Physics 101B. Modern Physics. Professor Dine

Matrix Mechanics and Band Structure

1 Matrix Mechanics

Heisenberg and Schrodinger, nearly simultaneously, proposed two, alternative formulations of quantum mechanics. Shortly afterwards, *Dirac* showed that these were equivalent, and gave a unified way to understand them.

We can use Heisenberg's matrix mechanics to understand, in a simple way, why the energy levels of crystals form bands. Matrix mechanics also illustrates some important features of quantum mechanics which we have not discussed up to now.

Heisenberg wanted to avoid discussing classical concepts, like position, and to formulate quantum theory in terms of objects which can be measured. In Heisenberg's picture in quantum mechanics, there are states, $i = 1, \ldots N$, where N may be large or infinite. For example, for the hydrogen atoms, i might denote the states of different n, ℓ, m and m_s, i.e. the states would be infinite. Measurable quantities, called "observables" are represented by matrices acting on these states. These matrices have eigenvectors and eigenvalues:

$$\mathcal{O} V_n = \lambda_n V_n \tag{1}$$

The result of any measurement of $\mathcal{O}$ is one of its eigenvalues, λ_n; after the measurement, the system is left in one of the eigenstates, V_n. Probably the most important observables is the energy; the corresponding matrix is the Hamiltonian matrix, H.

This is all rather abstract, and the idea of dealing with infinite dimensional matrices rather daunting, so let's look at something simpler – and very important – spin 1/2. In this case, there are just two basic states, spin up and spin down. We can represent these by the vectors:

$$\psi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \psi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2}$$

The matrix corresponding to S_z is then then very simple:

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

The eigenvectors are just $\psi_+ and \psi_-$, with eigenvalues $\pm\hbar/2$.

Now suppose we have a magnetic field in the z direction. Then the energy is $H = \mu_B B S_z$, where μ_B is the Bohr magneton. So as a matrix,

$$H = \frac{\hbar \mu_B B}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

The energy eigenstates are again $\psi_+ and \psi_-$, with eigenvalues $\pm\frac{\hbar\mu_B B}{2}$.

Heisenberg was very interested in how the states depend on time. His version of the Schrodinger equation (which is usually called the Schrodinger equation) is:

$$i\hbar \frac{\partial V}{\partial t} = HV \tag{5}$$

For an energy eigenstate, $HV = EV$, this is easy to solve:

$$V(t) = e^{-iEt/\hbar}V(0) \tag{6}$$

where $V(0)$ is the vector at time $t = 0$. Note the similarity to the time-dependent solutions of the Schrodinger equation you studied in chapter 6.

The Schrodinger equation is a linear equation, so any linear combination of solutions is a solution. E.g. if we have eigenvectors V_1 and V_2 with energy eigenvalues E_1 and E_2,

$$V(t) = a\ e^{-iE_1t/\hbar}V_1 + b\ e^{-iE_2t/\hbar}V_2 \tag{7}$$

is also a solution.

2 Oscillations

As an example, suppose we have a Stern-Gerlach apparatus which prepares a beam of electrons with spin up in the z direction. Now we pass the beam through a magnetic field in the x direction. The Hamiltonian is now

$$H = B\mu S_x \tag{8}$$

Claim:

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{9}$$

One check on this is to construct the eigenvectors and eigenvalues of this matrix.
Exercise: Check that

$$\psi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \psi_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{10}$$

are eigenvectors of this matrix. What are their eigenvalues?

Now, the general solution of the Schrodinger equation is:

$$V(t) = a\ e^{-iE_+t/\hbar}\psi_+ + b\ e^{-iE_-/\hbar}\psi_- \tag{11}$$

with $E_\pm = \pm\frac{\hbar\mu B}{2}$.
Exercise: verify this.

At $t = 0$, $V = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. So if we take $a = b = \frac{1}{\sqrt{2}}$, we have:

$$V(t) = \begin{pmatrix} \cos(\omega t) \\ i\sin(\omega t) \end{pmatrix}. \tag{12}$$

So the system oscillates between spin up and spin down. This sort of oscillation, between two *states*, is a common phenomenon in quantum mechanics. It has recently been discovered to take place among different types of neutrinos. Other examples are described in the attached handout from the Feynman lectures.

3 Band Structure

The matrix formulation provides a way of understanding the spectra of solids. Consider a system with a periodic potential (for simplicity, we will consider one dimension; you can generalize the argument to two or three dimensions). If the individual wells are reasonably deep, one can solve first the problem of an electron in each well. Call the ground state energy in each well E_o. However, there will be a non-zero amplitude (probability is the square of the amplitude) to tunnel from one

well to another. If this is small, the probability to tunnel in one step between two wells will be small. Call the amplitude to go from one well to another ϵ (strictly speaking, ϵ is an amplitude per unit time). What is the structure of the Hamiltonian for this system? If ϵ were zero, the Hamiltonian would just be diagonal, if we took the states to be the ground states in each well. In other words, as a matrix, it would look like:

$$H = \mathrm{diag}(E_o, E_o, E_o, \ldots). \tag{13}$$

But now there are off-diagonal terms, equal to ϵ, corresponding to the fact that the system will not remain for all time in the ground state. So the Hamiltonian matrix is more complicated:

$$H = \begin{pmatrix} E_0 & \epsilon & 0 & 0 & 0 & 0 & \ldots \\ \epsilon & E_o & \epsilon & 0 & 0 & 0 & \ldots \\ 0 & \epsilon & E_o & \epsilon & 0 & 0 & \ldots \\ 0 & 0 & \epsilon & E_o & \epsilon & 0 & \ldots \end{pmatrix} \tag{14}$$

Now we make a guess for the vector which diagonalizes this matrix:

$$V = \begin{pmatrix} e^{i\theta} \\ e^{2i\theta} \\ e^{3i\theta} \\ e^{4i\theta} \\ \ldots \end{pmatrix}. \tag{15}$$

If you plug in, you'll find:

$$HV = \begin{pmatrix} ** \\ (E_o + \epsilon(e^{i\theta} + e^{-i\theta}))e^{2i\theta} \\ (E_o + \epsilon(e^{i\theta} + e^{-i\theta}))e^{3i\theta} \\ (E_o + \epsilon(e^{i\theta} + e^{-i\theta}))e^{4i\theta} \\ \ldots \end{pmatrix} \tag{16}$$

Here the first entry indicates that this one doesn't work quite so nicely; but imagine that V has 10^{23} entries.

Exercise (for the brave): Verify this equation.

So, for any value of θ, V is an eigenvector of H with eigenvalue:

$$E = E_o + \epsilon \cos(\theta) \tag{17}$$

In what sense do these vectors correspond to plane waves? Calling the lattice spacing a, then $x = na$, where n is the row of the vector V. So the n'th entry in the vector is

$$V_n = e^{in\theta} = e^{ix\frac{\theta}{a}} = e^{ikx} \quad k = \frac{\theta}{a}. \tag{18}$$

So the energy eigenvalues depend on k as

$$\epsilon \cos(ka). \tag{19}$$

Note that because $0 < \theta < 2\pi$

$$0 < k < \frac{2\pi}{a}. \tag{20}$$

This is the promised band structure.

Finally, note that for k near zero, we can make a Taylor series expansion of the cosine:

$$E = E_o + \epsilon + \frac{|\epsilon|}{2\hbar^2} p^2 \tag{21}$$

This is the equation for the kinetic energy of a particle of mass $m^* = \frac{\hbar^2}{|\epsilon|}$. This is known as the "effective mass". It is typically of order 1/20. (The astute reader may note that we should really do this for states at the top of the band).

Real band calculations are complicated. There are more dimensions and more states in each well. But this little calculation makes clear why band structure forms.