Abstract

A single document copy of these notes, as well as a mirror of every note, can be found at `connorduncan.xyz/notes` We want to mix $|k\rangle, |-k\rangle$ at $\alpha|k\rangle + \beta|-k\rangle$, which comes down to solve the schroedinger equaltion in this degenerate subspace. This gives

$$\begin{bmatrix} \langle k| H |k\rangle & \langle k| H |k'\rangle \\ \langle k'| H |k\rangle & \langle k'| H |k'\rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

This becomes

$$\begin{bmatrix} E_0(k) + V_0 & V_n \\ V_n^* & E_0(k') + V_0 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

We know that $E_0(k) = E_0(k' = -k) = \frac{n^2\hbar^2\pi^2}{2ma^2}$, with after a bit of algebra gives us mixing

$$E = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n|$$

Case 3: Close to edge of BZ We want to take a "continuous" approach to the edge at each band. We're gonna take $k = \frac{n\pi}{a} + \delta$, and $k' = -\frac{n\pi}{a} + \delta'$. This is going to give us some state where $\exists$ matrix elements, but the gap between energy levels no longer be zero. Now, we want to solve the eigenvalue equaitons for

$$E_\pm = \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} \pm \delta^2\right) + V_0 \pm \sqrt{|V_n|^2 + \left(\frac{\hbar^2}{2m}\frac{2\pi n}{a}\delta\right)^2}$$

In the limit $\delta \to 0$, we justt get our original answer back, which is good. We can check out a few limits. First, let $\delta \gg V_n$. To first order, it becomes

$$E_\pm = E_0\left(\frac{n\pi}{a} \pm \delta\right) + V_0 \pm \frac{|V_n|^2}{E\left(\frac{n\pi}{a} + \delta\right) - E\left(\frac{n\pi}{a} - \delta\right)}$$

Limit 2 is for $\delta \ll V_n$,

$$E_\pi = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n| + \frac{\hbar^2}{2m}\left(1 + \frac{1}{|V_n|}\frac{n^2\hbar^2\pi^2}{ma^2}\right)^2$$

There are some things we should take away from this

1. for $k \ll \frac{\pi}{a}$, we have basically a free electron
2. for $k = \frac{\pi n}{a}$, the spectrum splits as $2|V_n|$.

1 Variational Method

In most cases, it's basically impossible to solve schroedingers equation, because we can't diagonalize that "big ass matrix"[1]. The idea is to find the ground state of some hamiltonian H. Then, we make the staement

$$\forall |\psi\rangle ; E(\psi) = \frac{\langle\psi| H |\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

i.e. any state's energy will be larger than the ground state energy. We can find some trial wavefunctions parameterized by $\{\alpha, \beta, \gamma \ldots\}$. Then, the goal becoems to minimize $E(\psi)$ with respect to these variational parameters which results in **a rigorous bound on the ground state energy**. In principle, we can always improve our bound by adding more variational parameters.

1.1 Ex: Free Particle

Let's take

$$H_0 = \frac{p^2}{2m} + \lambda x^4$$

The trial wavefunctions we are going to use are $\psi(x, \alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$. We choose our functions to be "nice" based on the hamiltonian. Prof. Yao wrote this on the board

1. Gaussians are easy for this H
2. Symmetric Function w/ nodes

We then calculate the variational energy

$$E(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int dx e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda x^4\right) e^{-\frac{\alpha x^2}{2}} = \frac{\hbar^2}{2m}\alpha + \frac{3\lambda}{4\alpha^2}$$

The latter term means that we have $\alpha \to \infty$ wants localized wavefunction to be minimal, and the former is minimzed by $\alpha \to 0$, saying that low momentum minimizes that component of the wf. We can solve this for

$$\alpha_0 = \left(\frac{6m\lambda}{\hbar^2}\right)^{1/3} \qquad E(\alpha_0) = \frac{3}{8}\left(\frac{6\hbar^4\lambda}{m^2}\right)^{1/3}$$

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[1] Norman Yao, circa 2019.