The Hopping Model Peter Hertel

Basic

Two states

Model crysta

More

Scattering

Binding

The Hopping Model

Peter Hertel

University of Osnabrück, Germany

Lecture presented at APS, Nankai University, China

March/April 2011

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States and amplitudes

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• The system has many distinct states

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States and amplitudes

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- The system has many distinct states
- There are amplitudes for hopping from one state to another

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States and amplitudes

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- Find eigenstates of energy H, they are stationary

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• Recall
$$\psi_t = e^{-\mathrm{i}\Omega t}\psi_0$$
 where $H = \hbar\Omega$

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- Example 1: ammonia molecule

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

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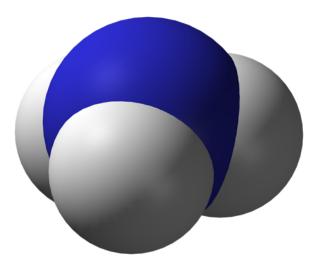
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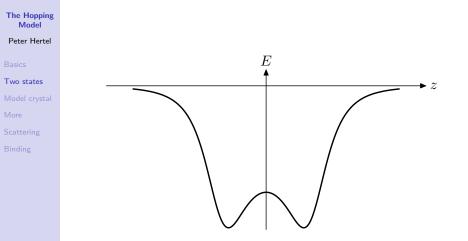
Scattering

Binding



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The ammonia molecule NH₃



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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The ammonia molecule

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- The nitrogen ion N^{3+} may be up or down with respect to the H^- plane

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- These states are u_{\uparrow} and u_{\downarrow}

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The ammonia molecule

- The nitrogen ion N^{3+} may be up or down with respect to the H^- plane
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- hopping up or down described by operators *U* and *D*, respectively

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- energy is H = EI V(U + D) where V is the transition amplitude

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- energy is H = EI V(U + D) where V is the transition amplitude
- V may be chosen positive

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Microwave standard

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$$H = \left(\begin{array}{cc} E & -V \\ -V & E \end{array}\right)$$

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Microwave standard

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• The energy is represented by matrix

$$H = \left(\begin{array}{cc} E & -V \\ -V & E \end{array} \right)$$

• its eigenvalues are $E_1 = E - V$ and $E_2 = E + V$

Microwave standard

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$$H = \left(\begin{array}{cc} E & -V \\ -V & E \end{array} \right)$$

- its eigenvalues are $E_1 = E V$ and $E_2 = E + V$
- resonance frequency f defined by $2\pi\hbar f = E_2 E_1$

Microwave standard

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- microwave standard, f = 23.87012 GHz

Microwave standard

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- resonance frequency f defined by $2\pi\hbar f = E_2 E_1$
- microwave standard, f = 23.87012 GHz
- Eigenstates are $\phi_1 = (u_\uparrow + u_\downarrow)/\sqrt{2}$ and $\phi_2 = (u_\uparrow u_\downarrow)/\sqrt{2}$

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Basics

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Stark effect

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• The dipole moment is proportional zu Z, i. e. P = d(U - D)

Basics

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Model crystal

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- The dipole moment is proportional zu Z, i. e. P = d(U - D)
- External electric field \mathcal{E} along the z axis

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- The dipole moment is proportional zu Z, i. e. P = d(U - D)
- External electric field \mathcal{E} along the z axis
- $H = EI + V(U+D) d\mathcal{E}(U-D)$

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- The dipole moment is proportional zu Z, i. e. P = d(U D)
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- The energy is now represented by the matrix

$$H=\left(egin{array}{cc} E-d\mathcal{E}&-V\ -V&E+d\mathcal{E}\end{array}
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• The energy eigenvalues are

$$E_{1,2}=E\pm\sqrt{V^2+(d\mathcal{E})^2}$$

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$$E_{1,2} = E \pm \sqrt{V^2 + (d\mathcal{E})^2}$$

• linear and quadratic Stark effect

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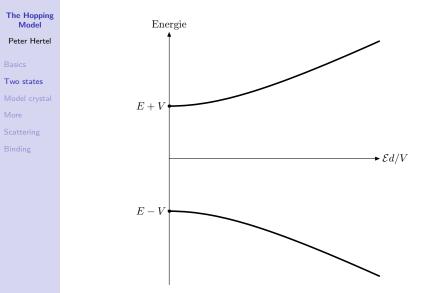
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- linear and quadratic Stark effect
- Ammonia maser...



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

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One-dimensional model crystal

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• sites labeled by $r = \ldots, -1, 0, 1, \ldots$, equal distances a

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One-dimensional model crystal

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$$Hu_r = E - V(u_{r-1} + u_{r+1})/2$$

Basics

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- V > 0 WLOG, E and V do not depend on r (translation symmetry)

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• left and right shift L and R

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- $Lu_r = u_{r-1}$ and $Ru_r = u_{r+1}$, respectively

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- [R, L] = 0, [X, R] = aR, [X, L] = -aL

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Stationary states

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• eigenstates $H\phi_k = E_k\phi_k$

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Stationary states

• eigenstates $H\phi_k = E_k\phi_k$

 $\phi_k = \sum_r e^{iakr} u_r$

 $E_k = E - V \cos ka$

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Stationary states

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- note $k \in [-\pi/a, \pi/a]$

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- energy band

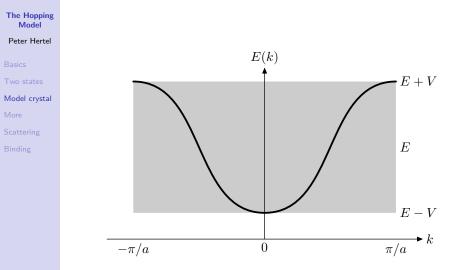
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- wave number k varies in Brillouin zone
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- dispersion relation $\omega = \omega(k)$ where $E_k = \hbar \omega(k)$



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Dispersion relation for next neighbor hopping

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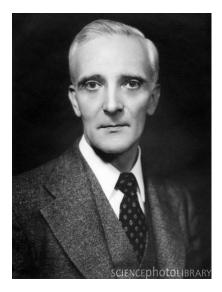
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Léon Brillouin, 1889-1969, French/US-american physicist

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• eigenstates cannot be normalized

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Wave packets

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- eigenstates cannot be normalized
- hence: wave packets

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- eigenstates cannot be normalized
- hence: wave packets

$$\psi_t = \int_k C(k) e^{-\mathrm{i}\omega(k)t} \phi_k = \sum_r c_r(t) u_r$$

$$\int_{k} = a \int_{-\pi/a}^{\pi/a} \frac{\mathrm{d}k}{2\pi}$$

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- eigenstates cannot be normalized
- hence: wave packets

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...

$$\int_{k} = a \int_{-\pi/a}^{\pi/a} \frac{\mathrm{d}k}{2\pi}$$
$$c_{r}(t) = \int_{-\pi/a} C(k) e^{ikar} e^{-ikar}$$

$$F_r(t) = \int_k C(k) e^{ikar} e^{-i\omega(k)t}$$

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$$c_r(t) = \int_k C(k) e^{ikar} e^{-i\omega(k)t}$$

• wave packet solves Schrödinger equation $\mathrm{i}\hbar\dot{\psi}_t=H\psi_t$

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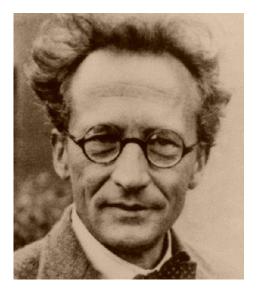
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Erwin Schrödinger, 1887-1961, Austrian physicist

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• If *M* is an observable,

$$\dot{M} = \frac{1}{\hbar}[H, M]$$

describes its temporal rate of change.

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• If *M* is an observable,

$$\dot{M} = \frac{1}{\hbar}[H, M]$$

describes its temporal rate of change.

• For our model

$$\dot{X} = \frac{Va}{\hbar} \frac{L-R}{2i}$$

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• If *M* is an observable,

$$\dot{M} = \frac{1}{\hbar}[H, M]$$

The Hopping Model

Peter Hertel

Model crystal

describes its temporal rate of change.

• For our model

$$\dot{X} = \frac{Va}{\hbar} \frac{L-R}{2i}$$

•
$$\dot{X}\phi_k = v(k)\phi_k$$

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$$v(k) = (Va/\hbar) \sin ka = \omega'(k)$$
 is group velocity

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Model crystal

The Hopping Model

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More

Scattering

Binding

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- $v(k) = (Va/\hbar) \sin ka = \omega'(k)$ is group velocity
- Velocity expectation value at time t is

$$\langle \dot{X}
angle_t = \int_k |C(k)|^2 \, \omega'(k) ext{ with } \int_k |C(k)|^2 = 1$$

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Basics

Two states

Model crystal

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Acceleration

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•
$$\ddot{X} = (i/\hbar)[H, \dot{X}] = 0$$

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• $\ddot{X} = (i/\hbar)[H, \dot{X}] = 0$

The Hopping Model

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· electron moves freely, velocity does not depend on time

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- · electron moves freely, velocity does not depend on time
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The Hopping Model

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- · electron moves freely, velocity does not depend on time
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$$H = EI - V(R + L) + e\mathcal{E}X$$

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The Hopping Model

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- · electron moves freely, velocity does not depend on time
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- $H = EI V(R + L) + e\mathcal{E}X$

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

•
$$m^* \langle \ddot{X} \rangle = -e\mathcal{E}$$
 where
 $\frac{1}{m^*} = \frac{1}{\hbar} \int_k |C(k)|^2 \omega''(k)$
defines effective mass m^*

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Model crystal More Scattering

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- $m^* \langle \ddot{X} \rangle = -e\mathcal{E}$ where $\frac{1}{m^*} = \frac{1}{\hbar} \int_k |C(k)|^2 \omega''(k)$ defines effective mass m^* .
- effective mass depends on the state, here C(k)
- effective mass depends on the interaction, here \boldsymbol{V}

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- effective mass can be negative!

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The Hopping Model

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- effective mass depends on the state, here C(k)
- effective mass depends on the interaction, here V
- effective mass can be negative!
- 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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Basics

Two states

Model crystal

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More on the hopping model

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• hopping to the next neigbor, to the second next neighbor, etc.

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Basics

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More on the hopping model

- hopping to the next neigbor, to the second next neighbor, etc.
- $H = EI V_1(R+L)/2 V_2(R^2 + L^2)/2 + \dots$

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Basics

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- Binding

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Basics

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- expressions for velocity and effective mass unchanged

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Basics

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More on the hopping model

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- valence band, conduction band, band gap, overlapping bands

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The Hopping Model

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Basics

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Scattering

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• One of many possibilities:

- One of many possibilities:
- the energy level at r = 0 is $E + \Delta$ instead of E

- wo states
- Model crystal

The Hopping Model

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Model Peter Hertel

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Model crystal

More

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- Binding

- One of many possibilities:
- the energy level at r = 0 is $E + \Delta$ instead of E
- $Hu_0 = (E + \Delta)u_0 V(u_{-1} + u_1)/2$

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Model Peter Hertel

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- One of many possibilities:
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- $Hu_r = Eu_r V(u_{r-1} + u_{r+1})/2$ elsewhere

- Model crystal

The Hopping Model

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- Scattering
- Binding

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- $Hu_r = Eu_r V(u_{r-1} + u_{r+1})/2$ elsewhere
- Try a superposition of a plane wave and a spherical wave $\phi = \sum_{r} e^{ikar} u_{r} + f \sum_{r} e^{ika|r|} u_{r}$

- Two state
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The Hopping Model

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

Defects ctd.

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Model Peter Hertel

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• solve
$$(H\phi)_0 = E(k)\phi_0$$

 $\Delta(1+f) - V\cos ka - f V e^{ika} = -V\cos ka(1+f)$

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Model crystal

The Hopping Model

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More

Scattering Binding

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$$(H\phi)_0 = E(k)\phi_0$$

 $\Delta(1+f) - V \cos ka - f V e^{ika} = -V \cos ka(1+f)$
• the scattering amplitude f is
 $f = -\frac{\Delta}{\Delta - iV \sin ka}$
 $\phi = \sum_r \phi_r u_r \text{ with } \phi_r = e^{ikar} + f e^{ika|r|}$

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Two state

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The Hopping Model

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More

Scattering Binding

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 $\phi = \sum_r \phi_r u_r \text{ with } \phi_r = e^{ikar} + f e^{ika|r|}$
• note $f = 0$ if $\Delta = 0$

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The Hopping Model

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 Recall $\phi = \sum_{r} e^{ikar} u_{r} + f \sum_{r} e^{ika|r|} u_{r}$

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The Hopping Model

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• Recall

$$\phi = \sum_{r} e^{ikar} u_{r} + f \sum_{r} e^{ika|r|} u_{r}$$

• reflexion coefficient $R = |f|^2$

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The Hopping Model

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- Recall $\phi = \sum_{r} e^{ikar} u_{r} + f \sum_{r} e^{ika|r|} u_{r}$
- reflexion coefficient $R = |f|^2$
- transmission coefficient $T = |1 + f|^2$

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The Hopping Model

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•
$$R+T=1$$

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- note that sign of Δ is irrelevant since

$$R = \frac{\Delta^2}{\Delta^2 + V^2 \sin^2 ka}$$

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- Recall $\phi = \sum_{r} e^{ikar} u_{r} + f \sum_{r} e^{ika|r|} u_{r}$
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- R + T = 1
- note that sign of Δ is irrelevant since

$$R = \frac{\Delta^2}{\Delta^2 + V^2 \sin^2 ka}$$

• slow electrons are more likely reflected than fast ones

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The Hopping Model

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Basic

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 Rewrite $\phi = \frac{1}{f(k)} \sum_{r} e^{ikar} u_r + \sum_{r} e^{ika|r|} u_r$

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The Hopping Model

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- Rewrite $\phi = \frac{1}{f(k)} \sum_{r} e^{ikar} u_{r} + \sum_{r} e^{ika|r|} u_{r}$
- plane wave vanishes if scattering amplitude f(k) is singular

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•
$$k = \mathrm{i}\kappa$$
 where sinh $\kappa a = -2\Delta/V$

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- $\kappa > 0$ for $\Delta < 0$

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- $\kappa > 0$ for $\Delta < 0$
- bound state, trapping

$$\phi = \sum_{r} e^{-\kappa a|r|}$$

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- Binding

• Rewrite

$$\phi = \frac{1}{f(k)} \sum_{r} e^{ikar} u_{r} + \sum_{r} e^{ika|r|} u_{r}$$

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• the deeper the defect, the smaller the bound state