# Summary



- Energy states indexed by $\vec{k}$ and $n$. The first index describes symmetry properties during translation, while the second distinguishes energy states with same symmetry.
- The eigenvalue corresponding to translation symmetry is

$$e^{i\vec{k}\cdot\vec{R}}, \tag{L1}$$

not $\vec{k}$. The eigenvalue and eigenstates are periodic functions of $\vec{k}$, unchanged when $\vec{k} \to \vec{k} + \vec{K}$.

- Essential result:

$$(\mathcal{E}^0_{\vec{q}} - \mathcal{E})\psi(\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q} - \vec{K}) = 0. \tag{L2}$$


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# Condition for scattering

$$k = \frac{K}{2\hat{k}\cdot\hat{K}} \Rightarrow \vec{k}\cdot\vec{K} = \frac{1}{2}K^2. \tag{L3}$$

➾ Energy degeneracy:

$$\frac{1}{2}k^2 = \frac{1}{2}k^2 - \vec{k}\cdot\vec{K} + \frac{1}{2}K^2 \tag{L4}$$

$$\Rightarrow \mathcal{E}^0_{\vec{k}} = \mathcal{E}^0_{\vec{k}-\vec{K}} \tag{L5}$$

➾ Geometry: Plane that bisects line between origin and $\vec{K}$ is given by

$$\vec{k}\cdot\hat{K} = \frac{K}{2} \Rightarrow \vec{k}\cdot\vec{K} = \frac{K^2}{2} \tag{L6}$$


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$$U_{\vec{K}} = \Delta w_{\vec{K}} \tag{L7}$$

Exercise:

Starting with

$$(\mathcal{E}^0_{\vec{q}} - \mathcal{E})\psi(\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q}-\vec{K}) = 0. \tag{L8}$$

and

$$\psi(\vec{q}) = \psi^{(0)}(\vec{q}) + \psi^{(1)}(\vec{q})\Delta + \ldots; \quad \mathcal{E} = \mathcal{E}^{(0)} + \Delta\mathcal{E}^{(1)} + \ldots. \tag{L9}$$

find the zero'th order solution $\psi^{(0)}$:

$$\psi^{(0)} ? \qquad\qquad ? = 0. \tag{L10}$$

$$\psi^{(0)}_{\vec{k}}(\vec{q}) = ? \quad ? \Rightarrow \psi^{(0)}_{\vec{k}}(\vec{r}) = ? \quad ? \tag{L11}$$

$$\Rightarrow \mathcal{E}^{(0)} = ? \quad ? \tag{L12}$$



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Exercise:

Next, expand Bloch's equation out to first order in $\Delta$ and find both the energy and wave function to this order:

$$[\mathcal{E}^0_{\vec{q}} - \mathcal{E}^0_{\vec{k}}]\psi^{(1)}_{\vec{k}}(\vec{q}) + \sum_{\vec{K}} w_{\vec{K}}\psi^{(0)}_{\vec{k}}(\vec{q}-\vec{K}) - \mathcal{E}^{(1)}\psi^{(0)}_{\vec{k}}(\vec{q}) = 0. \quad \text{(L13)}$$

$$\mathcal{E}^{(1)} = ? \qquad ? \quad \text{(L14)}$$

$$\left.\psi^{(1)}_{\vec{k}}(\vec{q}) \quad = \quad ? \qquad\qquad ?\right\} \quad \text{(L15)}$$

$$\Rightarrow \psi_{\vec{k}}(\vec{q}) \quad \approx \quad ? \qquad\qquad ? \quad \text{(L16)}$$


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# Perturbation theory breaks down



The condition for breakdown is

$$\mathcal{E}^0_{\vec{k}} = \mathcal{E}^0_{\vec{K}+\vec{k}} \tag{L17}$$


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$$\hat{\mathcal{H}}^{\text{eff}}_{ij} = \langle\psi_i|(\hat{\mathcal{H}} - \mathcal{E})|\psi_j\rangle \tag{L18}$$

$|\psi_1\rangle = |\vec{k}\rangle$

$|\psi_2\rangle = |\vec{k} + \vec{K}\rangle$

$$\hat{\mathcal{H}} = \sum_{\vec{q}'} |\vec{q}'\rangle \mathcal{E}^0_{\vec{q}'} \langle\vec{q}'| + \sum_{\vec{q}'\vec{K}'} |\vec{q}'\rangle U_{\vec{K}'} \langle\vec{q}' - \vec{K}'|. \tag{L19}$$

Exercise: Find off-diagonal components of matrix.

$$\begin{vmatrix} \mathcal{E}^0_{\vec{k}} - \mathcal{E} & ? & ? \\ ? & ? & \mathcal{E}^0_{\vec{k}+\vec{K}} - \mathcal{E} \end{vmatrix}. \tag{L20}$$

Exercise: find eigenvalues of matrix

$$\mathcal{E} = ? \qquad\qquad ? \tag{L21}$$


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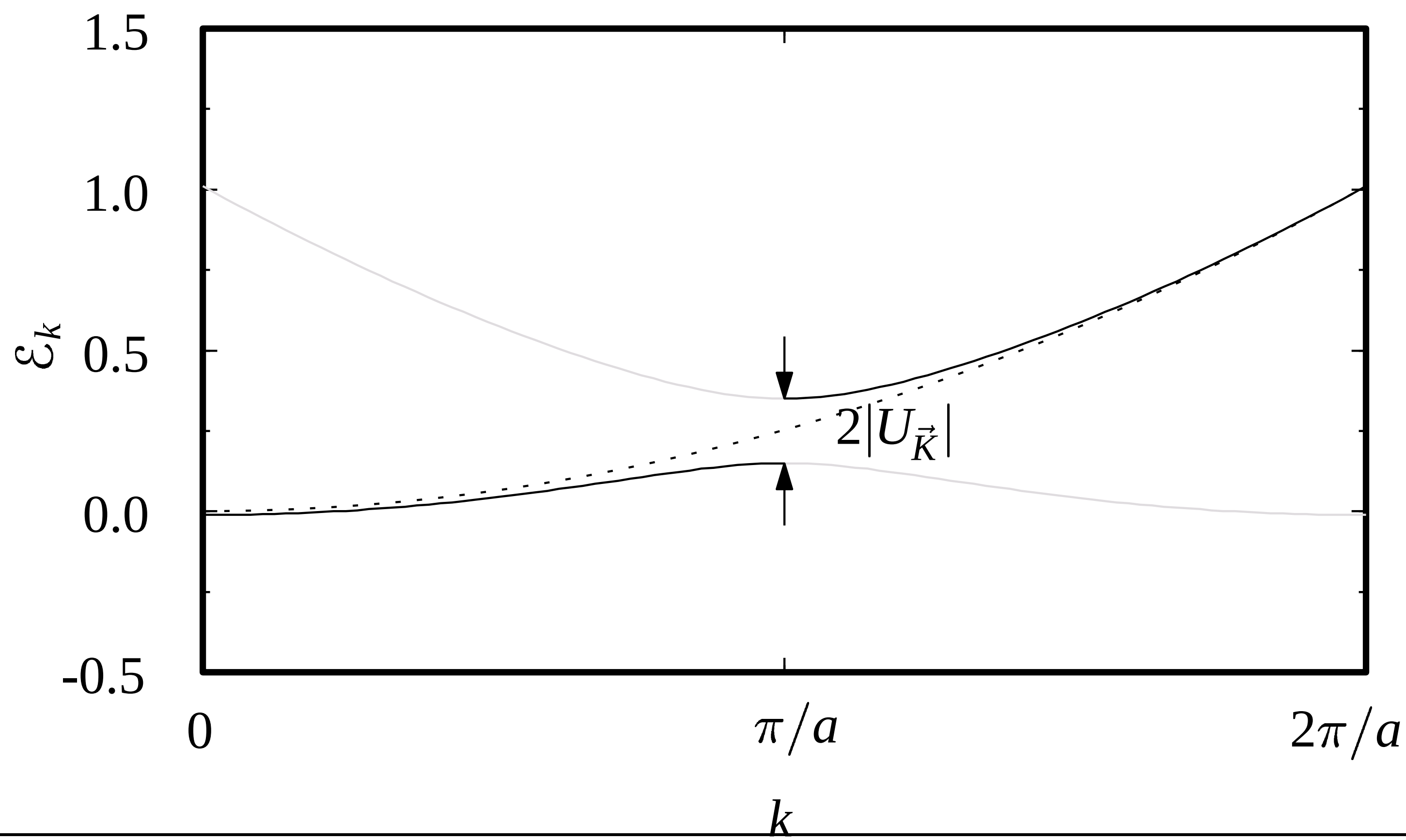
Right at $\vec{k} = \vec{K}$ have

$$\mathcal{E} = \mathcal{E}^0_{\vec{k}} \pm \|U_{\vec{K}}|. \quad \text{(L22)}$$

$$\mathcal{E}_g = 2|U_{\vec{K}}|. \quad \text{(L23)}$$





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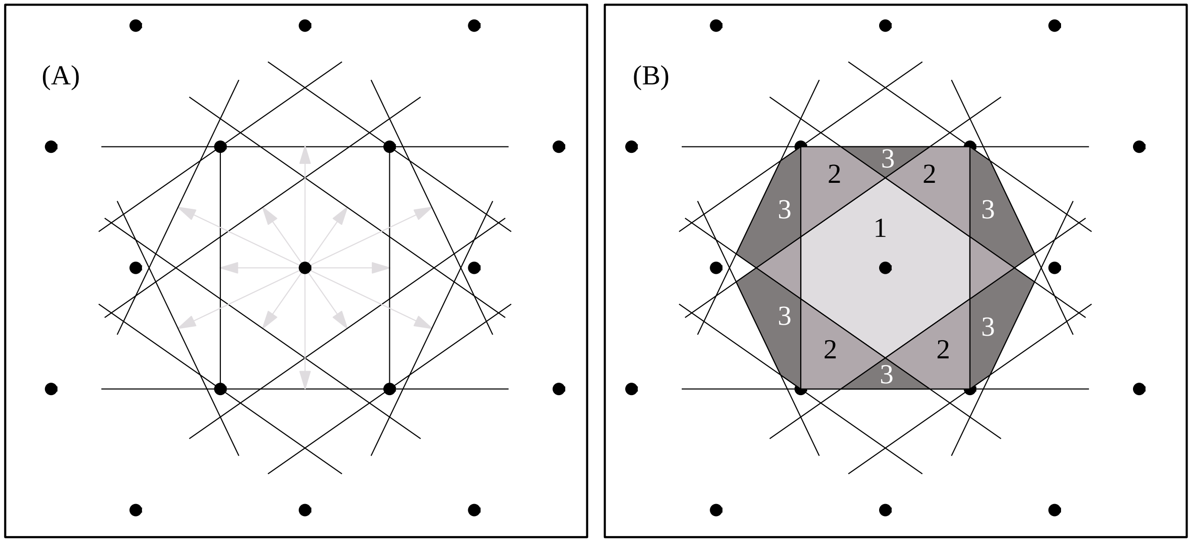
# Geometrical view



$$\vec{k} \cdot \frac{\vec{K}}{K} = \frac{1}{2} K. \qquad \text{(L24)}$$





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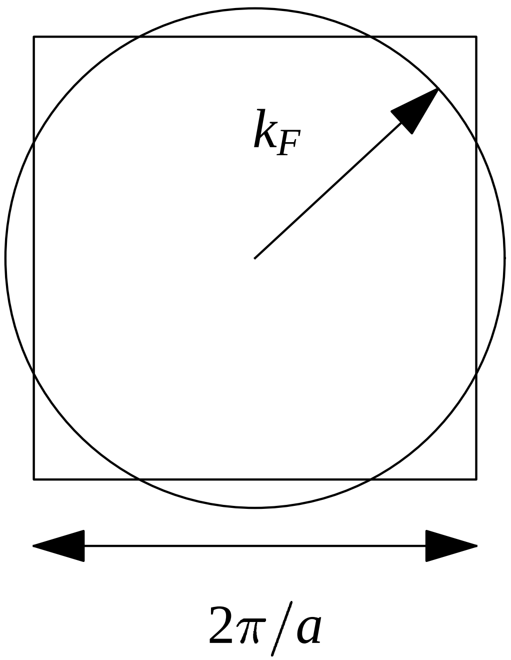
# Example in two dimensions




$$\pi k_F^2 = 4\pi^2/a^2$$

$$\Rightarrow k_F = 2\pi/\sqrt{\pi}a = 1.128\pi/a$$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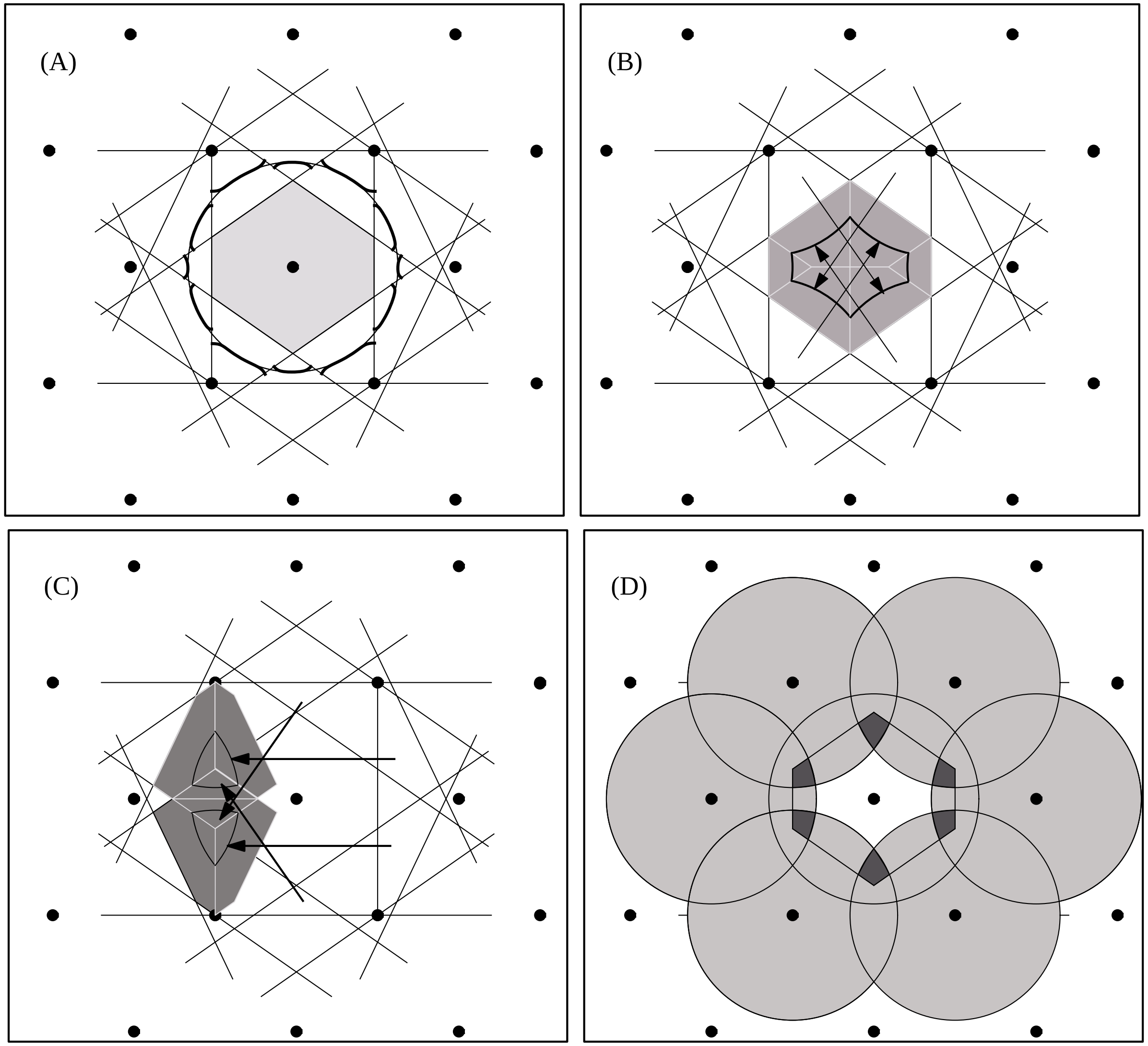
# Example in two dimensions







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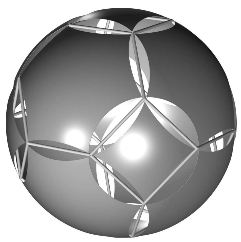
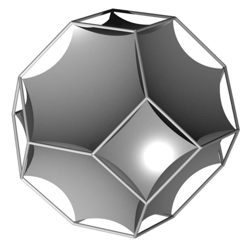
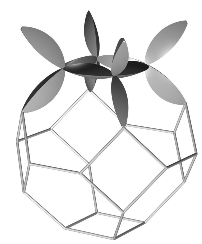
# Nearly Free Electron Fermi Surface Gallery 

| Brillouin zone | Extended zone scheme | Reduced zone scheme |
|---|---|---|
| First | Empty | Empty |
| Second |  |  |
| Third |  |  |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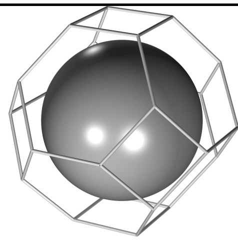
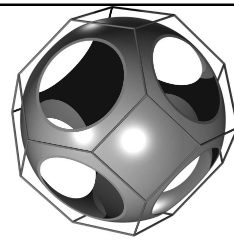
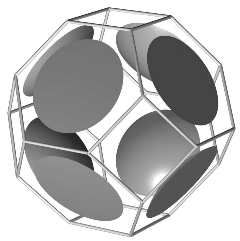
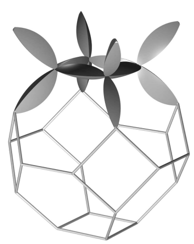
# Nearly Free Electron Fermi Surface Gallery

| Brillouin zone | 1 electron/cell | 2 electrons/cell | 3 electrons/cell |
|---|---|---|---|
| First |  |  | |
| Second | |  |  |
| Third | | |  |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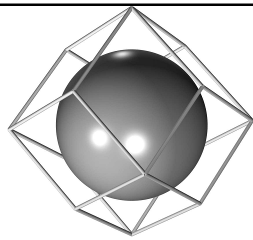
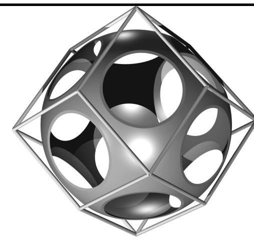
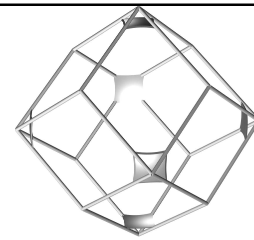
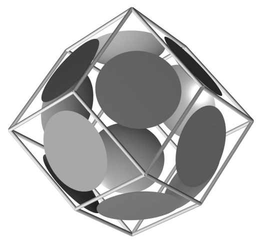
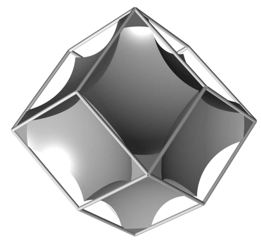
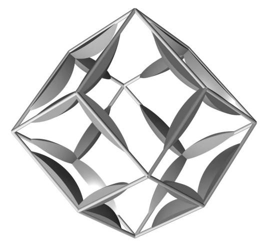
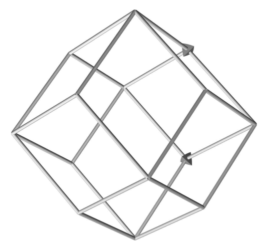
# Nearly Free Electron Fermi Surface Gallery 

| Brillouin zone | 1 electron/cell | 2 electrons/cell | 3 electrons/cell |
| --- | --- | --- | --- |
| First |  |  |  |
| Second | |  |  |
| Third | | |  |
| Fourth | | |  |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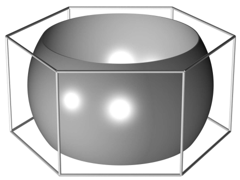
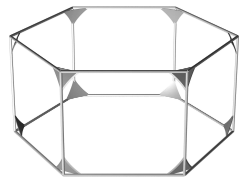
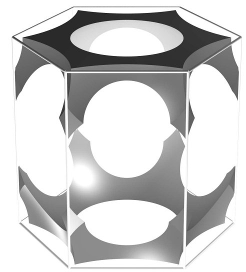
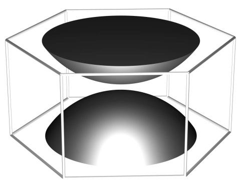
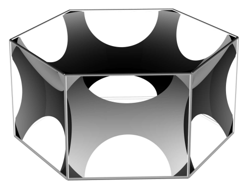
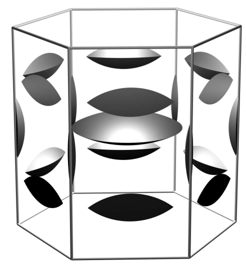
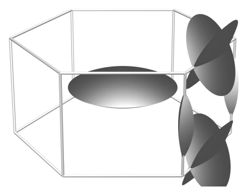
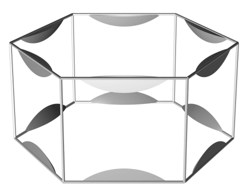
# Nearly Free Electron Fermi Surface Gallery



| Brillouin zone | 2 electrons/cell | 4 electrons/cell | 4 electrons/cell with hcp extinction |
|---|---|---|---|
| First |  |  |  |
| Second |  |  |  |
| Third | |  | |
| Fourth | |  | |



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# Actual Fermi Surfaces of All the Elements 

Periodic Table of Fermi Surfaces, University of Florida


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$$\langle\vec{r}|\vec{R}\rangle \equiv w_n(\vec{R},\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}}\psi_{n\vec{k}}(\vec{r}). \quad \text{(L25)}$$

$$\int d\vec{r}\, w_n(\vec{R},\vec{r})w_m^*(\vec{R}',\vec{r}) = ?$$

$$? \quad \text{(L27)}$$

$$= \quad \delta_{\vec{R},\vec{R}'}\delta_{n,m}. \quad \text{(L28)}$$

$$\frac{1}{\sqrt{N}}\sum_{\vec{R}} w_n(\vec{R},\vec{r})e^{i\vec{k}\cdot\vec{R}} = \psi_{n\vec{k}}(\vec{r}). \quad \text{(L29)}$$

$$w_n(\vec{R},\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}+i\phi(\vec{k})}\psi_{n\vec{k}}(\vec{r}), \quad \text{(L30)}$$


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# Tight Binding Hamiltonian

$$\hat{\mathcal{H}} = \sum_{\vec{R}\vec{R}'} |\vec{R}'\rangle\langle\vec{R}'|\hat{\mathcal{H}}|\vec{R}\rangle\langle\vec{R}|. \tag{L31}$$

$$\mathcal{H}_{\vec{R}\vec{R}'} \equiv \langle\vec{R}'|\hat{\mathcal{H}}|\vec{R}\rangle = \int d\vec{r}\, w_n^*\left(\vec{R}',\vec{r}\right)[-\frac{\hbar^2\nabla^2}{2m} + U(\vec{r})]w_n(\vec{R},\vec{r}) \tag{L32}$$

$$\mathcal{H}_{\vec{R}\vec{R}'} = \sum_{\vec{k}} \frac{1}{N}\mathcal{E}_{n\vec{k}}e^{-i\vec{k}\cdot(\vec{R}-\vec{R}')}. \tag{L33}$$

$$\hat{\mathcal{H}}_{\mathrm{TB}} = \sum_{\vec{R}\vec{\delta}} |\vec{R}\rangle\, \mathfrak{t}\, \langle\vec{R}+\vec{\delta}| + \sum_{\vec{R}} |\vec{R}\rangle U \langle\vec{R}|. \tag{L34}$$


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$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} |\vec{R}\rangle, \tag{L35}$$

$$|\vec{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} |\vec{k}\rangle, \tag{L36}$$

$$\hat{\mathcal{H}}_{\text{TB}} = ? \qquad ? \tag{L37}$$

$$= \sum_{\vec{k}} \mathcal{E}_{\vec{k}} |\vec{k}\rangle \langle \vec{k}| \tag{L38}$$

$$\mathcal{E}_{\vec{k}} = ? \qquad ? \tag{L39}$$

$$2\mathcal{W} = 2z\mathfrak{t}. \tag{L40}$$



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$$\hat{P}_n = \sum_k |\psi_{nk}\rangle\langle\psi_{nk}|. \tag{L41}$$

$$R|R\rangle = \hat{P}\hat{R}\hat{P}|R\rangle. \tag{L42}$$

$$w(R,k) = \langle\psi_k|R\rangle. \tag{L43}$$

$$Rw(R,k) = \sum_{k'} \langle\psi_k|\hat{R}|\psi_{k'}\rangle w(R,k'). \tag{L44}$$

$$\psi_k(x) = e^{ikx}u_k(x), \tag{L45}$$

$$\begin{aligned}\langle\psi_k|\hat{R}|\psi_{k'}\rangle = \quad & 2\pi i\left[\frac{\partial}{\partial k}\delta(k-k')\right]\int_0^a \frac{dx}{a}u_k^*(x)u_k(x) \\ & +2\pi\delta(k-k')\int_0^a \frac{dx}{a}u_k^*(x)i\frac{\partial}{\partial k}u_k(x).\end{aligned} \tag{L46}$$


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$$\tilde{u}_k(x) = e^{-i\phi(k)} u_k(x) \tag{L47}$$

$$\int_0^a \frac{dx}{a} \tilde{u}_k^*(x) i \frac{\partial}{\partial k} \tilde{u}_k(x) = 0, \tag{L48}$$

$$w(R,x) = \langle x | R \rangle \tag{L49}$$

$\psi_{k+2\pi/a}(x) = \exp[i\chi]\psi_k(x)$

$\exp[-i\gamma(k)]$

$\gamma(2\pi/a) = \chi$

$$\tilde{\psi}_{k+2\pi/a}(x) = e^{i\Gamma} \tilde{\psi}_k(x). \tag{L50}$$

$$R = \frac{\Gamma a}{2\pi} + la. \tag{L51}$$



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