H. Empty Lattice Approximation emphasizes effects of Periodicity.

- Consider an $\underbrace{\text{infinitisemally weak}}$ Periodic $U(\vec{r})$

$U(\vec{r}) \to 0$ [Yet, think about there is periodicity]

Easy to illustrate a One-Dimension (1D)

$U(x) \to 0$ [Yet, there is a "periodicity" of $\underbrace{\text{lattice constant } a}$]

- $U(x) = 0$, free particle Hamiltonian

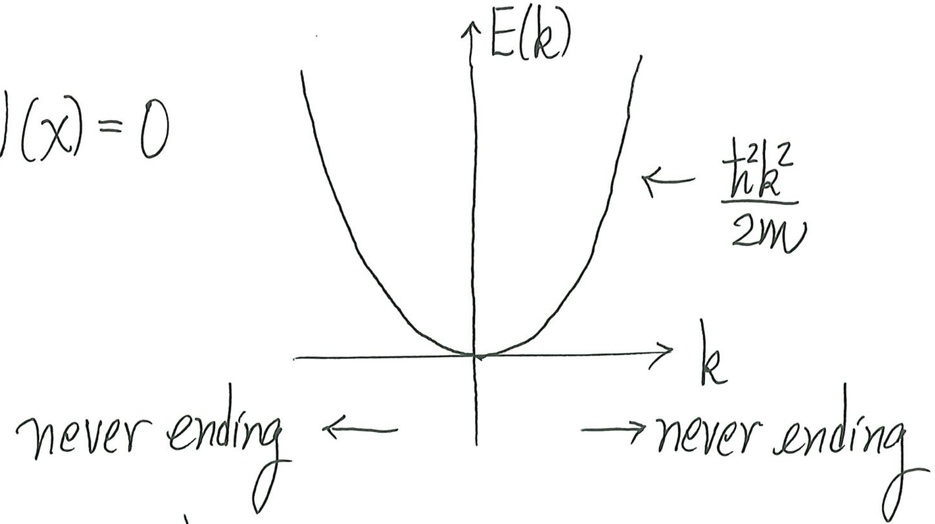
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_k(x) = E\,\psi_k(x)$$

$$\vec{G}_1 = \frac{2\pi}{a}\hat{x}$$

1st B.Z. is $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

$$\psi_k(x) \sim \underbrace{e^{ikx}}_{k \text{ can be +ve and -ve}} \quad \text{and} \quad E(k) = \frac{\hbar^2 k^2}{2m}$$

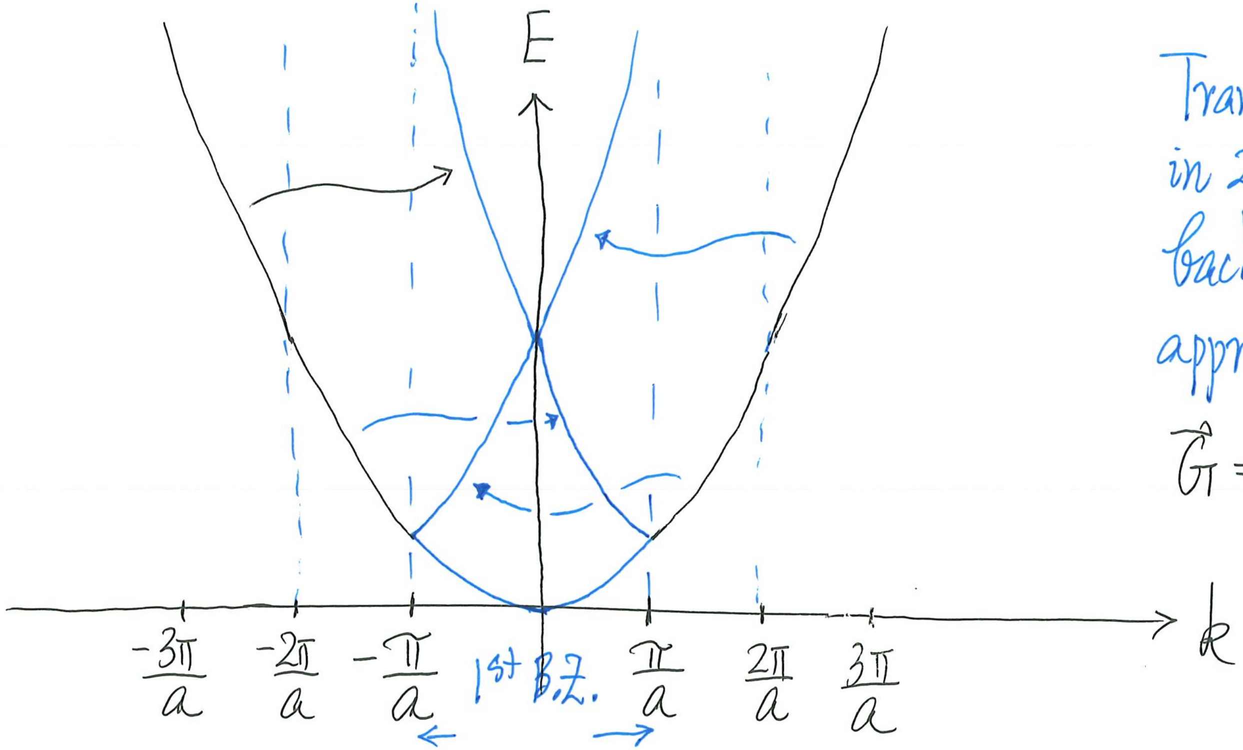
Strictly $U(x) = 0$



<u>Empty Lattice Approximation</u> $U(x) \to 0$, but hidden there is a periodic a

Then k can be chosen $k \in 1^{st}$ B.Z.

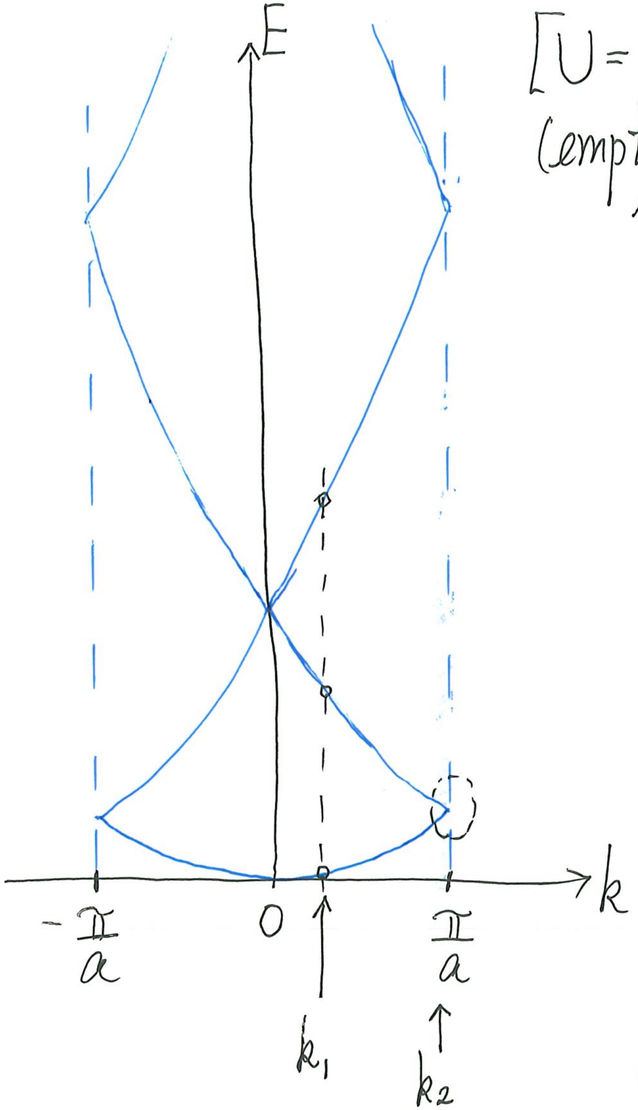
"Band Folding"



Translate E(k) in 2^{nd}, 3^{rd}, ... zones back to 1^{st} B.Z. by appropriate $\vec{G}$'s

$$\vec{G} = n\left(\frac{2\pi}{a}\hat{x}\right) = n\vec{b}_1$$

After Band Folding into 1st B.Z. [thus focused only on periodicity of $U(x)$],
we started to see <u>bands</u> (no band gaps yet)



$[U=0]$
(empty lattice)

$\boxed{\text{Turn On strength of } U(x), \text{ what will happen?}}$

$$U(x) = \sum_{\vec{G}} U_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

Each k is a separate Problem

<u>k_1 problem</u>

"n=3" ∘ $E^{(0)}(k_1 + \underbrace{\tfrac{2\pi}{a}}_{+G_1})$

"n=2" ∘ $E^{(0)}(k_1 - \underbrace{\tfrac{2\pi}{a}}_{-G_1})$

"n=1" ∘ $E^{(0)}(k_1)$

k_1

$U=0$ | $U\neq 0$ (add in some terms)

<u>Problem is:</u>

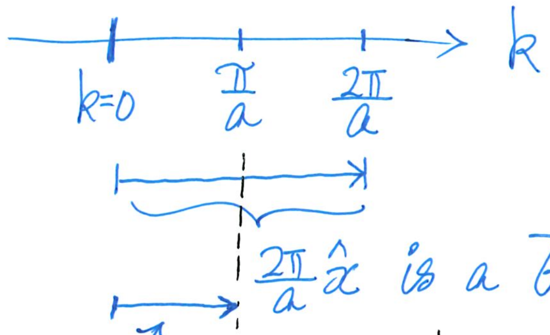
$$\begin{pmatrix} E^{(0)}(k_1) & U_{-G_1} & U_{+G_1} & \\ U^*_{-G_1} & E^{(0)}(k_1 - \frac{2\pi}{a}) & U_{G_2} & \\ U^*_{+G_1} & U^*_{G_2} & E^{(0)}(k_1 + \frac{2\pi}{a}) & \\ & & & \ddots \end{pmatrix} \qquad (39)$$

U_G will modify the eigenvalues only slightly ($\because$ E^0 values are far from eachother) for the k_1 problem

---

<u>How about the problem at k_2?</u> [$k_2 \approx \frac{\pi}{a}$] (Key concept here)

(a) What is so special at $k_2 = +\frac{\pi}{a}$ (or $k_3 = -\frac{\pi}{a}$)?



$\frac{2\pi}{a}\hat{x}$ is a $\vec{G}$ vector (shortest one except $\vec{G}=0$)

$\frac{\pi}{a}$ (bisect a $\vec{G}$, i.e. it is $\frac{\vec{G}}{2}$ for some $\vec{G}$)

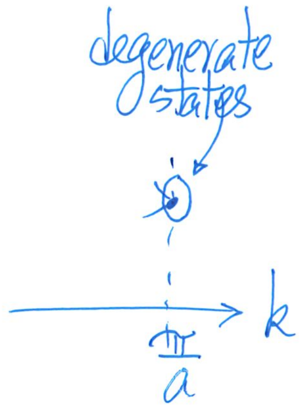
$\vec{k}_2$

same for $\vec{k}_3 = -\frac{\pi}{a}$

(b) so what?

There will be a state with degenerate energy in the empty lattice approximation

$$\underbrace{\frac{\hbar^2}{2m}\left(\frac{+\pi}{a}\right)^2}_{k_2} = \underbrace{\frac{\hbar^2}{2m}\left(\frac{-\pi}{a}\right)^2}_{-k_2}$$



two $\vec{k}$-values in 1st B.Z. edge connected by $\vec{G}_1$

(c) <u>so so what?</u> ($U \neq 0$ add in some terms)

$$\begin{pmatrix}
E^{(0)}(k_2) = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 & U_{-G_1} & U_{+G_1} & \cdots \\
U^*_{-G_1} & E^{(0)}\left(k_2 - \frac{2\pi}{a}\right) = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 & U_{+G_2} & \\
U^*_{+G_1} & U^*_{+G_2} & E^{(0)}\left(k_2 + \frac{2\pi}{a}\right) = \frac{\hbar^2}{2m}\left(\frac{3\pi}{a}\right)^2 \text{ (very high)} & U_{G_2} \\
\vdots & \vdots & U^*_{G_2} & E^{0}\left(k_2 - \frac{4\pi}{a}\right) = \frac{\hbar^2}{2m}\left(\frac{3\pi}{a}\right)^2 \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix} \quad (40)$$

What is the effect?

When there are degenerate states, $U_{\vec{G}}$ will be most apparent in its effect!

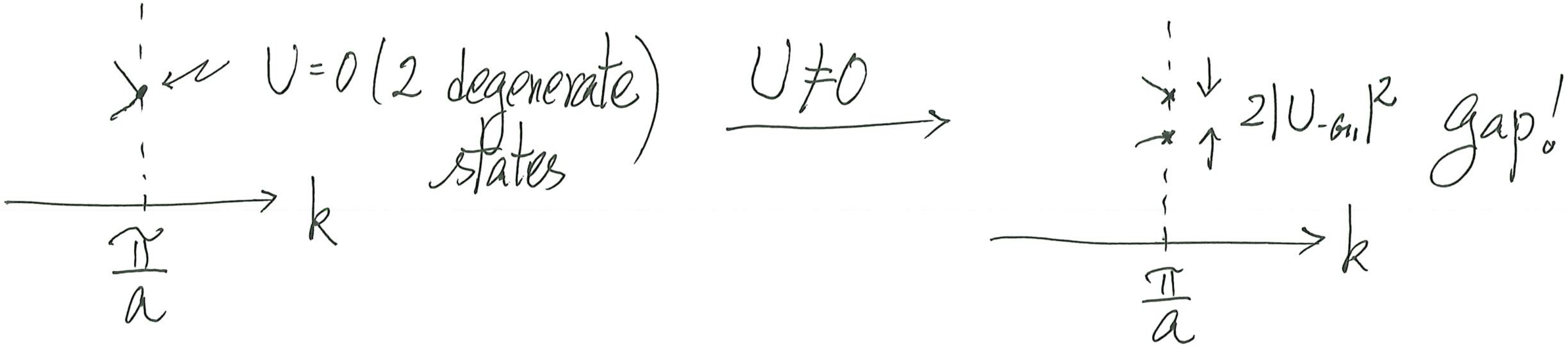
$$\begin{vmatrix} \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 - E & U_{-G_1} \\ U^*_{-G_1} & \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 - E \end{vmatrix} = 0$$

gives dominating effect of $U(x)$

$$\Rightarrow E = \begin{cases} \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + |U_{-G_1}| \\ \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 - |U_{-G_1}| \end{cases}$$

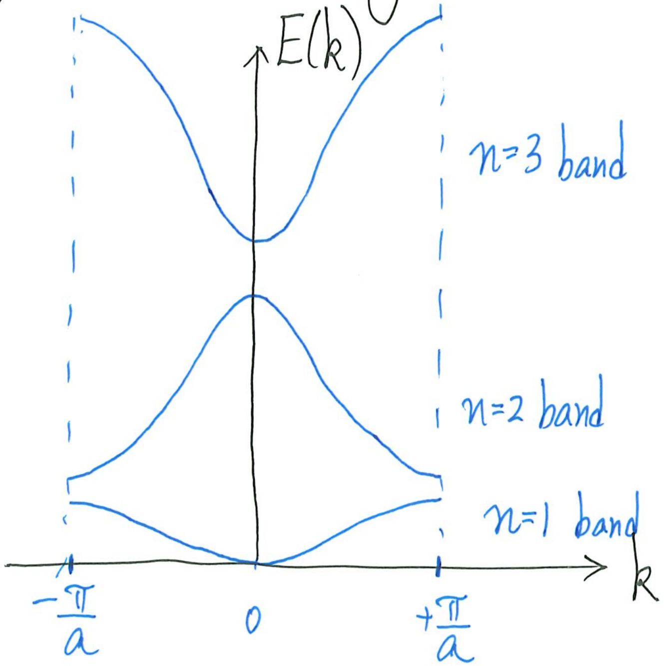
(lift the degeneracy!)

This is eigenvalue problem of $\begin{pmatrix} \varepsilon_0 & \Delta \\ \Delta^* & \varepsilon_0 \end{pmatrix}$



[Similar effect for k's near $\pm\frac{\pi}{a}$, and other k's with degeneracy in empty lattice]

After considering $U(x) \neq 0$ and Periodic, we expect to have



So, $\psi_{n\vec{k}}(\vec{r})$ makes sense!

The Band Folding and Qualitative effects of $U(\vec{r})$ are important concepts for understanding bands/band gaps and proposing creative ideas with applications.

(It is related to waves in periodic structures)

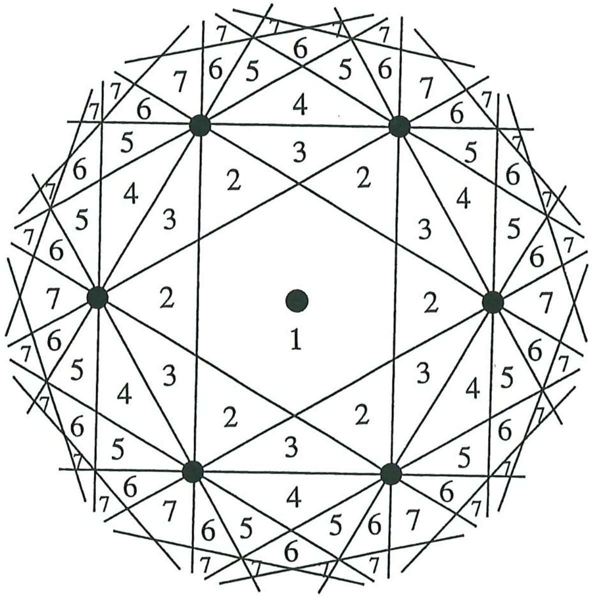
The Idea can be carried over to 2D and 3D.

B.Z.'s of 2D Hexagonal Lattice

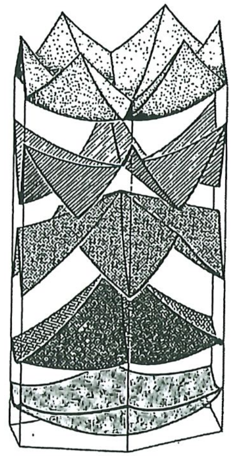
Higher Dimension, points with Higher degeneracy

Band Folding (U=0)

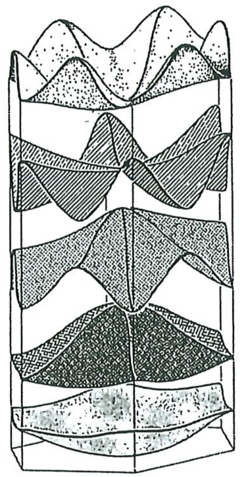
U ≠ 0



(a)

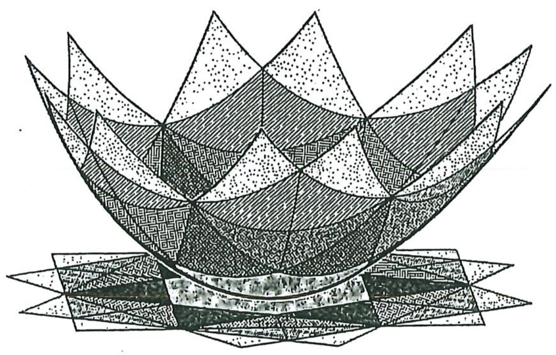


(c)



(d)

$E(k) = \frac{\hbar^2 k^2}{2m}$

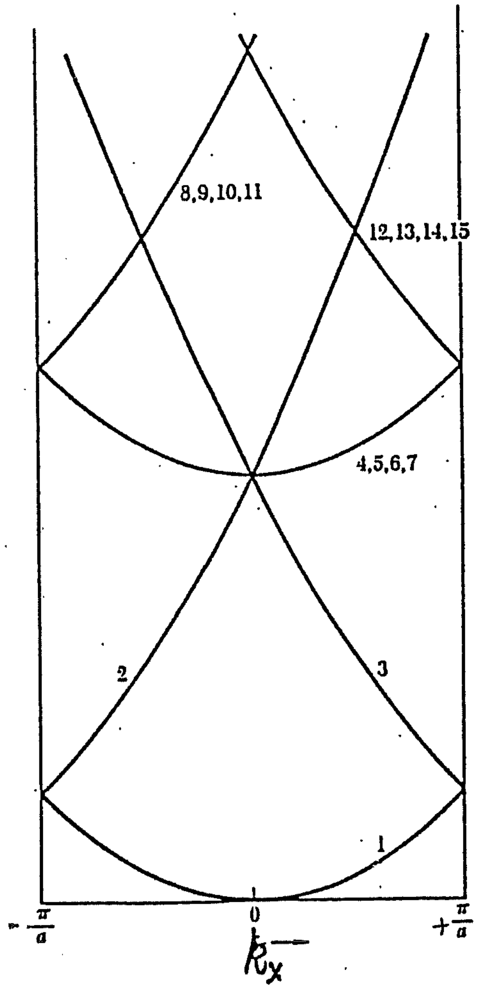


(b)

a) Brillouin zones for a two-dimensional hexagonal lattice. b) Energy paraboloid for free electrons ($E = \hbar^2k^2/2m$) above the k-plane for the two-dimensional hexagonal lattice. Regions of the free-electron energy surface falling in different Brillouin zones are shaded differently. c) The energy paraboloid of (b) reduced to the first Brillouin zone. d) The bands of (c) smoothed by the effect of a weak lattice potential.

[Taken from Snoke, "Solid State Physics". See also Madelung, "Introduction to Solid State Theory"]

A "simple" 3D example: Simple Cubic Lattice (can't draw 4D diagrams)



band crossings

$\vec{k} = (k_x, 0, 0)$

Band	$Ga/2\pi$	$\epsilon(000)$	$\epsilon(k_x00)$
1	000	0	k_x^2
2,3	100,$\bar{1}00$	$(2\pi/a)^2$	$(k_x \pm 2\pi/a)^2$
4,5,6,7	010,$0\bar{1}0$,001,$00\bar{1}$	$(2\pi/a)^2$	$k_x^2 + (2\pi/a)^2$
8,9,10,11	110,101,$1\bar{1}0$,$10\bar{1}$	$2(2\pi/a)^2$	$(k_x + 2\pi/a)^2 + (2\pi/a)^2$
12,13,14,15	$\bar{1}10$,$\bar{1}01$,$\bar{1}\bar{1}0$,$\bar{1}0\bar{1}$	$2(2\pi/a)^2$	$(k_x - 2\pi/a)^2 + (2\pi/a)^2$
16,17,18,19	011,$0\bar{1}1$,$01\bar{1}$,$0\bar{1}\bar{1}$	$2(2\pi/a)^2$	$k_x^2 + 2(2\pi/a)^2$

$G = \frac{2\pi}{a}(\uparrow\uparrow\uparrow)$

Energies at $k=0$

factors of $\frac{\hbar^2}{2m}$ are ignored.

Energies along $(k_x, 0, 0)$

factors of $\frac{\hbar^2}{2m}$ are ignored.

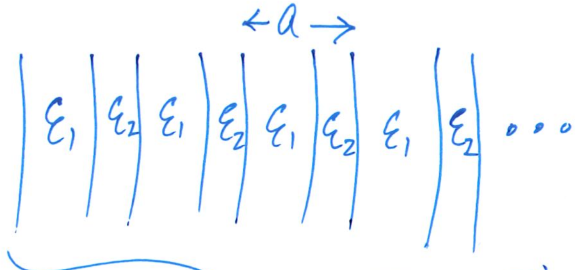
Low-lying free electron energy bands of the empty sc lattice, as transformed to the first Brillouin zone and plotted vs. (k_x00). The free electron energy is $\hbar^2(\mathbf{k}+\mathbf{G})^2/2m$, where the G's are given in the second column of the table. The bold curves are in the first Brillouin zone, with $-\pi/a \leq k_x \leq \pi/a$. Energy bands drawn in this way are said to be in the reduced zone scheme.

[Taken from Kittel, "An introduction to Solid State Physics"]

Applications of the Idea

- Photonic Crystals

"1D case"
(usually photonic crystals refer to 2D/3D structures)

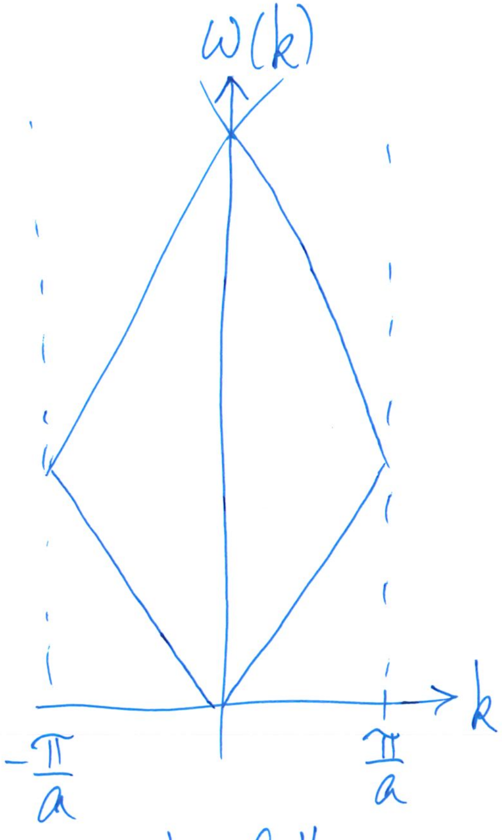


EM waves propagation

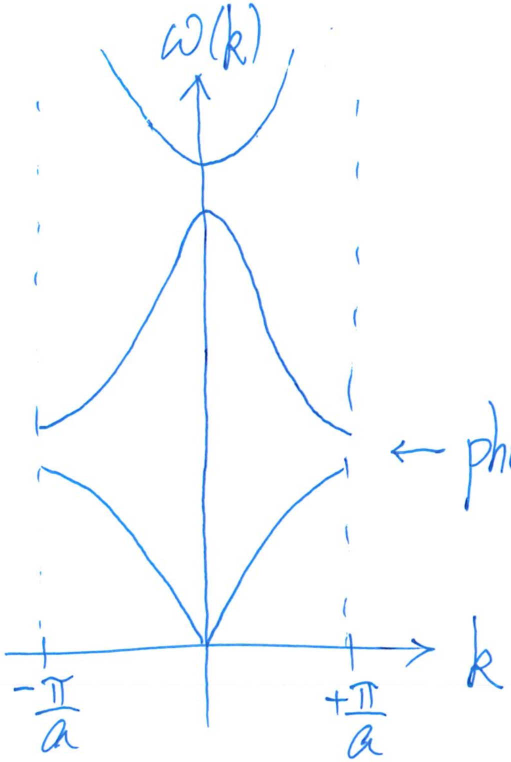
$$\underbrace{\epsilon(x) = \epsilon(x+na)}_{\text{periodic dielectric function}}$$

c.f. $\left[\nabla^2 + \frac{\omega^2}{c^2}\epsilon(\vec{r})\right]\psi(\vec{r}) = 0$

↑ $\mathcal{E}$-field

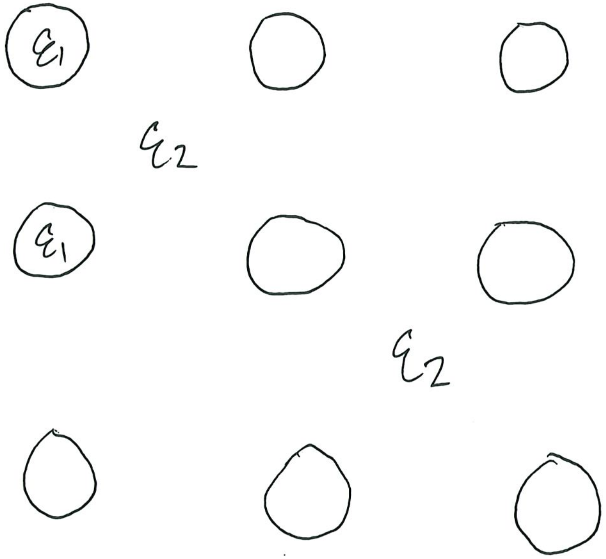


empty lattice

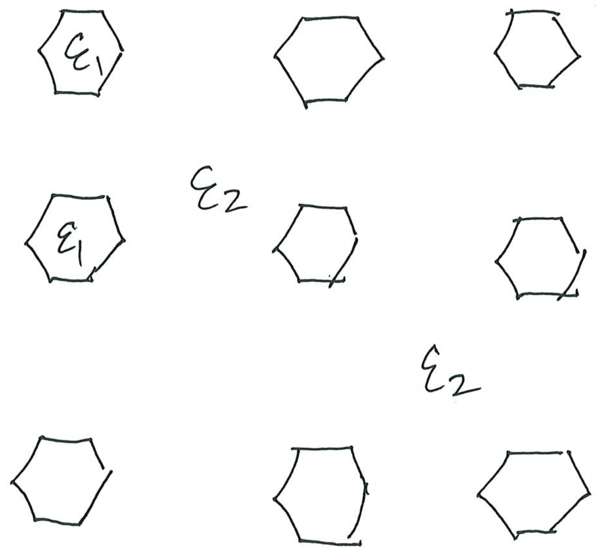


← photonic bandgap
(No "normal modes" in gap for EM waves to propagate through the structure)

3D



OR



stacking it up

stacking it up

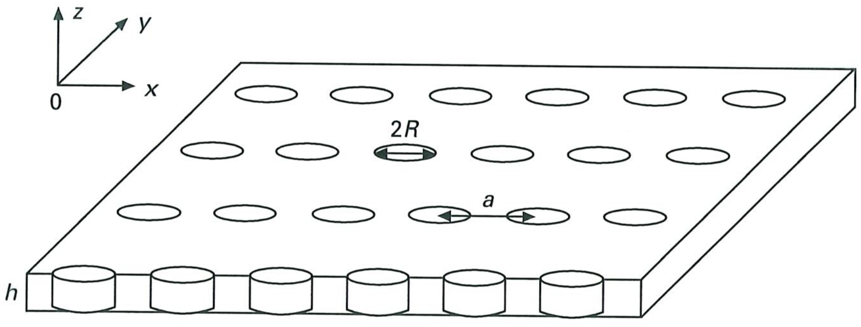
or more complicated structures

Maxwell's equations in Periodic Structures

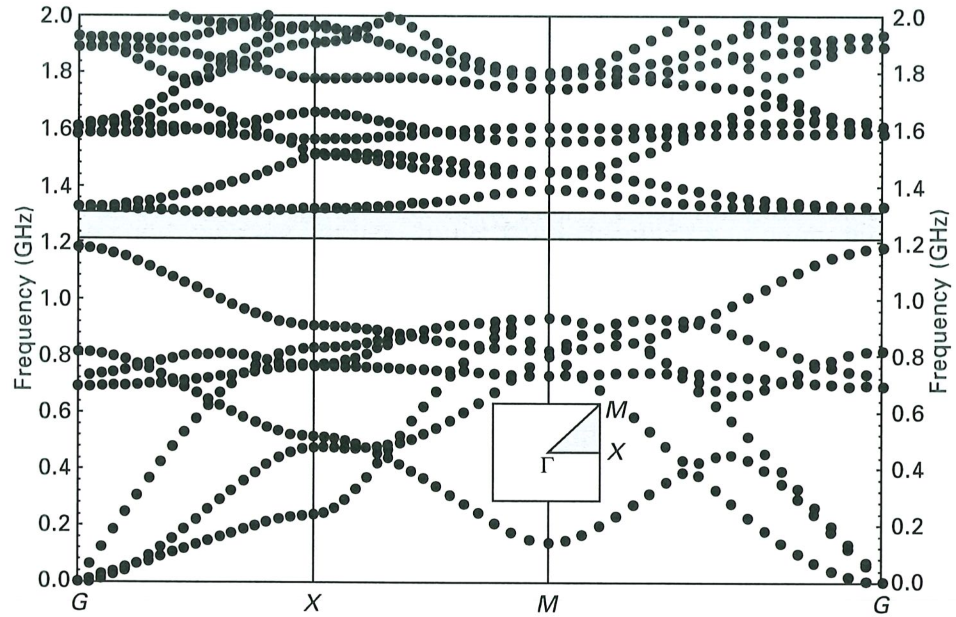
• Phononic Crystals

Sound Waves propagating through "softer" and "harder" periodic structures

different elastic modulus



Phononic crystal plate of thickness h. The basic phononic crystal is composed of a square array of parallel cylindrical air inclusions (holes) of radius R drilled in a piezoelectric matrix. The lattice parameter is a.



Elastic band structures calculated with the ATILA code. The phononic crystal plate of thickness $h = a = 0.77$ µm is made of a square array of holes drilled in a PZT5A piezoelectric matrix with a filling fraction of 0.7. The inset represents the Brillouin zone (ΓXM) of the square array.

Taken from Hladky-Hennion, in Applications of ATILA FEM Software to Smart Materials, 2013

"Photonic Crystal (PC) applications of ATILA"

These two fields have evolved into hot areas called <u>metamaterials</u>[+]
and <u>Smart Materials</u>.

- Use different (available) materials <u>AND</u> artificial structures to manipulate wave propagations (e.g. negative refractive index, invisible cloaking, focusing, ...)

<u>e.g.</u> Schrüch and Philipee, "Composite Metamaterials: Types and Synthesis", in Encyclopedia of Materials: Composites (2021)

[+] Photonic metamaterials and acoustic metamaterials

I. The Method of Plane Wave Expansion

- A general method to set up Band Structure Calculations
- The way to put the discussion in Empty Lattice Approximation into math

General Structure

$\hat{H}\psi = E\psi$ standard QM problem (TISE)

Pick a set of basis functions $\{\phi_i\}$, expand $\psi = \sum_i c_i \phi_i$ (c_i: unknowns; ϕ_i: knowns)

Then TISE becomes a huge matrix problem

$$\begin{pmatrix} \text{Typically} \\ \infty \times \infty \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_i \\ \vdots \end{pmatrix} = 0$$

with Matrix Elements $(H_{ji} - E S_{ji})$

$$H_{ji} = \int \phi_j^* \hat{H} \phi_i \, d^3r \; ; \; S_{ji} = \int \phi_j^* \phi_i \, d^3r$$

Solid State Energy Band Problems

$$\hat{H}\,\psi_{\vec{k}}(\vec{r}) = E(\vec{k})\,\psi_{\vec{k}}(\vec{r}) \qquad (1)$$

take on the Bloch Form

For each $\vec{k}$, it is a separate problem.

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\,u_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} e^{i\vec{k}\cdot\vec{r}}\,u_{\vec{k}+\vec{G}}\,e^{i\vec{G}\cdot\vec{r}}$$

($\because$ $u_{\vec{k}}(\vec{r})$ is periodic)

$$= \sum_{\vec{G}} \underbrace{u_{\vec{k}+\vec{G}}}_{\text{unknowns}}\,e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

SAME

$$= \sum_{\vec{G}} u_{\vec{k}}(\vec{G})\,e^{i(\vec{k}+\vec{G})\cdot\vec{r}} \qquad (41)$$

labelling the problem of a particular $\vec{k}$ under consideration

$\therefore$ Basis Functions are:

For a given $\vec{k}$: $\{e^{i\vec{k}\cdot\vec{r}}, e^{i(\vec{k}+\vec{G}_1)\cdot\vec{r}}, e^{i(\vec{k}+\vec{G}_2)\cdot\vec{r}}, \dots\}$ Plane Waves (but only $\vec{G}$-components due to periodicity)

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \equiv -\frac{\hbar^2}{2m}\nabla^2 + \underbrace{V(\vec{r})}_{\text{using } V(\vec{r}) \text{ to avoid confusion}^{+}}$$

(i) $$-\frac{\hbar^2}{2m}\nabla^2 \psi_{\vec{k}}(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2\left(\sum_{\vec{G}} u_{\vec{k}}(\vec{G})\, e^{i(\vec{k}+\vec{G})\cdot\vec{r}}\right)$$

$$= e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \frac{\hbar^2}{2m}|\vec{k}+\vec{G}|^2 e^{i\vec{G}\cdot\vec{r}}\, u_{\vec{k}}(\vec{G})$$

(ii) $V(\vec{r})$ is periodic (given)

$$V(\vec{r}) = \sum_{\vec{G}'} V_{\vec{G}'}\, e^{i\vec{G}'\cdot\vec{r}} = \sum_{\vec{G}'} V(\vec{G}')\, e^{i\vec{G}'\cdot\vec{r}} \quad (8)$$

knowns

$$V(\vec{G}') = \frac{1}{\Omega_c}\int_{\Omega_c} e^{-i\vec{G}'\cdot\vec{r}}\, V(\vec{r})\, d^3r \; ; \text{ in particular } \underset{\vec{G}'=0}{V(\vec{0})} = \underbrace{\frac{1}{\Omega_c}\int V(\vec{r})\, d^3r}_{\text{average of } V(\vec{r})} = \bar{V} \quad (42)$$

Ω_c: one primitive cell

$^{+}$ as "u" is used for $u_{\vec{k}}(\vec{r})$, the cell function in Bloch Form.

$$V(\vec{r})\,\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \sum_{\vec{G}'} V(\vec{G}')\, u_{\vec{k}}(\vec{G})\, e^{i(\vec{G}+\vec{G}')\cdot\vec{r}}$$

$$= e^{i\vec{k}\cdot\vec{r}}\, \overline{V} \sum_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}\, u_{\vec{k}}(\vec{G})$$ ← $\vec{G}'=0$ term

$$+ e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \sum_{\substack{\vec{G}' \\ (\vec{G}'\neq 0)}} V(\vec{G}')\; u_{\vec{k}}(\vec{G})\, e^{i(\vec{G}+\vec{G}')\cdot\vec{r}}$$

(iii) RHS of TISE

$$E(\vec{k})\,\psi_{\vec{k}}(\vec{r}) = E(\vec{k})\; e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} u_{\vec{k}}(\vec{G})\, e^{i\vec{G}\cdot\vec{r}}$$

TISE $\Rightarrow$ (i) + (ii) = (iii)

Cancelling "$e^{i\vec{k}\cdot\vec{r}}$" that appears in every term

TISE becomes:

$$\sum_{\vec{G}} \left[\frac{\hbar^2}{2m}|\vec{k}+\vec{G}|^2 + \overline{V}\right] u_{\vec{k}}(\vec{G})\, e^{i\vec{G}\cdot\vec{r}} + \sum_{\vec{G}}\sum_{\vec{G}'} V(\vec{G}')\, u_{\vec{k}}(\vec{G})\, e^{i(\vec{G}+\vec{G}')\cdot\vec{r}}$$

$$= E(\vec{k}) \sum_{\vec{G}} u_{\vec{k}}(\vec{G})\, e^{i\vec{G}\cdot\vec{r}} \qquad (43) \quad \text{(Exact)}$$

(to solve for $\underset{\uparrow\,\text{all } \vec{G}\text{'s}}{u_{\vec{k}}(\vec{G})} \leftrightarrow E(\vec{k})$ pairs (many of them))

- left multiply by $e^{-i\vec{G}''\cdot\vec{r}}$ [select a $\vec{G}$ (call it $\vec{G}''$) and do it]
- $\frac{1}{\Omega_c}\int_{\Omega_c} (\cdots)\, d^3r$ over a unit cell
- $\frac{1}{\Omega_c}\int_{\Omega_c} d^3r\, e^{i(\vec{G}-\vec{G}'')\cdot\vec{r}} = \delta_{\vec{G},\vec{G}''}$

do these on TISE

TISE becomes:

$$\left[\frac{\hbar^2}{2m}|\vec{k}+\vec{G}''|^2+\overline{V}\right]u_{\vec{k}}(\vec{G}'') + \sum_{\substack{\vec{G}' \\ (\vec{G}'\neq 0)}} V(\vec{G}')\, u_{\vec{k}}(\vec{G}''-\vec{G}') = E(\vec{k})\, u_{\vec{k}}(\vec{G}'') \quad (44)$$

- Central Equation (exact so far, need truncation in practice)
- a $\infty \times \infty$ matrix Problem for every $\vec{k}$ ($\vec{k} \in 1^{st}$ B.Z.) $\Rightarrow E_n(\vec{k})$

  $\uparrow$ labelling solutions
- This is the equation for the math. of the physical picture discussed in Sec. H.

$^+$ Eq. (44) is in fact a matrix problem of elements $(H_{ji} - E\delta_{ji})$ multiplying into a column vector of $u_{\vec{k}}(\vec{G})$'s. See following pages.

Analyzing the equation:

$$\left[\frac{\hbar^2}{2m}|\vec{k}+\vec{G}''|^2+\bar{V}\right]u_{\vec{k}}(\vec{G}'')+\sum_{\vec{G}'(\vec{G}'\neq 0)} V(\vec{G}')\,u_{\vec{k}}(\vec{G}''-\vec{G}') = E(\vec{k})\,u_{\vec{k}}(\vec{G}'') \qquad (44)$$

"IF it were not here"

$$\overbrace{\left[\underbrace{\frac{\hbar^2}{2m}|\vec{k}+\vec{G}''|^2}_{\text{free electron}}+\bar{V}\right]}^{\text{diagonal terms}} u_{\vec{k}}(\vec{G}'') = E(\vec{k})\,u_{\vec{k}}(\vec{G}'')$$

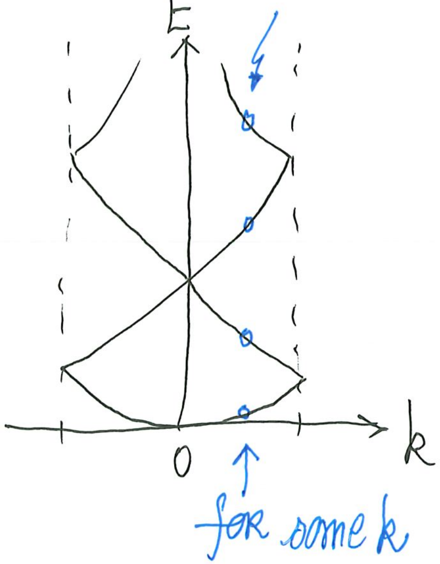
free electron

↓

these are the values

$\bar{V}$: just a constant (1st order perturbation)

[lowest order effect of $V(\vec{r})$]



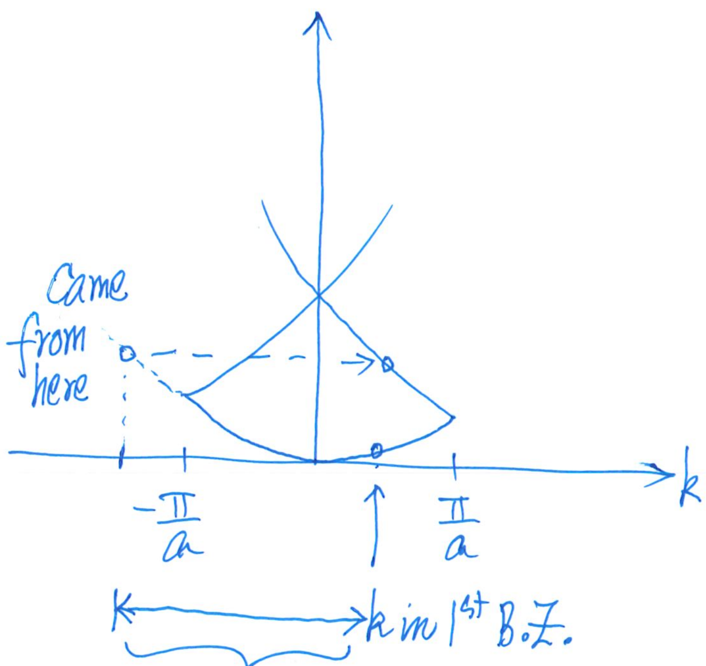
$$\varepsilon^0(k) \equiv \frac{\hbar^2 k^2}{2m}$$

$$\begin{pmatrix} \varepsilon^0(\vec{k})+\bar{V} & & & & \\ & \varepsilon^0(\vec{k}+\vec{G}_1)+\bar{V} & & & \\ & & \ddots & & \\ & & & \varepsilon^0(\vec{k}+\vec{G}'')+\bar{V} & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ \vdots \\ u_{\vec{k}}(\vec{G}'') \\ \vdots \end{pmatrix} = E(\vec{k}) \begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ \vdots \\ u_{\vec{k}}(\vec{G}'') \\ \vdots \end{pmatrix}$$

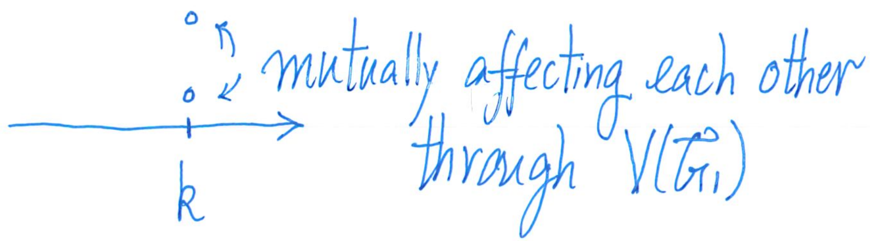
(if ignoring terms with $V(\vec{G}')$, $\vec{G}'\neq 0$)

$\therefore \sum_{\vec{G}'(\vec{G}'\neq 0)} V(\vec{G}')\, U_{\vec{k}}(\vec{G}''-\vec{G}')$ represents the coupling between plane waves basis functions due to the various Fourier components $V(\vec{G}')$ of $V(\vec{r})$

$V(\vec{G}')$ can connect $\underbrace{e^{i\vec{k}\cdot\vec{r}}\, e^{i\vec{G}''\cdot\vec{r}} \text{ to } e^{i\vec{k}\cdot\vec{r}}\, e^{i(\vec{G}''-\vec{G}')\cdot\vec{r}}}_{\text{differs by } \vec{G}'}$



connected by $\vec{G}_1 = \frac{2\pi}{a}\hat{x}$, thus $V(\vec{G}_1)$ serves to couple them.



The whole Matrix can be visualized as

$$\begin{array}{cc}
 & \begin{array}{ccccc} e^{i\vec{k}\cdot\vec{r}} & e^{i(\vec{k}+\vec{G}_1)\cdot\vec{r}} & e^{i(\vec{k}+\vec{G}_2)\cdot\vec{r}} & e^{i(\vec{k}+\vec{G}_3)\cdot\vec{r}} & \cdots \leftarrow \text{help you think} \end{array} \\
\begin{array}{c} e^{i\vec{k}\cdot\vec{r}} \\ e^{i(\vec{k}+\vec{G}_1)\cdot\vec{r}} \\ e^{i(\vec{k}+\vec{G}_2)\cdot\vec{r}} \\ e^{i(\vec{k}+\vec{G}_3)\cdot\vec{r}} \\ \vdots \\ \uparrow \\ \text{Basis} \\ \text{functions} \end{array} &
\begin{pmatrix}
\varepsilon^0(\vec{k})+\bar{V} & V(-\vec{G}_1) & V(-\vec{G}_2) & V(-\vec{G}_3) & \cdots \\
V(\vec{G}_1) & \varepsilon^0(\vec{k}+\vec{G}_1)+\bar{V} & V(\vec{G}_1-\vec{G}_2) & V(\vec{G}_1-\vec{G}_3) & \cdots \\
V(\vec{G}_2) & V(\vec{G}_2-\vec{G}_1) & \varepsilon^0(\vec{k}+\vec{G}_2)+\bar{V} & V(\vec{G}_2-\vec{G}_3) & \cdots \\
V(\vec{G}_3) & V(\vec{G}_3-\vec{G}_1) & V(\vec{G}_3-\vec{G}_2) & \varepsilon^0(\vec{k}+\vec{G}_3)+\bar{V} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\end{array} \qquad (45)$$

Eigenvalues of this Matrix give $\underbrace{E(\vec{k})\ [\text{many values}]}_{E_n(\vec{k})}$

Done!

Band Index → n

$\uparrow$ counting from lowest energy up

TISE is equivalent† to:

$$\begin{pmatrix} & & \\ & \text{Last Page} & \\ & & \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ u_{\vec{k}}(\vec{G}_2) \\ \vdots \end{pmatrix} = E(\vec{k}) \begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ u_{\vec{k}}(\vec{G}_2) \\ \vdots \end{pmatrix} \quad (46)$$

- This finishes the general set up for band structure problems
- "Exact" (if retaining $\infty \times \infty$); Practice (depending on # bands required, truncations)
- <u>Viewpoint</u>: Starts with Plane Waves (although exact mathematically), the picture is "what does periodic $V(\vec{r})$ do to otherwise free electrons"?
- Good for electronic bands, photonic bands, phononic bands, ...

---

† This is the quantitative treatment behind the physical pictures introduced in Sec. H (see Eqs. (39) and (40))