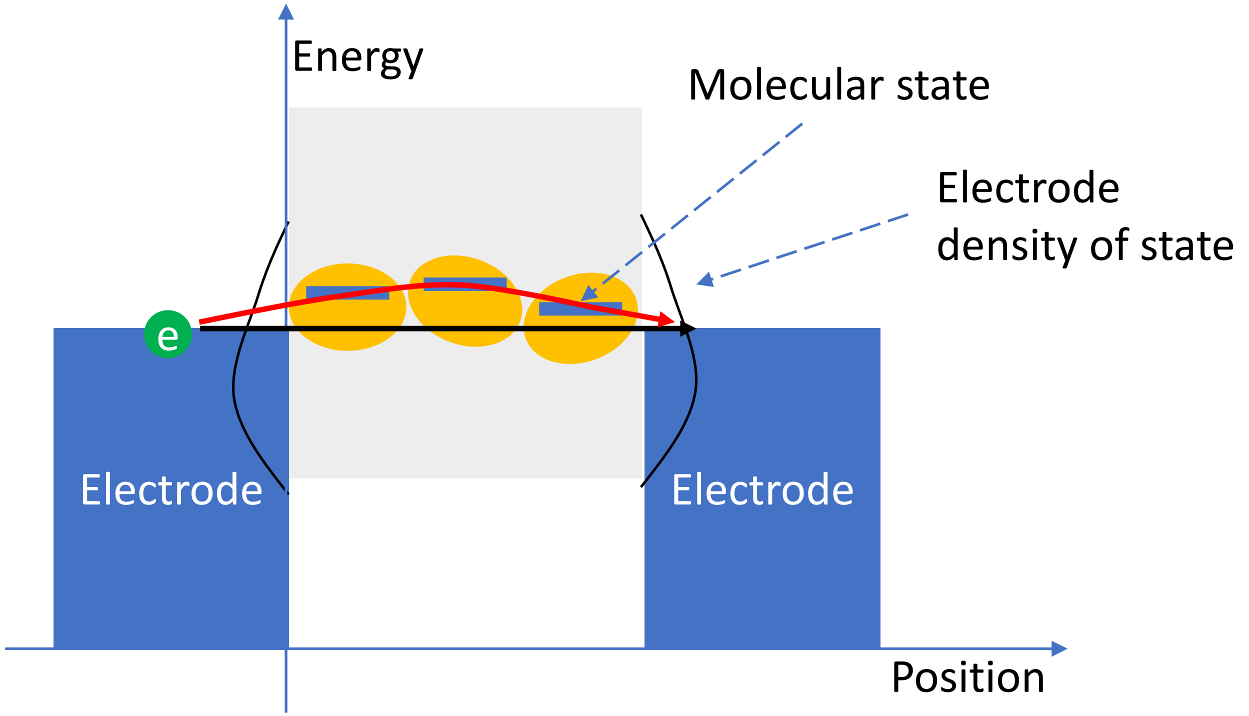
Analyzing Resonant Tunneling using Green’s Function

Xiaoshan Xu

2019/05/30

J. Chem. Phys. **101**, 6849 (1994)
NATURE PHYSICS, **6**, 615, (2010)
PRL 82, 4288 (1999)

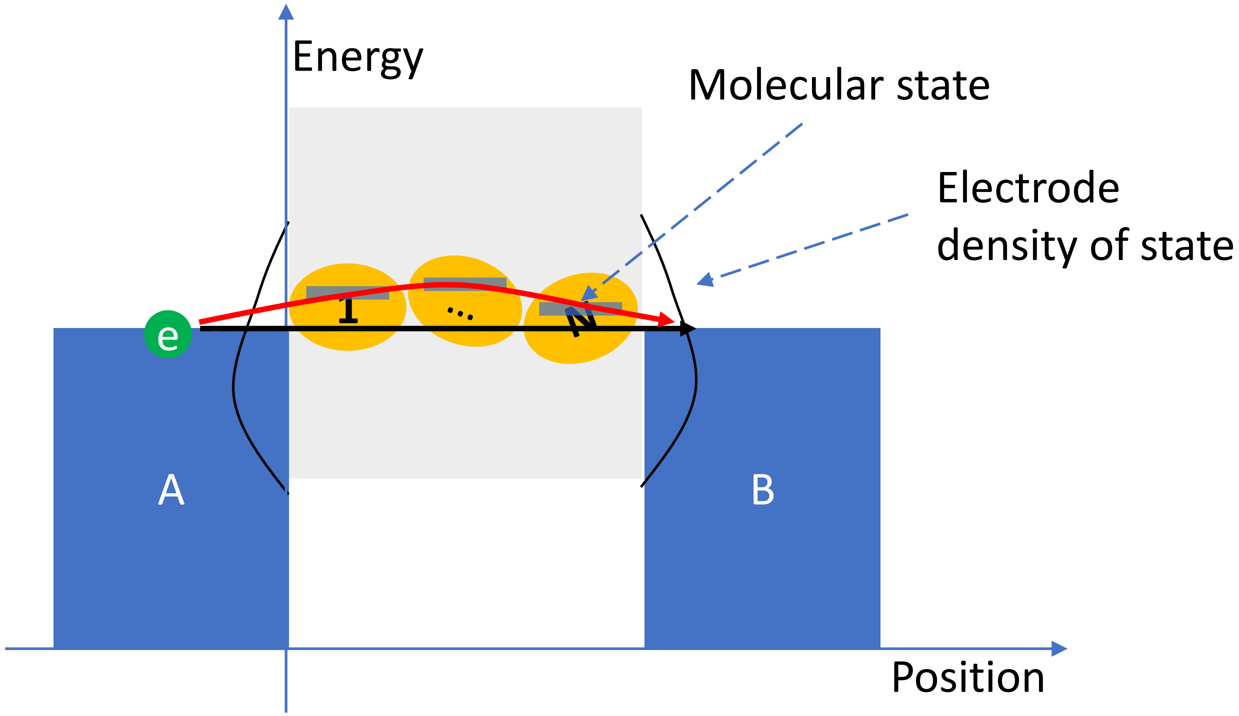
Resonant tunneling problem



→Direct tunneling: tunneling without interacting with the states in the barrier

→Resonant tunneling: tunneling with the help of the states in the barrier

Quantum mechanical description



State: ϕ_i^A, E_i^A | ϕ_i^M, E_i^M | ϕ_i^B, E_i^B

$$H = H_0 + V$$

Interaction: $V_{i,0}^A$ | $V_{i,j}^M$ | $V_{i,N}^B$

$$V = \sum_i V_{i,0}^A + \sum_{i,j} V_{i,j}^M + \sum_i V_{i,N}^B$$

Continuum A only in contact with molecule 0

Continuum B only in contact with molecule N

Introduction to the Green's function

Green's function: $G(E) = \frac{1}{E-H}$, $G_0(E) = \frac{1}{E-H_0}$

Transition operator: $T = V + VG_0T = V + VGV$

According to the scattering theory (no approximation), transition probability from initial $|i\rangle$ state to final state $|f\rangle$ is:

$$\nu = \frac{2\pi}{\hbar}\left|T_{fi}\right|^2 \rho(E_f)$$

$\rho(E_f)$ is the density of state of the final state.

The electric current:

$$j = e\nu = \frac{2\pi e}{\hbar}\left|T_{fi}\right|^2 f(E_i)\left[1 - f\left(E_f\right)\right]\delta\left(E_i - E_f\right)$$

$$\boldsymbol{j = \sum_{i,f} \frac{2\pi e}{\hbar}\left|T_{fi}\right|^2 \delta(E_i - E_F)\delta\left(E_f - E_F\right)}$$

$f(E_i)$ is the Fermi function, V is the bias voltage.

Transition operator T

$$j = \sum_{\boldsymbol{i,f}} \frac{\boldsymbol{2\pi e}}{\boldsymbol{\hbar}} \left|\boldsymbol{T_{fi}}\right|^{\boldsymbol{2}} \boldsymbol{\delta(E_i - E_F)\delta\left(E_f - E_F\right)}$$

$$T_{fi} = \langle f|T|i\rangle$$

Recall $T = V + VGV$

$$T_{fi} = \langle f|V + VGV|i\rangle$$
$$= \langle f|V|i\rangle + \langle f|VGV|i\rangle$$

Through-space tunneling, approximation in Fermi's golden rule.
In this model $\langle f|V|i\rangle = 0$

Resonant tunneling, important when through-space tunneling is too small.

Resonant tunneling

$$j = \sum_{\boldsymbol{i,f}} \frac{\boldsymbol{2\pi e}}{\boldsymbol{\hbar}} \left|\boldsymbol{T_{fi}}\right|^2 \boldsymbol{\delta(E_i - E_F)\delta\left(E_f - E_F\right)}$$

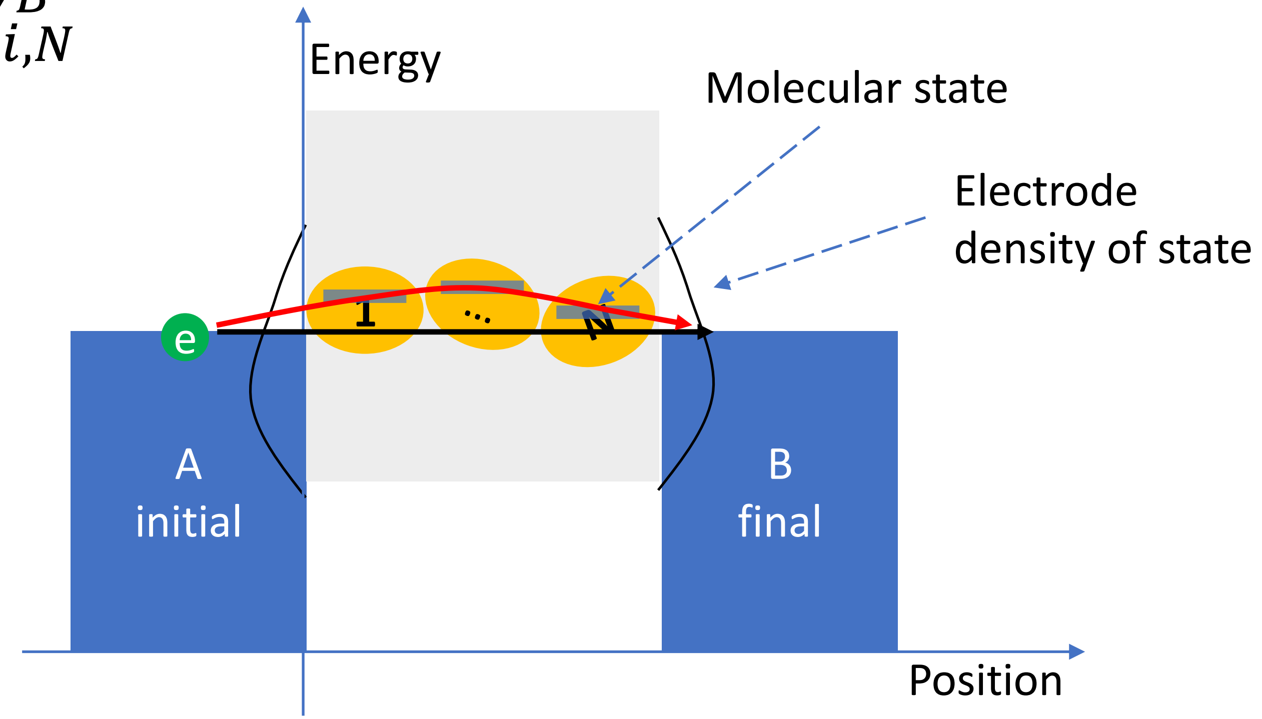
$$T_{fi} = \langle f|VGV|i\rangle$$

Recall $$V = \sum_i V_{i,0}^A + \sum_{i,j} V_{i,j}^M + \sum_i V_{i,N}^B$$

$$T_{fi} = \sum_{i1,i2} \langle f|V|i1\rangle\langle i1|G|i2\rangle\langle i2|V|i\rangle$$

$|i1\rangle, |i2\rangle$ run through all states.

$$T_{fi} = \langle f|V|N\rangle\langle N|G|1\rangle\langle 1|V|i\rangle$$
$$= V_{f,N}G_{N,1}V_{1,i}$$



Resonant tunneling

$$j = \sum_{i,f} \frac{2\pi e}{\hbar} \left|T_{fi}\right|^2 \delta(E_i - E_F)\delta\left(E_f - E_F\right)$$

$$T_{fi} = V_{f,N} G_{N,1} V_{1,i}$$

$$j = \sum_{i,f} \frac{2\pi e}{\hbar} \left|V_{f,N}\right|^2 \left|G_{N,1}\right|^2 \left|V_{1,i}\right|^2 \delta(E_i - E_F)\delta\left(E_f - E_F\right)$$

$$= \sum_{i,f} \frac{2\pi e}{\hbar} \left|G_{N,1}\right|^2 \left[\left|V_{1,i}\right|^2 \delta(E_i - E_F)\right] \left[\left|V_{f,N}\right|^2 \delta\left(E_f - E_F\right)\right]$$

Spectra density (weighted density of state):

$$\Delta_1 = \sum_{i\in A} \pi \left|V_{1,i}\right|^2 \delta(E_i - E_F)$$

$$\Delta_N = \sum_{j\in B} \pi \left|V_{f,N}\right|^2 \delta\left(E_f - E_F\right)$$

$$\boldsymbol{j = \frac{2e}{\hbar\pi} \left|G_{N,1}\right|^2 \Delta_1^2 \Delta_N^2}$$

How to find $\boldsymbol{G_{N,1}}$

$$G(E) = \frac{1}{E - H}$$

$$H = \begin{bmatrix} H_A & H_{AM} & 0 \\ H_{MA} & H_M & H_{MB} \\ 0 & H_{BM} & H_B \end{bmatrix}$$

$$H - E = \begin{bmatrix} H_A - E & H_{AM} & 0 \\ H_{MA} & H_M - E & H_{MB} \\ 0 & H_{BM} & H_B - E \end{bmatrix}$$

This can be converted to finite dimensional problem:

$$h' = H - E = \begin{bmatrix} H_{1,1}^M - E - S_1 & H_{1,i}^M & 0 \\ H_{i,1}^M & H_{i,i}^M - E & H_{i,N}^M \\ 0 & H_{N,i}^M & H_{N,N}^M - E - S_N \end{bmatrix}$$

$$\boldsymbol{S_1 = \sum_i \frac{V_{i0}^2}{E_i - E}}$$

$$\boldsymbol{S_N = \sum_i \frac{V_{fN}^2}{E_f - E}}$$

$$\boldsymbol{G_{N,1} = \frac{|h'(1|N)|}{|h'|}}$$

$\boldsymbol{h'(1|N)}$ is the cofactor of $\boldsymbol{h'}$.

Conclusion

- The resonant tunneling is another route of tunneling beside tunneling through space described by the Fermi's golden rule
- The resonant tunneling can be calculated using the Green's function