The Hopping Model

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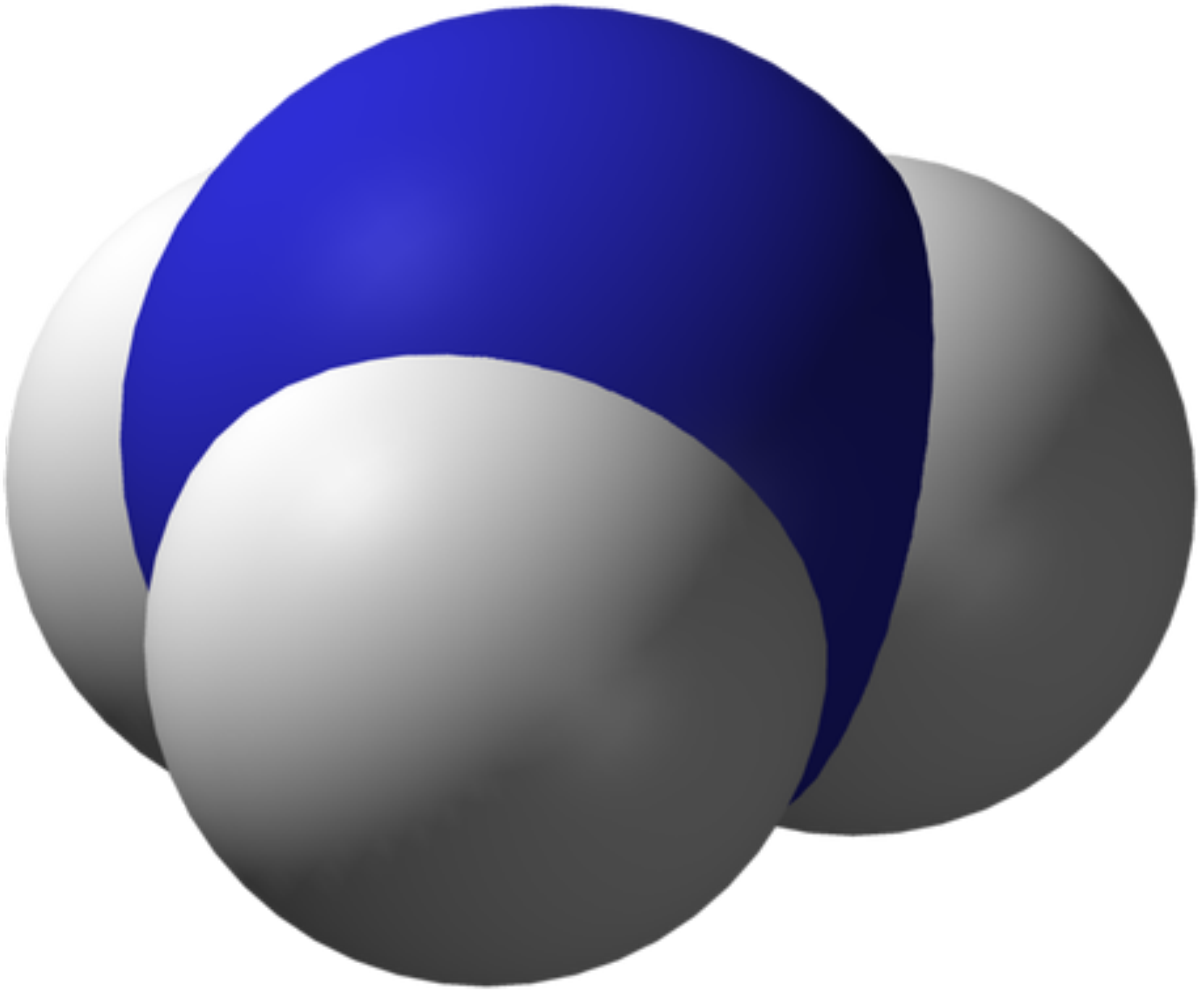
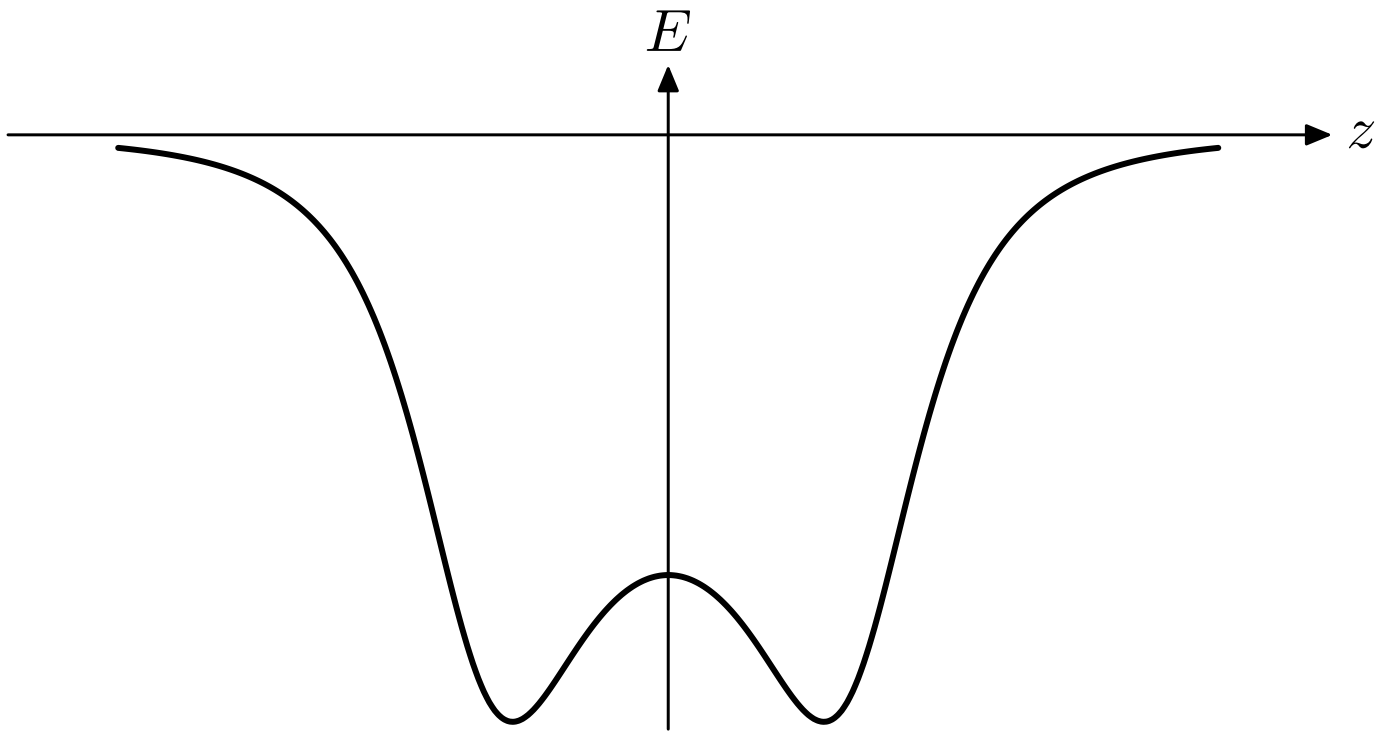
- Example 1: ammonia molecule
- Example 2: free quasi-electrons



The ammonia molecule NH_3



Total energy of the ammonia molecule as a function of the position of the nitrogen ion on the symmetry axis. There are two positions with minimal energy.

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- V may be chosen positive

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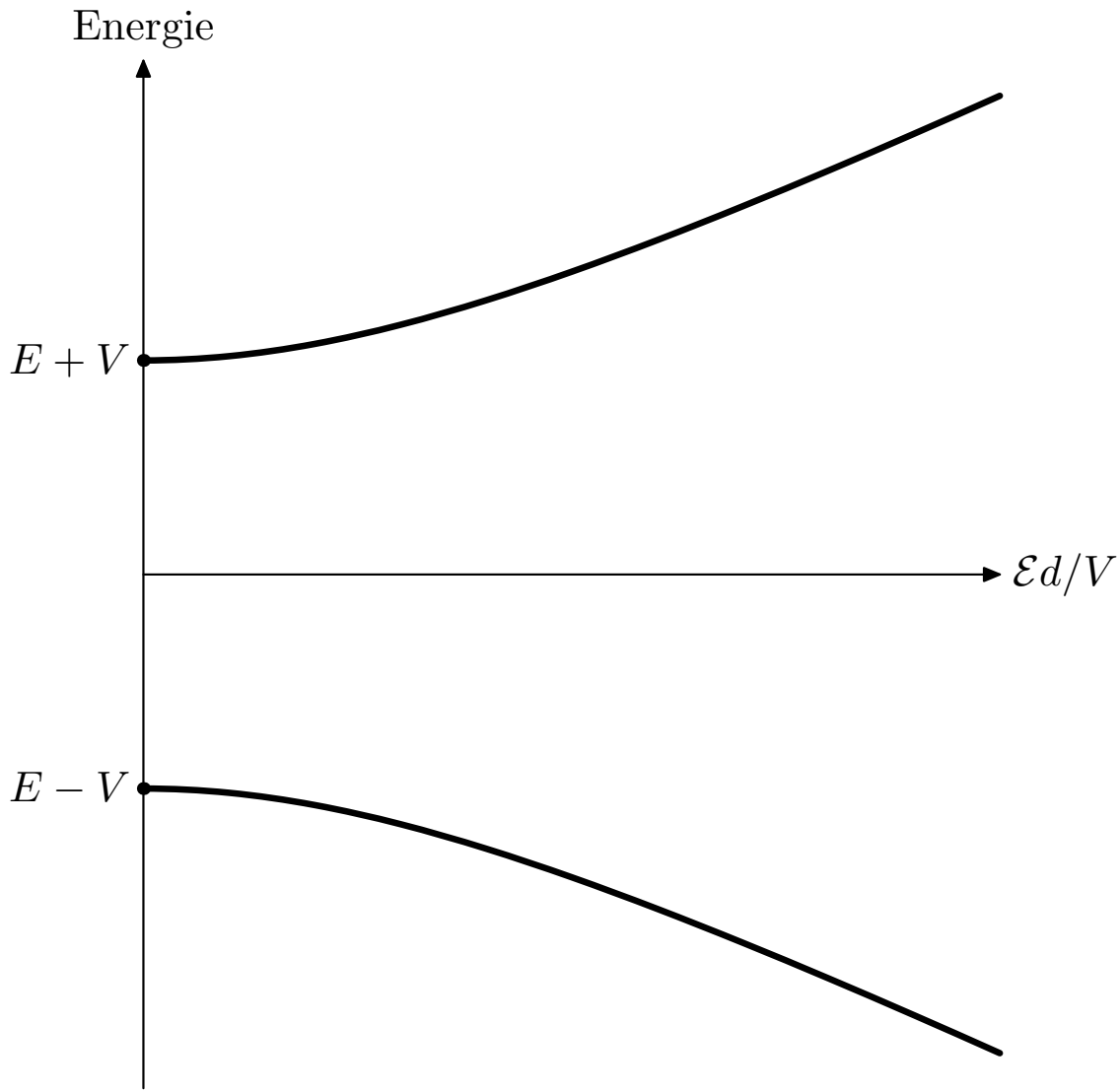

The two energy states of the ammonia model as functions of an external electric field.

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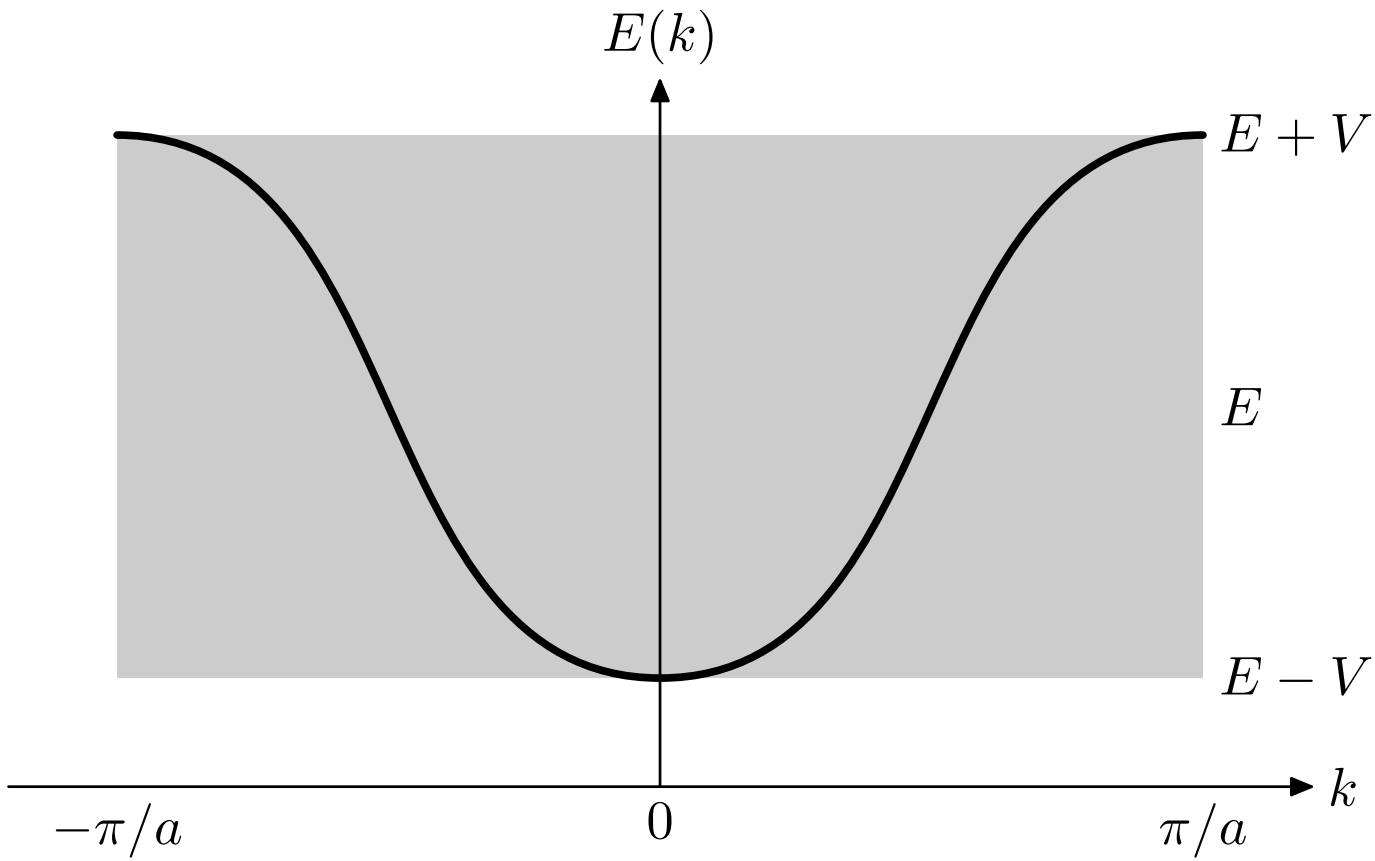
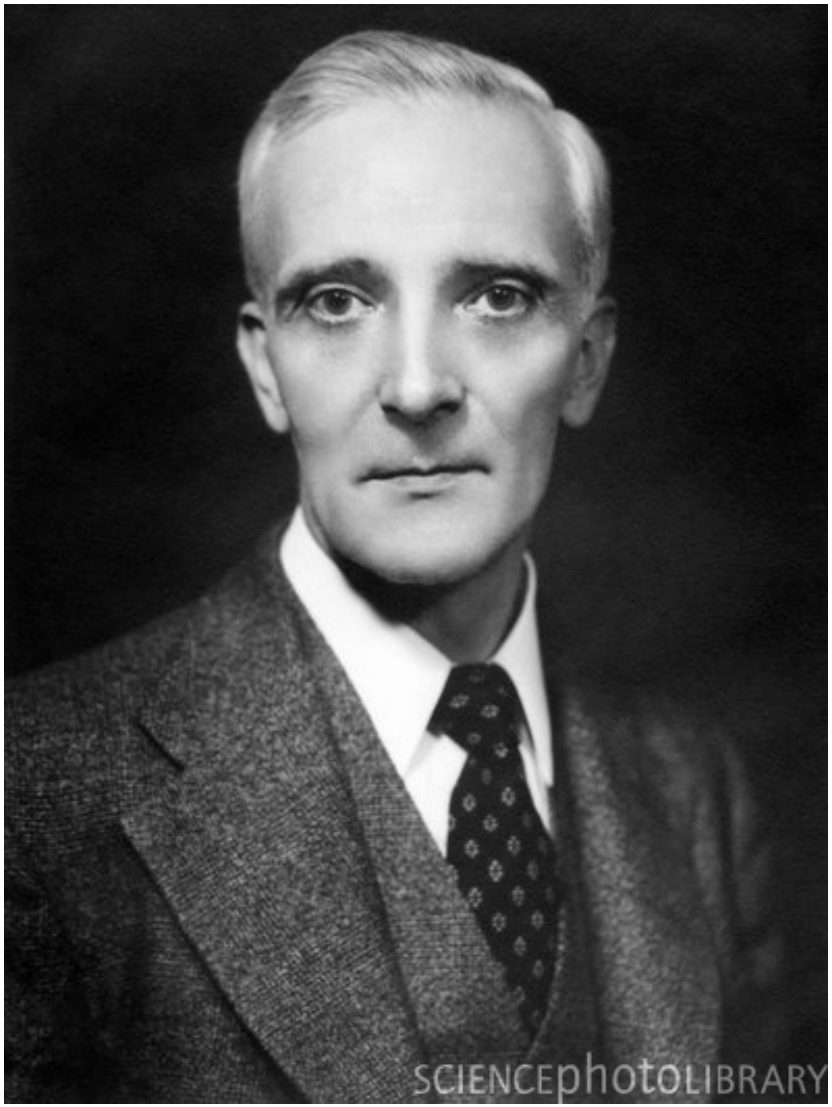
- dispersion relation $\omega = \omega(k)$ where $E_k = \hbar\omega(k)$



Dispersion relation for next neighbor hopping



Léon Brillouin, 1889-1969, French/US-american physicist

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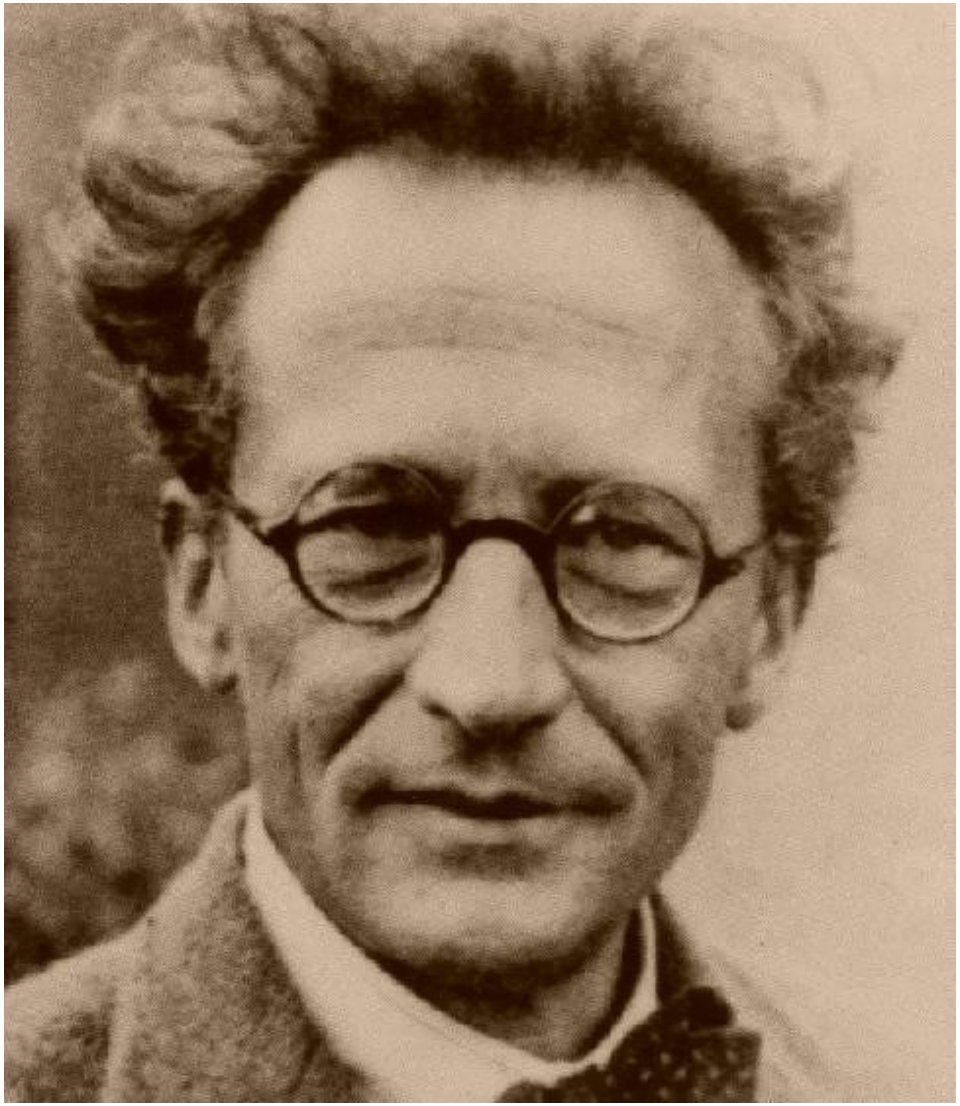

Erwin Schrödinger, 1887-1961, Austrian physicist

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- Velocity expectation value at time t is
  $\langle\dot{X}\rangle_t = \int_k |C(k)|^2\,\omega'(k)$ with $\int_k |C(k)|^2 = 1$

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- $\dot{X}$ unchanged, but now

$$\ddot{X} = -\frac{Va^2}{2\hbar^2} e\mathcal{E}(R + L)$$

$$\ddot{X}\,\phi_k = -\frac{Va^2}{\hbar^2} e\mathcal{E}\cos ka\;\phi_k = -e\mathcal{E}\frac{E''(k)}{\hbar^2}\phi_k$$

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- in three dimensions it is a tensor:
  $$\left(\frac{1}{m^*} \right)_{ij} = \int_{\mathbf{k}} |C(|\mathbf{k}|)|^2 \, \frac{\partial^2 \omega(\mathbf{k})}{\partial k_i \partial k_j}$$

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- valence band, conduction band, band gap, overlapping bands
- dielectrica, conducters, semi-conducters ...
- defects

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- for $r \neq 0$: ok with $E(k) = E - V \cos ka$ as before

Defects ctd.

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- note $f = 0$ if $\Delta = 0$

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- slow electrons are more likely reflected than fast ones

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- the deeper the defect, the smaller the bound state