\cos k \end{cases}$$

$$\begin{cases} \varepsilon_s = \int dr^3 \varphi_s^*(r) H \varphi_s(r) \\ t_s = \int dr^3 \varphi_s^*(r) H \varphi_s(r+a) \end{cases}$$

(Onsite and overlap energies for s-orbitals: φ_s)

$$I(\mu) = -e\int_{-\pi}^{\pi} \underbrace{D(k)}_{\frac{1}{\pi}} \times \underbrace{v(k)}_{\frac{1}{\hbar}\frac{\partial E}{\partial k}} \times \underbrace{f_{FD}(k)}_{\text{Occ.Prob.}} dk = -2\frac{e}{h}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} f_{FD}(E-\mu)\,dE$$

Dens. of states velocity

Chemical potential

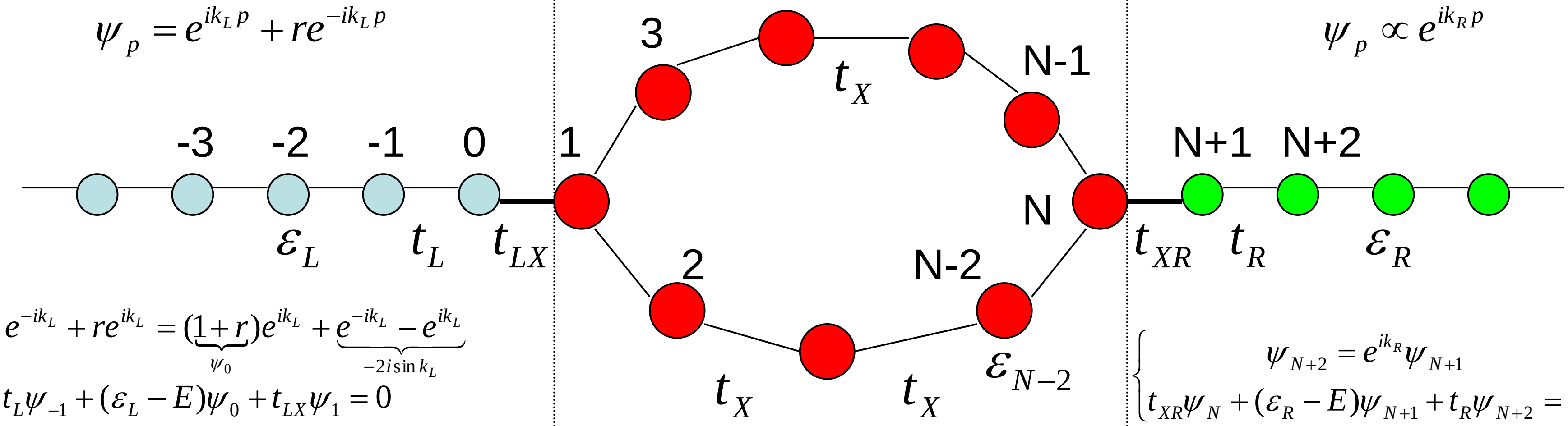
Fermi-Dirac distribution

$$I_{tot} = I_{Left}(\underbrace{\mu_L}_{\mu+eV/2}) - I_{Right}(\underbrace{\mu_R}_{\mu-eV/2}) = I(V) = \frac{2e}{h}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \left(\frac{1}{1+e^{\frac{E-\mu+eV/2}{kT}}} - \frac{1}{1+e^{\frac{E-\mu-eV/2}{kT}}} \right) dE$$

Left Lead	Molecule	Right Lead

$$\psi_p = e^{ik_L p} + re^{-ik_L p}$$

$$\psi_p \propto e^{ik_R p}$$



Left Lead:

$$\begin{cases} \psi_{-1} = e^{-ik_L} + re^{ik_L} = (\underbrace{1+r}_{\psi_0})e^{ik_L} + \underbrace{e^{-ik_L} - e^{ik_L}}_{-2i\sin k_L} \\ t_L\psi_{-1} + (\varepsilon_L - E)\psi_0 + t_{LX}\psi_1 = 0 \end{cases}$$

$$\Rightarrow -2it_L \sin k_L + (t_L e^{ik_L} \underbrace{+\varepsilon_L - E}_{-t_L(e^{ik_L}+e^{-ik_L})})\psi_0 + t_{LX}\psi_1 = 0$$

$$\Rightarrow \psi_0 = \frac{t_{LX}}{t_L} e^{ik_L}\psi_1 - 2ie^{ik_L}\sin k_L$$

Molecule:

$$\begin{cases} t_{LX}\psi_0 + (\varepsilon_1 - E)\psi_1 + t_X\psi_2 + t_X\psi_3 = 0 \\ \vdots \\ t_X\psi_{N-2} + t_X\psi_{N-1} + (\varepsilon_N - E)\psi_N + t_{XR}\psi_{N+1} = 0 \end{cases}$$

Right Lead:

$$\begin{cases} \psi_{N+2} = e^{ik_R}\psi_{N+1} \\ t_{XR}\psi_N + (\varepsilon_R - E)\psi_{N+1} + t_R\psi_{N+2} = 0 \end{cases}$$

$$\Rightarrow t_{XR}\psi_N + (\underbrace{\varepsilon_R - E}_{-t_R(e^{ik_R}+e^{-ik_R})} + t_R e^{ik_R})\psi_{N+1} = 0$$

$$\Rightarrow \psi_{N+1} = \frac{t_{XR}}{t_R} e^{ik_R}\psi_N$$

$$\underbrace{\begin{pmatrix} \frac{t_{LX}^2}{t_L}e^{ik_L}+\varepsilon_1-E & t_X & t_X & 0 & \cdots & 0 \\ t_X & \varepsilon_2-E & 0 & t_X & \cdots & 0 \\ \vdots & & \ddots & & & \vdots \\ 0 & \cdots & & & & \varepsilon_N-E+\frac{t_{XR}^2}{t_R}e^{ik_R} \end{pmatrix}}_{H_X+\Sigma-E} \underbrace{\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}}_{\psi} = \underbrace{\begin{pmatrix} 2it_{LX}e^{ik_L}\sin k_L \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_{-J_L}$$

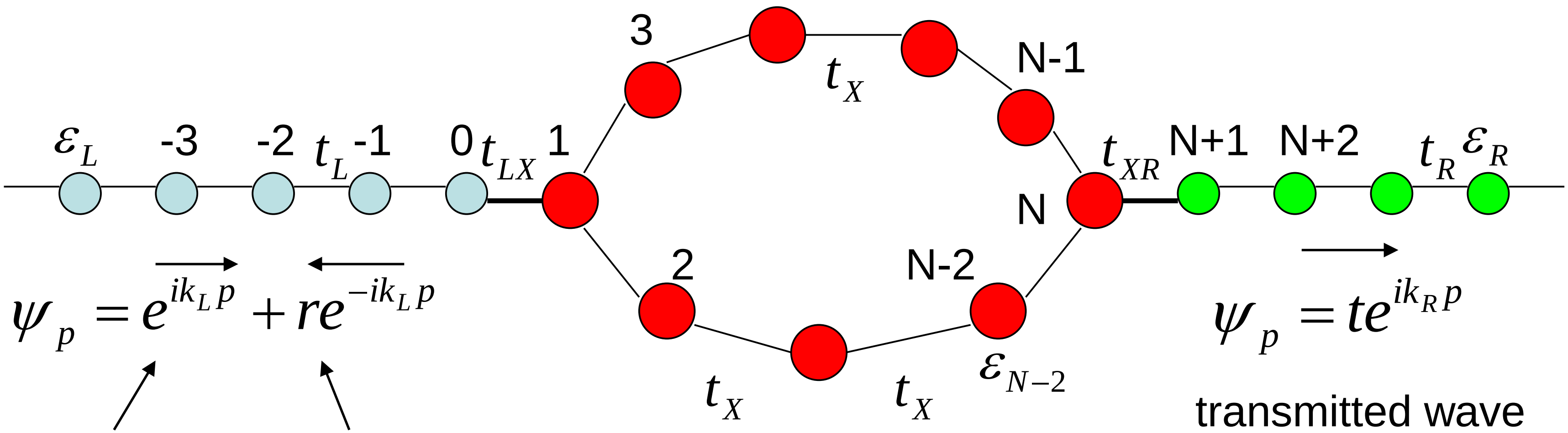
Hamiltonian of X | Self-energy | Energy | Wavefunction | Source function

$$H_X=\begin{pmatrix} \varepsilon_1 & t_X & \cdots & 0 \\ t_X & \varepsilon_2 & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & \varepsilon_N \end{pmatrix} \quad \Sigma=\begin{pmatrix} \frac{t_{LX}^2}{t_L}e^{ik_L} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & \frac{t_{XR}^2}{t_R}e^{ik_R} \end{pmatrix} \quad E=\begin{pmatrix} E & 0 & \cdots & 0 \\ 0 & E & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & E \end{pmatrix}$$

$$\begin{cases} (H_X+\Sigma-E)\psi=-J_L \\ \Rightarrow \psi = \underbrace{(E-H_X-\Sigma)^{-1}}_{G(E)} J_L \end{cases}$$

(Green's function)

$$\psi_n=\left[G(E)\right]_{(n,1)}(-2it_{LX}e^{ik_L}\sin k_L)$$



$$\psi_p = e^{ik_L p} + re^{-ik_L p}$$

Incoming and reflected wave

$$\psi_p = te^{ik_R p}$$

transmitted wave

$$j_L = \frac{2it_L}{\hbar}\sin k_L \times (1 - r^2) \longleftarrow \text{Current probabilities} \longrightarrow j_R = \frac{2it_R}{\hbar}\sin k_R \times (t^2)$$

$$\left(j = \frac{i\hbar}{2m}\left[\psi \nabla \psi^* - \psi^* \nabla \psi\right] \right)$$

But current probablities are conserved:

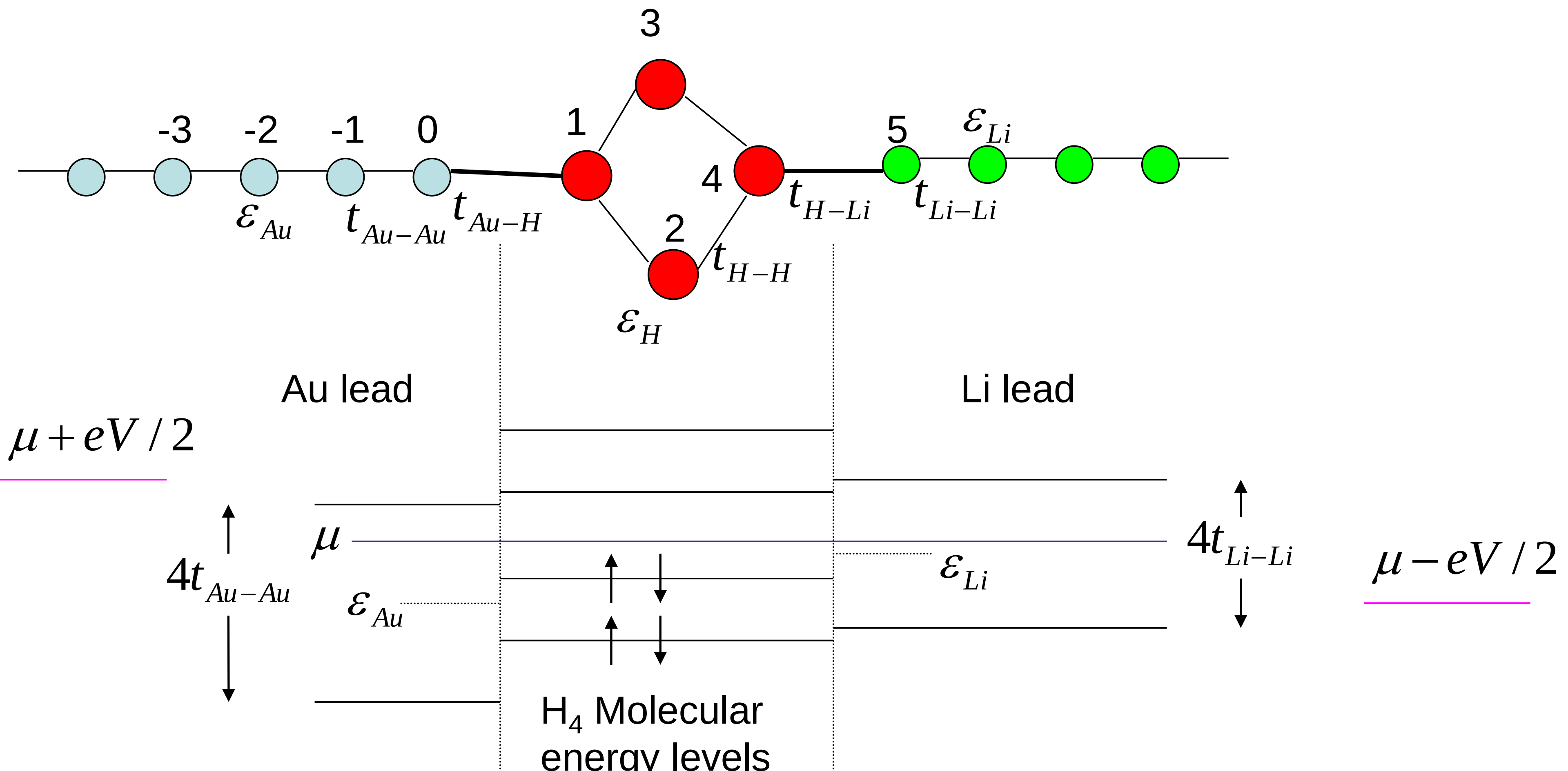
$$\Rightarrow t^2 = \left| \frac{t_L \sin k_L}{t_R \sin k_R} \right| \underbrace{(1 - r^2)}_{T(E)} = \left| \psi_{N+1} \right|^2$$

$$\Rightarrow T(E) = \left| \psi_{N+1} \right|^2 \times \left| \frac{t_R \sin k_R}{t_L \sin k_L} \right|$$

$$T(E)=\left|\psi_{N+1}\right|^2\times\left|\frac{t_R\sin k_R}{t_L\sin k_L}\right|=\left|\frac{t_{XR}^2 t_{LX}^2\,4\sin k_R\sin k_L\left|\left[G(E)\right]_{(N,1)}\right|^2}{t_R t_L}\right|$$

$$\begin{cases}\psi_{N+1}=\dfrac{t_{XR}}{t_R}e^{ik_R}\psi_N\\ \psi_N=\left[G(E)\right]_{(N,1)}(-2it_{LX}e^{ik_L}\sin k_L)\end{cases}$$

$$\Rightarrow I(V)=\frac{2e}{h}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}T(E)\left(\frac{1}{1+e^{\frac{E-\mu+eV/2}{kT}}}-\frac{1}{1+e^{\frac{E-\mu-eV/2}{kT}}}\right)dE$$



$$\mathrm{E} = \varepsilon_{Au} + 2t_{Au-Au} \cos k_{Au}$$

$$\Rightarrow \varepsilon_{Au} - 2t_{Au-Au} < E < \varepsilon_{Au} + 2t_{Au-Au}$$

$$\Rightarrow T(E) = 0 \ \text{ outside this range}$$

$$\mathrm{E} = \varepsilon_{Li} + 2t_{Li-Li} \cos k_{Li}$$

$$\Rightarrow \varepsilon_{Li} - 2t_{Li-Li} < E < \varepsilon_{Li} + 2t_{Li-Li}$$

$$\Rightarrow T(E) = 0 \ \text{ outside this range}$$

$$\Rightarrow I(V) = \frac{2e}{h}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} T(E)\left(\frac{1}{1+e^{\frac{E-\mu+eV/2}{kT}}} - \frac{1}{1+e^{\frac{E-\mu-eV/2}{kT}}}\right)dE$$

$$\begin{cases} \varepsilon_{\min} = \varepsilon_{Li} - 2t_{Li-Li} \\ \varepsilon_{\max} = \varepsilon_{Au} + 2t_{Au-Au} \end{cases}$$

Numerical procedure

- 1st step: Chose units (Energy and kT in eV, 1 meV = 11.6 K)
- 2nd step: Chose a voltage V=V1 and assume you know T(E)
- 3rd step: Perform the integral

$$\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} f(E)dE \cong step \times \sum_{i=0}^{(\varepsilon_{\max}-\varepsilon_{\min})/step} f(\varepsilon_{\min} + step \times i) \quad \text{Matlab}: \begin{cases} E = [\varepsilon_{\min} : step : -\varepsilon_{\max}] \\ Int = step \times sum(f(E)) \end{cases}$$

- 4th step: Repeat for different voltages

$$T(E)=\left|\frac{t_{H-Li}^2 t_{Au-H}^2\, 4\sin k_{Au}\sin k_{Li}\left|\left[G(E)\right]_{(4,1)}\right|^2}{t_{Li-Li}t_{Au-Au}}\right|$$

$$\mathrm{E}=\varepsilon_{Au}+2t_{Au-Au}\cos k_{Au}$$

$$\Rightarrow k_{Au}=a\cos\left((E-\varepsilon_{Au})/2t_{Au-Au}\right)$$

$$\text{and } k_{Li}=a\cos\left((E-\varepsilon_{Li})/2t_{Li-Li}\right)$$

$$G(E)=\begin{pmatrix} E-\varepsilon_H-\frac{t_{Au-H}^2}{t_{Au-Au}}e^{ik_{Au}} & -t_{H-H} & -t_{H-H} & 0 \\ -t_{H-H} & E-\varepsilon_H & 0 & -t_{H-H} \\ -t_{H-H} & 0 & E-\varepsilon_H & -t_{H-H} \\ 0 & -t_{H-H} & -t_{H-H} & E-\varepsilon_H-\frac{t_{H-Li}^2}{t_{Li-Li}}e^{ik_{Li}} \end{pmatrix}^{-1}$$

In Matlab:

X=[1 2 3 4;5 6 7 8;9 10 11 12;13 14 15 16]=

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

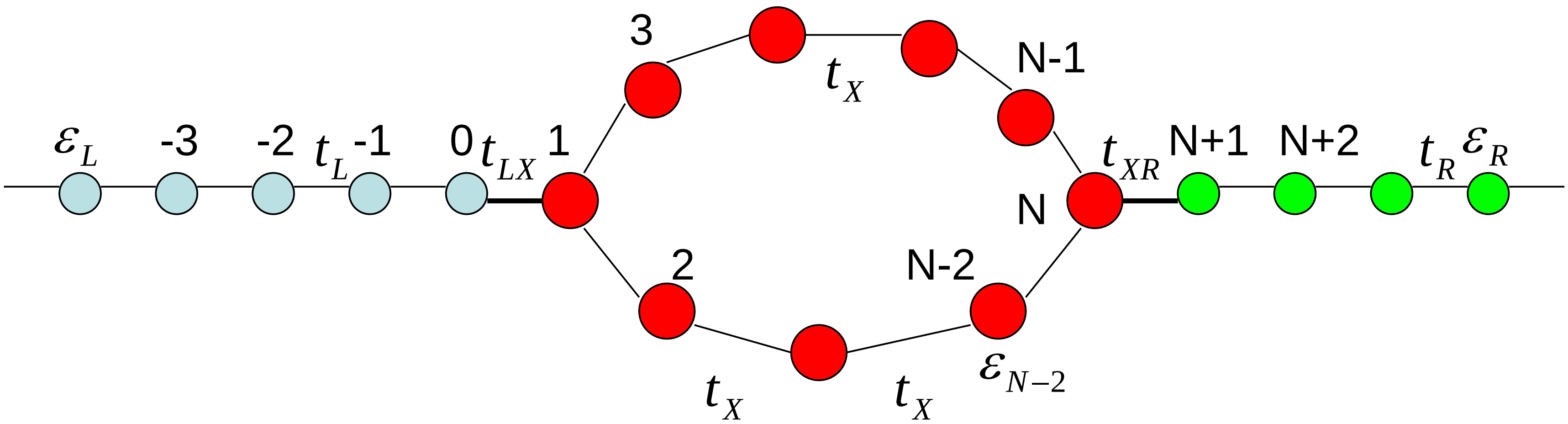
X^{-1}=inv(X); $\left[G(E)\right]_{(4,1)}$ =G(4,1);

Putting it all together:

- Chose a voltage (for example: V=1)
- Define the step for your energies; (for example: step=.0001)
- Define all your coefficients: $\varepsilon_{Li}, t_{Li-Li}, \varepsilon_{\min}, k_{Au}, \ldots$
- Define your energy interval: $E = [\varepsilon_{\min} : step : -\varepsilon_{\max}]$
- Calculate $\left[G(E)\right]_{(4,1)}$ for each E (use a loop)
- Calculate T(E) for each E
- Calculate I(V) (using the expression for the integral)
- Start over for different V (use a loop)

Loop example:

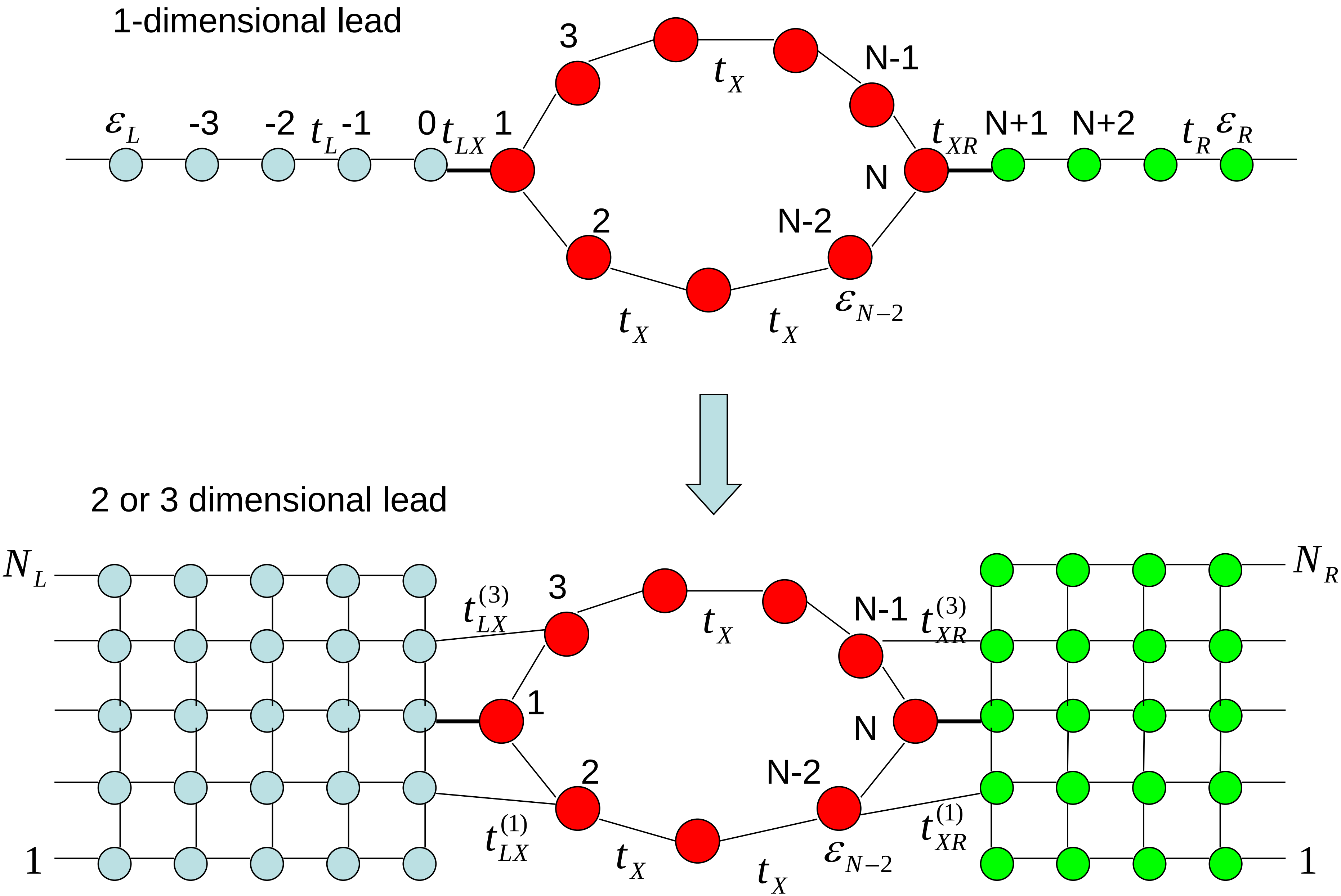
```
n=1;
for V=-5:.1:5,
I(n)=sin(V);n=n+1;
end;
```



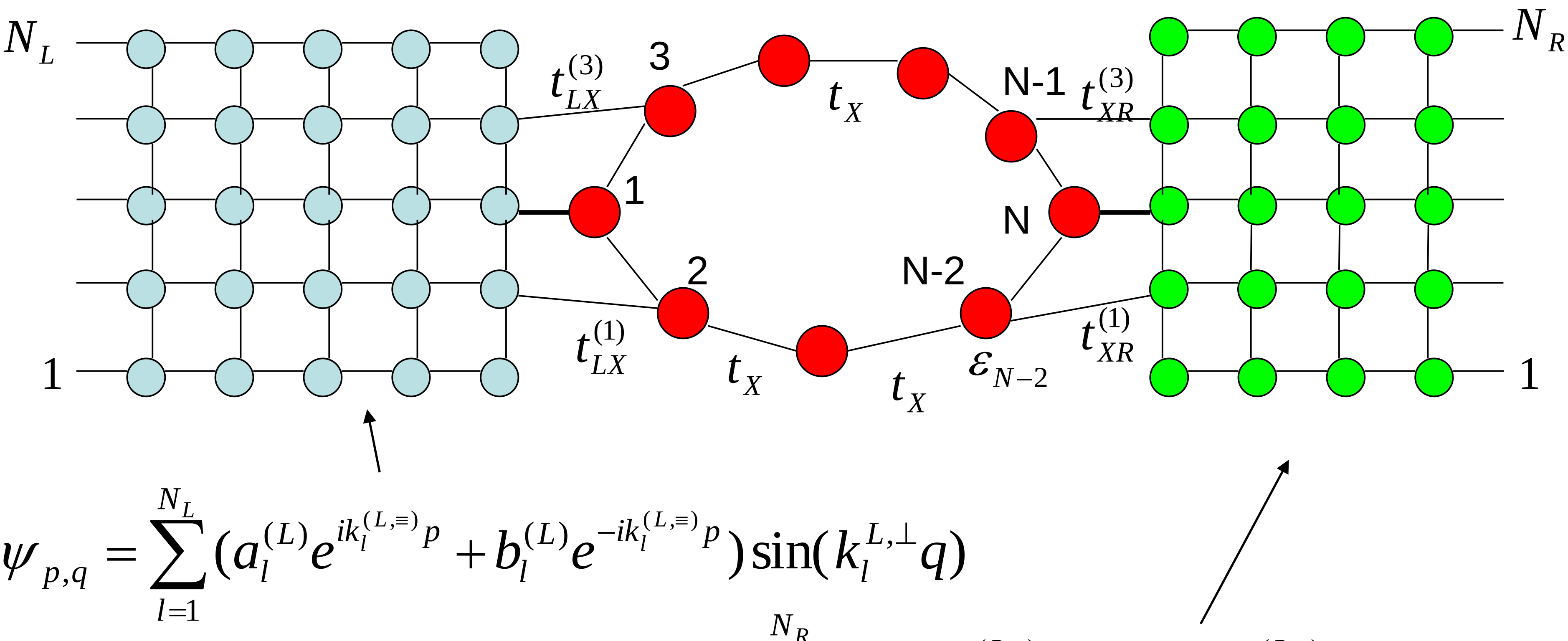
$$\begin{cases} T(E) = \left|\psi_{N+1}\right|^2 \times \left|\dfrac{t_R \sin k_R}{t_L \sin k_L}\right| = \left|\dfrac{t_{XR}^2 t_{LX}^2\, 4 \sin k_R \sin k_L \left|\left[G(E)\right]_{(N,1)}\right|^2}{t_R t_L}\right| \\ = 4 \cdot Tr\left[\Gamma_L G \Gamma_R G^+\right] \text{ (Fisher} - \text{Lee)} \end{cases}$$

$$\Gamma_L = \mathrm{Im}(\Sigma_L)$$
$$\Gamma_R = \mathrm{Im}(\Sigma_R)$$

$$\Sigma = \Sigma_L + \Sigma_R; \Sigma_L = \begin{pmatrix} \dfrac{t_{LX}^2}{t_L} e^{ik_L} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}; \Sigma_R = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & \dfrac{t_{XR}^2}{t_R} e^{ik_R} \end{pmatrix}$$



1-dimensional lead
2 or 3 dimensional lead
ε_L
-3
-2
t_L
-1
0
t_{LX}
1
2
3
t_X
N-1
N
N-2
ε_{N-2}
t_{XR}
N+1
N+2
t_R
ε_R
N_L
N_R
$t_{LX}^{(3)}$
$t_{LX}^{(1)}$
$t_{XR}^{(3)}$
$t_{XR}^{(1)}$



$$\psi_{p,q} = \sum_{l=1}^{N_L} \left(a_l^{(L)} e^{ik_l^{(L,\equiv)} p} + b_l^{(L)} e^{-ik_l^{(L,\equiv)} p}\right) \sin(k_l^{L,\perp} q)$$

$$\psi_{p,q} = \sum_{r=1}^{N_R} \left(a_r^{(R)} e^{ik_r^{(R,\equiv)} p} + b_r^{(R)} e^{-ik_r^{(R,\equiv)} p}\right) \sin(k_r^{R,\perp} q)$$

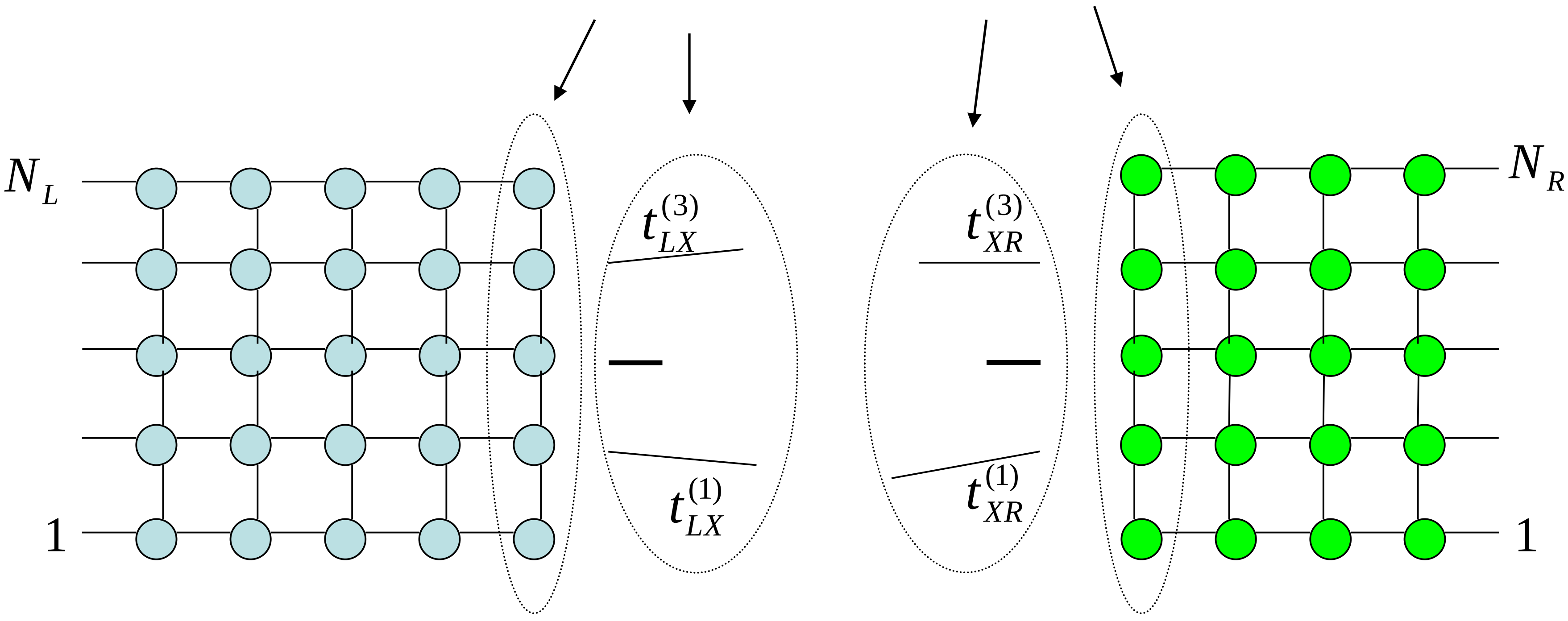
$$\begin{cases} t_L \psi_{p-1,q} + (\varepsilon_L - E)\psi_{p,q} + t_L \psi_{p+1,q} + t_L \psi_{p,q-1} + t_L \psi_{p,q+1} = 0 \\ \Rightarrow \psi_{p,q} \propto e^{ik^{(L,\equiv)} p} \sin(\mathrm{k}^{(\mathrm{L},\perp)} \mathrm{q}) \text{ and } \mathrm{E} - \varepsilon_L = 2t_L \left[\cos(k^{(L,\equiv)}) + \cos(k^{(L,\perp)})\right] \\ k_l^{(L,\perp)} = l \dfrac{\pi}{N_L + 1} ; k_r^{(R,\perp)} = r \dfrac{\pi}{N_R + 1} \end{cases}$$

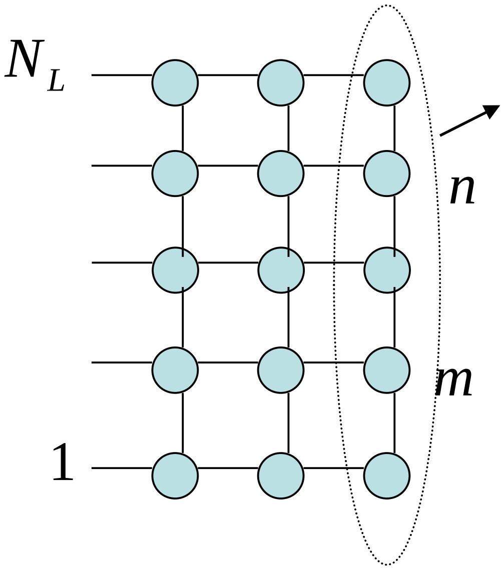
$$T(E) = 4 \cdot Tr\left[\Gamma_L G \Gamma_R G^+\right]$$

$$\Gamma_L = \mathrm{Im}(\Sigma_L)$$

$$\Gamma_R = \mathrm{Im}(\Sigma_R)$$

$$\Sigma_L = T_{XL} G_L^S T_{LX}; \Sigma_R = T_{XR} G_R^S T_{RX}$$

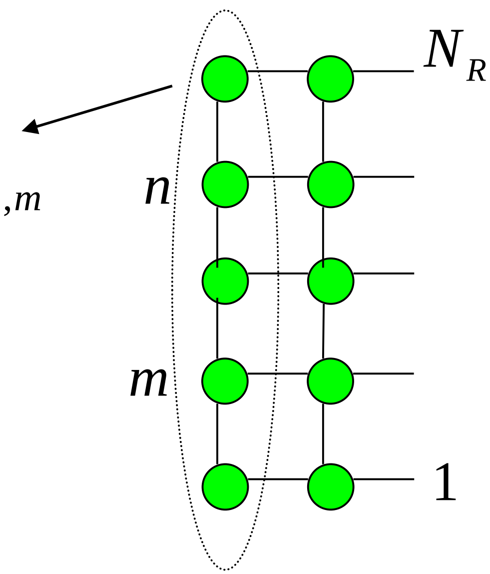




$$\left[G_L^S\right]_{n,m} = (-1)^{n-m}\frac{2}{L+1}\sum_{l=1}^{N_L}\frac{e^{ik_l^{(L,\equiv)}}}{t_L}\sin(k_l^{L,\perp}n)\sin(k_l^{L,\perp}m)$$

$$\begin{cases} \mathrm{E} - \varepsilon_L = 2t_L\left[\cos(k_l^{(L,\equiv)}) + \cos(k_l^{(L,\perp)})\right] \\ k_l^{(L,\perp)} = l\dfrac{\pi}{N_L+1} \end{cases}$$

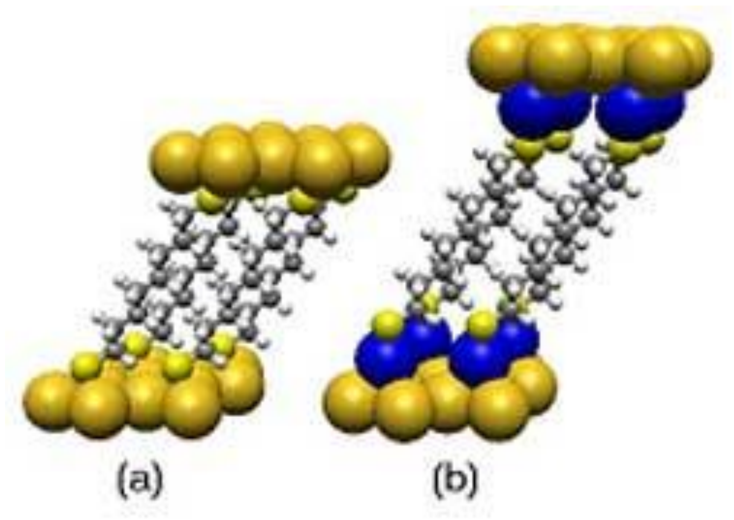
$$(-1)^{n-m}\frac{2}{R+1}\sum_{l=1}^{N_R}\frac{e^{ik_r^{(R,\equiv)}}}{t_R}\sin(k_r^{R,\perp}n)\sin(k_r^{R,\perp}m) = \left[G_R^S\right]_{n,m}$$

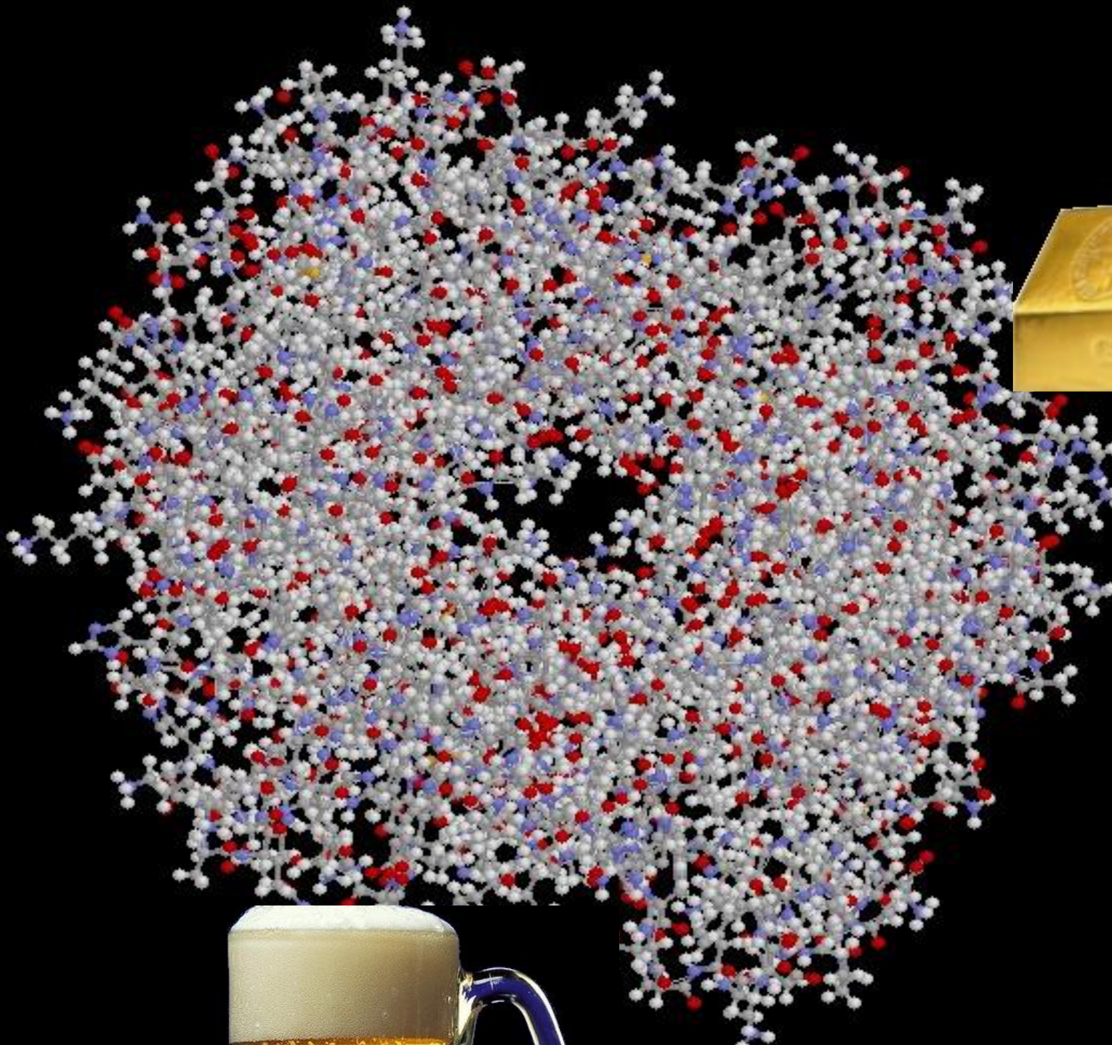


$$\begin{cases} \mathrm{E} - \varepsilon_R = 2t_R\left[\cos(k_r^{(R,\equiv)}) + \cos(k_r^{(R,\perp)})\right] \\ k_r^{(R,\perp)} = r\dfrac{\pi}{N_R+1} \end{cases}$$

$$\Rightarrow I(V)=\frac{2e}{h}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} T(E)\left(\frac{1}{1+e^{\frac{E-\mu+eV/2}{kT}}}-\frac{1}{1+e^{\frac{E-\mu-eV/2}{kT}}}\right)dE$$

$$\left(T(E)=4\cdot Tr\left[\Gamma_L G \Gamma_R G^{+}\right]\right)$$






GOLD