Quadratic eigenvalue problem.

* An electron in magnetic field along z-direction.

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{i\hbar e}{c}\left(\nabla\cdot\vec{A} + \vec{A}\cdot\nabla\right) + \frac{e^2A^2}{c^2}$$

using Coulomb gauge $\nabla\cdot\vec{A} = 0$

and choose $\vec{A} = Bx\hat{j} \equiv B\vec{A}_0$ and set

$$E = \frac{\hbar^2}{2m}e_0$$

$$b = \frac{eB}{\hbar c}$$

We have

$$\left(-\nabla^2 + 2ib\vec{A}_0\cdot\nabla + b^2A_0^2\right)\psi = e_0\psi$$

use finite difference method to discretize the system,

in the tight-binding representation, we write

$$\left(M_1 + ibM_2 + b^2M_3\right)\psi = e_0\psi$$

where M_1, M_2, M_3 are matrices

* eigenvalue problem. (1). given B or b, we can find e_0

(2). given e_0, we want to find b

$\Downarrow$

quadratic eigenvalue problem

$\psi = \phi e^{-ibt}$

$\phi = \psi e^{ibt}$

$\dot{\phi} = \psi ib e^{ibt}$

$\ddot{\phi} = \psi b^2 e^{ibt}$

Let $\Psi(t) = e^{ibt}\psi$

We have

$$M_1 \Psi + M_2 \dot{\Psi} - M_3 \ddot{\Psi} = e\Psi$$

* recall classical mechanics.

Lagrange equation of motion

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \quad \Rightarrow \quad m\ddot{x} = F$$

second order diff. eq.

$x(t)$ as variable.

Hamilton's equation of motion

use $q(t)$, $p(t)$, two sets of variables.

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad -\dot{p}_i = \frac{\partial H}{\partial q_i}$$

2 - 1^{st} order diff. equ.

* $m\ddot{x} = F$, $y = \dot{x}$

$$\begin{cases} m\dot{y} = F \\ \dot{x} = y \end{cases}$$

use x, y as variables,

One second order diff. equ

becomes two 1^{st} order diff. equ.

set $\Phi = \dot{\Psi}$, we have

$$\begin{cases} M_1 \Psi + M_2 \Phi - M_3 \dot{\Phi} = e \Psi \\ \Phi = \dot{\Psi} \end{cases}$$

Since $\Psi = e^{ibt}\psi$, $\dot{\Psi} = ib e^{ibt}\psi$

$$\dot{\Phi} \Rightarrow \ddot{\Psi} = -b^2 e^{ibt}\psi = ib\dot{\Psi} = ib\Phi$$

$\therefore$

$$\begin{cases} M_1 \Psi + M_2 \Phi - ib M_3 \Phi = e_0 \Psi \\ \Phi = ib\Psi \end{cases}$$

or

$$\begin{cases} \Phi = ib\Psi \\ \underbrace{M_3^{-1}(M_1 - e_0)}_{N_1}\Psi + \underbrace{M_3^{-1}M_2}_{N_2}\Phi = ib\Phi \end{cases}$$

finally we have $\begin{pmatrix} 0 & I \\ N_1 & N_2 \end{pmatrix}\begin{pmatrix} \Psi \\ \Phi \end{pmatrix} = ib\begin{pmatrix} \Psi \\ \Phi \end{pmatrix}$

it is a non-Hermitian matrix,

the eigenvalues are in general complex.

physical solution: all real b.