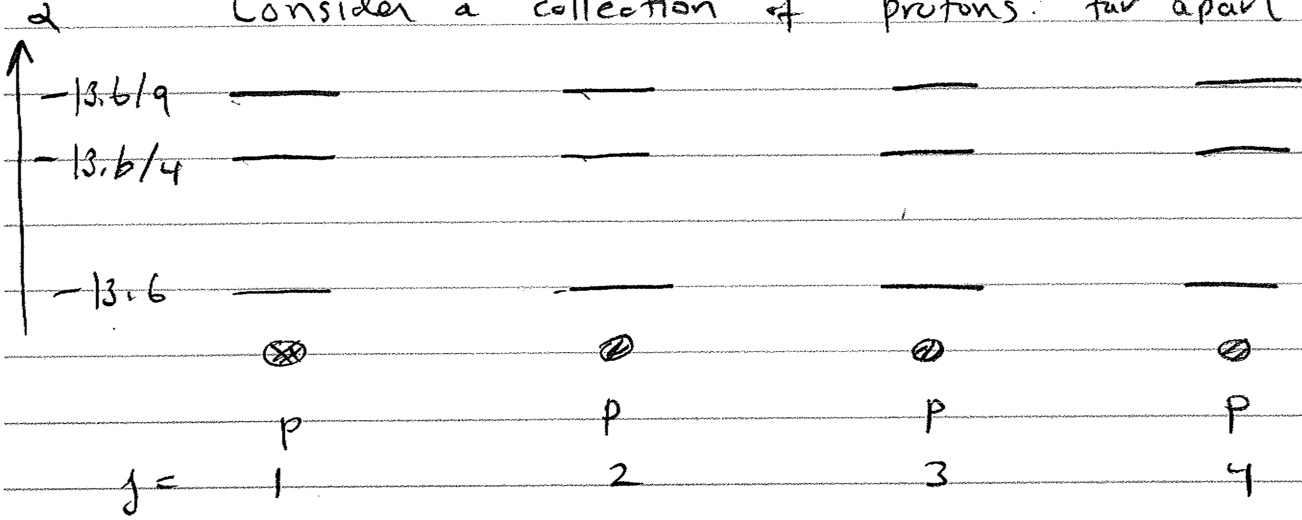
BB-1

BAND STRUCTURE BACKGROUND

Consider a collection of protons far apart



We know there are energy levels (Hydrogen atom levels)

for an electron to sit near each proton $E_n = \frac{-13.6}{n^2}$ eV

If protons really far apart, the state of the system

is described by $|j\ \alpha\rangle$

which proton (j) — which level (α)

BB-2.

The Hamiltonian in this basis is

$$\begin{array}{c c}
\begin{array}{c}\alpha=1\\ \text{block}\end{array} & \left[\begin{array}{cccc|cccc}
-13.6 & & & & & & & \\
 & -13.6 & & & & & & \\
 & & -13.6 & & & & & \\
 & & & \ddots & & & & \\
\hline
 & & & & -13.6/4 & & & \\
 & & & & & -13.6/4 & & \\
 & & & & & & -13.6/4 & \\
 & & & & & & & \ddots
\end{array}\right] \\
 & \underbrace{\qquad\qquad\qquad}_{N \text{ protons}} \qquad \begin{array}{c}\alpha=2\\ \text{block}\end{array}
\end{array}$$

Each level α is
Highly degenerate
(N identical
eigenvalues)

What happens if protons get closer? The completely
Isolated wave functions of a single proton (nucleus) begin to mix with neighbors

We can describe this process mathematically via

$$\begin{pmatrix} E & & \\ & E & \\ & & E \end{pmatrix} \rightarrow \begin{pmatrix} E & -t & \\ -t & E & -t \\ & -t & E \end{pmatrix}$$

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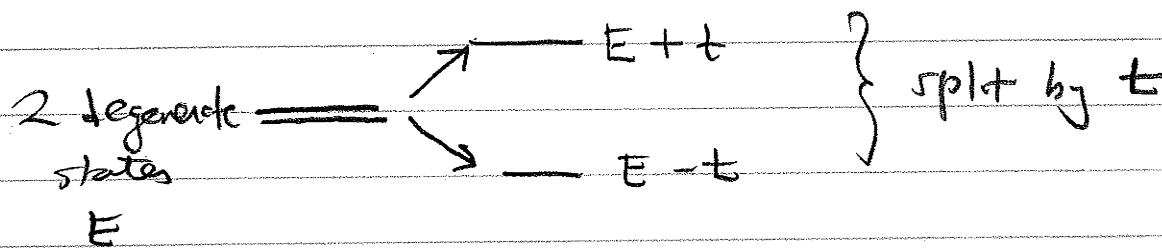
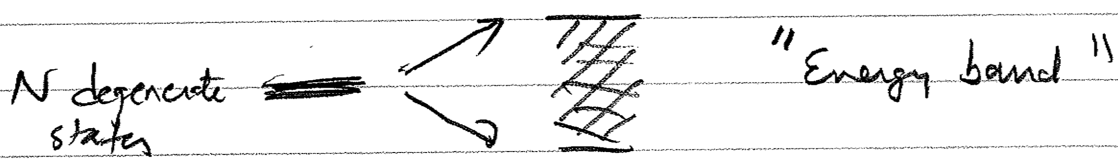
2×2 Example

$$\begin{pmatrix} E & -t \\ -t & E \end{pmatrix} \qquad (E-\lambda)^2 - t^2 = 0$$

$$\lambda = E \pm t$$

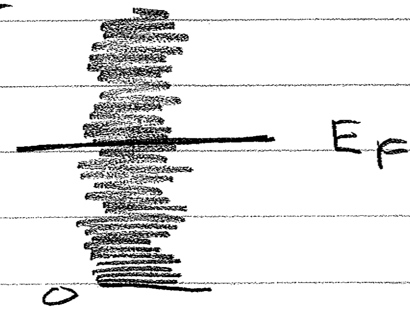


Larger system $\quad E \Rightarrow E - 2t\cos q$



Explains Metal vs insulator

Particle in a box picture:



unbroken set of levels

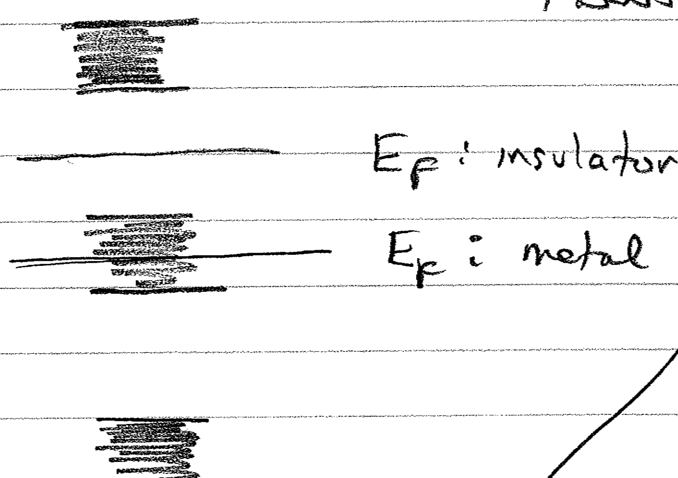
$$E_n = \frac{\hbar^2}{2m}\frac{\pi n^2}{L^2} \to \frac{\hbar^2 k^2}{2m}$$

k continuous as $L \to \infty$

No matter where E_F is always levels which are empty just above it.

Electric field applied e^- can move to those higher k levels → current flows

New picture:



no levels into which e^- can be shifted by Electric field: no current flow

like $C(T) = k_B \to k_B \frac{k_B T}{E_F}$

Similar "Pauli Blocking"

Actually, different types of insulators exist

This one is called <u>Band</u> <u>insulator</u>

General Rule: Materials with odd # valence electrons expected to be metallic. Reason is that really can put $2e^-$ in each level (spin up/spin dn) if odd # of electrons on each atom can never completely fill a band.

<u>Mott</u> <u>insulator</u> (from $e^- e^-$ interactions)

<u>Anderson</u> <u>insulator</u> ← disordered system and e^- get stuck in localized states. HW problem

$\boxed{\text{Discuss HW problem}}$

$$
\begin{array}{ccccccc}
E & -t & & & & & \\
-t & E & -t & & & & \\
 & -t & E_* & -t & & & \\
 & & -t & E & -t & & \\
 & & & -t & E & -t & \\
 & & & & -t & E_* & -t \\
 & & & & & -t &
\end{array}
$$

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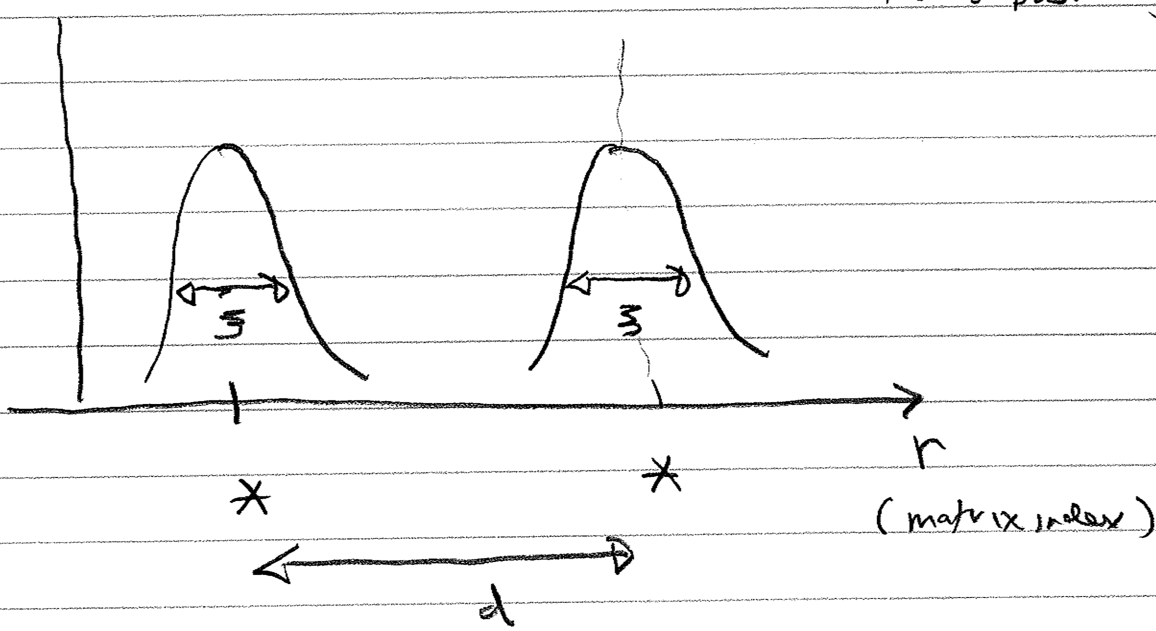
Can we make any guess at physics?

Perhaps insulator as long as distance between E_* levels $>$ localization length ξ ← Participation ratio is basically ξ



$d \gg \xi$ insulator

$d \sim \xi$ metal

control with $\frac{E_*}{E}$ ratio

or with defect density

Further
Analogy with Quantum Oscillator — Stark Effect

$$H_0 = \hbar\omega(a^\dagger a + 1/2) \longleftrightarrow H_0 = \tfrac{1}{2}m\omega^2 x^2 + p^2/2m$$

$$V = e\mathcal{E}\sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger) \longleftrightarrow V = e\mathcal{E}x$$

$$H_0 = \hbar\omega\begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 \\ 0 & 0 & 5/2 & 0 \\ 0 & 0 & 0 & 7/2 \end{pmatrix} \quad \text{in } |n\rangle \text{ basis}$$

$$V = e\mathcal{E}\sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & \sqrt{2} & & \\ & \sqrt{2} & 0 & \sqrt{3} & \\ & & \sqrt{3} & 0 & \sqrt{4} \\ & & & \sqrt{4} & 0 \end{pmatrix}$$

Similar Mathematical structure of perturbation V adding off diagonal $(n, n+1)$ $(n+1, n)$ elements to H_0.

Do not want to push analogy too far since V mixes states of different E_0 whereas in our band structure problem highly degenerate states are mixed.

$\nabla^2 - 1$

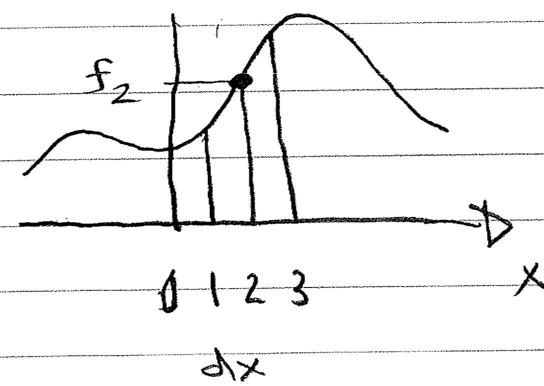
Tridiagonal Matrix

Tridiagonal Matrix arises for us in soln of Mass spring problem (phonons) and now also in trying to understand Energy bands of electrons in solids

In fact it is absolutely ubiquitous. why?

$$f''(x) = \frac{d^2 f}{dx^2} \qquad f(x) \rightarrow$$

continuous



$$f(x) \rightarrow \begin{pmatrix} \vdots \\ f_{-2} \\ f_{-1} \\ f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}$$

$$f(x+\Delta x) = f(x) + \Delta x\, f'(x) + \tfrac{1}{2}\Delta x^2 f''(x) + \ldots$$

$$f(x-\Delta x) = f(x) - \Delta x\, f'(x) + \tfrac{1}{2}\Delta x^2 f''(x) + \ldots$$

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + \Delta x^2\, f''(x)$$

$\Delta^2 - 2$

$$f''(x) = \frac{1}{\Delta x^2}\left[f(x+\Delta x) - 2f(x) + f(x-\Delta x)\right]$$

$$\frac{d^2 f}{dx^2} = -\frac{1}{\Delta x^2}\begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 & \\ & & & & & & \end{bmatrix}\begin{pmatrix} \vdots \\ f_{-2} \\ f_{-1} \\ f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}$$

Matrix for our mass spring problem

$$\frac{k}{m}\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & & \ddots & \\ & & & & & \end{bmatrix}$$

Actually this is basis of connection of discrete mass spring problem to the wave eqn which is alternate way of describing lattice vibrations/sound

$$x_n(t) = a_n e^{i\omega t}$$

$$\frac{\partial^2 f}{\partial x^2} + \frac{1}{v^2}\frac{\partial^2 f}{\partial t^2} = 0$$