

Quantum Mechanics

06/10/98

The M.A.P. Monkeys and Animals Principal

All Monkeys are necessarily animals, but
Animals are not necessarily monkeys.

The L.A.G. (Feynmann)

Light at the bottom of the garden principal.
Forcing a potentially inappropriate body of knowledge onto an new
problem.

The P.S. (Dirac)

"Principal of Simplicity"
In essence, nature always takes the simplest path.

Quotes

Einstein

"A good physics education is such that the student will never
believe anything anyone tells them."

At the turn of this century, there were three phenomena that could
not be explained,
(1)Black-Body radiation.
(2)Existance of the Ether (lead to special relativity when it could not be
found in the Michelson Morley experiment).
(3)Advance of the perihelion of Mercury (4 arc seconds per century!).

Number 3, was solved by general relativity.

De Broglie equated Einstein's and Plank's work as a foot note to his
PhD thesis. This brought about Wave Particle duality!

Davisson & Germer - Electron diffraction (De Broglie)

Bohr used classical mechanics (P.S. circular orbits and L.A.G. in actually using classical mechanics) to postulate,

$$\begin{aligned} \mathbf{I} &= n \cdot \hbar \\ \mathbf{I} &= \frac{h}{2\pi} \cdot n \quad (n=1) \\ &\text{(Angular momentum of electrons orbiting nucleus)} \end{aligned}$$

Schrödinger derived what Bohr postulated using what De Broglie stated.

$$2\pi r / \lambda = n$$

13/10/98

Schrödinger's Wave equations

We try to replace a particle with a wave. To work out what happens to the wave and assumes that is what happens to the particle. Called it Wave mechanics.

How is it worked out?

If it was true in general would it be true in particular! Choose the simplest thing in particular.

A Free particle

BUT! Replace with a free wave i.e. no P.E. only K.E. (plane wave).

Plane wave of vector \mathbf{k} travelling along the x direction with a speed \mathbf{v} ,

ψ - a function which describes a wave. It is a **wave function**

$$\begin{aligned} \psi &= A e^{i(kx - \omega t)} \\ k &= 2\pi / \lambda \\ \omega &= 2\pi \nu \end{aligned}$$

Also, $\mathbf{E} = h\nu$

To try and get the energy out of ψ , Schrödinger differentiated,

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= ? \\ \psi &= A \cdot e^{i \cdot \theta} \\ \frac{\partial \psi}{\partial t} &= \frac{\partial \psi}{\partial \theta} \cdot \frac{\partial \theta}{\partial t} \\ \theta &= 2\pi \left(\frac{x}{\lambda} - \nu t \right) \end{aligned}$$

$$\begin{aligned} \frac{\partial \psi}{\partial \theta} &= i A e^{i \theta} \\ \frac{\partial \theta}{\partial t} &= 2\pi(-v) \end{aligned}$$

Therefore we can say,

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= -i \cdot 2 \cdot \pi \cdot v \cdot \psi \\ i \cdot \frac{\partial \psi}{\partial t} &= 2\pi v \cdot \psi \end{aligned}$$

Finally,

$$i \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = \hbar v \cdot \psi$$

Hence we get the **energy operator**

$$i \cdot \hbar \cdot \frac{\partial}{\partial t} .$$

To get the momentum to agree with the De Broglie relationship, we do the following,

$$\begin{aligned} P &= h / \lambda \\ \frac{\partial \psi}{\partial x} &= \frac{\partial \psi}{\partial \theta} \cdot \frac{\partial \theta}{\partial x} \\ &= i \cdot \psi \cdot \frac{2\pi}{\lambda} \\ &= i \cdot \frac{2\pi}{\lambda} \cdot \psi \\ -i \cdot \hbar \cdot \frac{\partial \psi}{\partial x} &= h / \lambda \cdot \psi \end{aligned}$$

So the **momentum operator**,

$$P_x = -i \cdot \hbar \cdot \frac{\partial}{\partial x}$$

These are derived from classical physics, momentum and energy are operators, not algebraic variables.

In classical physics, quantities are commutative, $\mathbf{x} \cdot \mathbf{P} = \mathbf{P} \cdot \mathbf{x}$. In classical physics the commutator of x and P_x is zero.

eq 1

The commutator of the momentum operator is

$$P_x \cdot x - x \cdot P_x = -i \cdot \hbar$$

In classical mechanics, the Hamiltonian, H is the sum of the potential and kinetic energy.

Note,

in classical mechanics, mass and velocity are two important variables. In quantum mechanics however, mass and momentum are the most important variables. Velocity is not well defined in quantum mechanics.

$$\begin{aligned}
 H &= \frac{1}{2}mv^2 + V(x) \\
 &= \frac{1}{2}m\dot{y}^2 + V(x) \\
 &= \frac{1}{2}P^2 + V(x)
 \end{aligned}$$

To recap,

$$\begin{aligned}
 \text{energy} \cdot \psi &= \text{energy} \cdot \psi \\
 \text{energy} \cdot \psi &= \text{energy} \cdot \psi
 \end{aligned}$$

Using the Hamiltonian on ψ gives us "SCHRÖDINGER'S TIME DEPENDENT WAVE EQUATION". (This is the general *animal*),

$$H \cdot \psi = i \cdot \hbar \cdot \frac{\partial \psi}{\partial t}$$

This is a non-relativistic wave equation. It is always correct. The classical version however is not correct on a relativistic scale.

We know,

$$H = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} + V(x) = H(x)$$

$$H(x) \cdot \psi(x, t) = A(t) \cdot \psi(x, t)$$

Now, using the method of separation of variables (which gives a particular solution, or a *monkey*),

$$\begin{aligned}
 H(x) \cdot \psi(x, t) &= A(t) \cdot \psi(x, t) \\
 \psi(x, t) &= \psi(x) \cdot n(t) \\
 \text{(this is in particular)} \\
 H(x) \cdot \psi(x) \cdot n(t) &= A(t) \cdot \psi(x) \cdot n(t) \\
 n(t) \cdot H(x) &= A(t) \cdot n(t) \\
 (n/n) \cdot H(x) &= (A/n) \cdot A \cdot n \\
 (1/n) \cdot H(x) &= (1/n) \cdot A \cdot n = \text{constant} \\
 \text{(H is a function of x and A is a function of t)} \\
 (1/n) \cdot H(x) &= E \\
 H(x) &= E \cdot n
 \end{aligned}$$

This is SCHRODINGERS TIME INDEPENDANT EQUATION (a particular monkey!).

20/10/98

Schrödinger Time independant wave equation (particular solution)

$$H \Psi = E \Psi$$

Schrödinger Time dependant wave equation (STIWE).

$$\mathbf{H \Psi = i \cdot \hbar \cdot \partial \Psi / \partial t}$$

We will now apply STIWE to a Hydrogen atom. If we model this as a proton with an electron orbiting at a distance \mathbf{r} . Now apply the Hamiltonian,

$$\begin{aligned} \mathbf{H} &= (\mathbf{p}^2 / 2m) - e^2 / r \\ \mathbf{p}^2 &= p_x^2 + p_y^2 + p_z^2 \\ \mathbf{r} &= r_x + r_y + r_z \end{aligned}$$

$$\begin{aligned} \mathbf{p}_x^2} &= -\hbar^2 \cdot \partial^2 / \partial x^2 \\ \mathbf{p}_y^2} &= -\hbar^2 \cdot \partial^2 / \partial y^2 \\ \mathbf{p}_z^2} &= -\hbar^2 \cdot \partial^2 / \partial z^2 \end{aligned}$$

$$\text{Therefore,} \\ \mathbf{[(-\hbar^2 / 2m) \cdot (\partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2) - e^2 / r] \Psi = E \Psi}$$

$$\begin{aligned} \mathbf{E} &= -R_n / n^2 \\ (\mathbf{n} &= 1, 2, 3, \dots) \\ \mathbf{R_n} &= \text{Rydberg constant} \\ &= (e, \hbar, m) \end{aligned}$$

This equation agrees with experimental observation. For this there is any solution from $E = -\infty$ to $E = +\infty$. However for most Ψ approaches infinity as r approaches infinity. These solutions are rejected by physicists. The solutions which are taken are when Ψ approaches 0 as r approaches infinity.

Ground state of Hydrogen atom, $n=1$, $E = -R_H$. Mathematicians say that the energy has a lower bound. Bohr limits the boundary on electron orbit.

I = n · ħ : Postulate

The equation yields $\Psi = \exp(-r/a_0)$, $a_0 = \text{constant}$ which Bohr orbit.

If we now use quantum mechanics to solve for a particle on a string. Recall SHM formulae,

$$\begin{aligned} \mathbf{f} &= -kx \\ \mathbf{f} &= m \cdot (\partial^2 x / \partial t^2) \\ -k \cdot x &= m \cdot (\partial^2 x / \partial t^2) \\ \partial^2 x / \partial t^2 &= -\omega^2 \cdot x \\ \omega &= k / m \end{aligned}$$

Now,

$$\begin{aligned} \mathbf{F} \cdot dx &= -dV \\ \mathbf{F} &= -dV / dx = -kx \\ dV / dx &= kx \end{aligned}$$

$$V = \alpha kx$$

$$KE = p_x^2 / 2m = -(\hbar^2 / 2m) \cdot (\partial^2 / \partial x^2)$$

Now for,

$$H \Psi = E \Psi$$

We only keep the solution for $\Psi \rightarrow 0$ as $x \rightarrow \infty$. It can be shown that,

$$E = (n + \frac{1}{2}) \cdot \hbar \omega = (n + \frac{1}{2}) \cdot h \nu$$

$$\omega / 2\pi = \nu$$

Even at absolute zero, all atoms in solids **will vibrate**. This is seen in the above equation for $n=0$. This is called the **zero point energy**. This means that there is no such thing as a universe with no energy.

Now consider a particle of mass m in a potential well of width L , with infinitely high barriers. So, $E=0$ and $E=\infty$. Now solve,

$$H \Psi = E \Psi$$

$$-(\hbar^2 / 2m) \cdot (\partial^2 / \partial x^2) \Psi = E \Psi$$

$$\partial^2 / \partial x^2 \Psi = \alpha \Psi$$

$$\alpha = 2mE / \hbar^2$$

$$\Psi = 0 \text{ at } 0 \text{ and } L$$

The condition of constructive interference is,

$$n \cdot (\lambda / 2) = L$$

Note,

$$E = p^2 / 2m$$

and from DeBroglie,

$$p = h / \lambda$$

$$E = h^2 / 2m \cdot \lambda^2$$

$$\lambda = 2L / n$$

$$E = (h^2 / 2m) \cdot (n^2 / 4L^2)$$

$$= (h^2 / 8mL^2) \cdot n^2$$

$$E = \hbar^2 \cdot n^2$$

$$\hbar^2 = h^2 / 8mL^2$$

27/10/98Probability density and Probability current density

Equation of continuity from fluid mechanics, $\frac{D\rho}{Dt} + \nabla \cdot (\rho \mathbf{v}) = 0$
 ρ is density of fluid and $\rho \mathbf{v}$ is the mass flow rate in.

03/11/98

$$\hat{H} \Psi = i\hbar \frac{d\Psi}{dt}$$

$$\Psi = \Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}, t)$$

$$\hat{H} \Psi = E \Psi$$

The latter can only be solved for 2 cases. One, for the Hydrogen atom ($\Psi = \exp\{-r/a_0\}$ and $\Psi\Psi^*$ gives the probability density) and Two, for atomic oscillators (using SHM, which gives $E = (n + \frac{1}{2})\hbar\omega$). For the Hydrogen atom, the probability interpretation of the wave function (by the Copenhagen school)

Einsten Quote :if you can't explain physics to a bar man you don't understand it!

Heisenberg

From quantum mechanics,

$$[\hat{p}_x, \hat{x}] = -i\hbar$$

From classical mechanics,

$$p_x \cdot x - x \cdot p_x = 0$$

By the definition of error (partly made by Heisenberg)

$$\begin{aligned} (\Delta p)^2 &= \langle p^2 \rangle - \langle p \rangle^2 \\ (\Delta x)^2 &= \langle x^2 \rangle - \langle x \rangle^2 \end{aligned}$$

Heisenberg showed that,

$$\langle (\Delta P)(\Delta x) \rangle = \hbar/2$$

The corresponding result in classical physics the greater than is ignored and \hbar is not present.

So,

$$\begin{aligned} \langle dP \cdot dx \rangle &= 0 \\ \text{then,} \\ \langle dP \rangle &= 0 \\ \langle dx \rangle &= 0 \end{aligned}$$

This meant that both quantities could be measured simultaneously with arbitrary accuracy. What Heisenberg showed is that both quantities could not be measured together with no uncertainty. if dP is small then dx is large!

We now apply this to S.H.M.

$$\begin{aligned} \text{SHM} &= \text{KE} + \text{PE} \\ E &= \langle mv^2 \rangle + \langle kx^2 \rangle \\ E &= \langle p^2 \rangle / 2m + \langle kx^2 \rangle \\ \langle E \rangle &= (1/2m) \cdot \langle p^2 \rangle + \langle kx^2 \rangle \end{aligned}$$

The average of p and x are always zero in SHM.

Hence,

$$\begin{aligned} \langle dp \rangle &= \langle p \rangle \\ \text{and} \\ \langle dx \rangle &= \langle x \rangle \end{aligned}$$

So we now write,

$$\langle E \rangle = (1/2m) \cdot \langle dp \rangle^2 + \langle k(dx) \rangle^2$$

Suppose, $x = L_0$

$$dp = \hbar/2L_0$$

So we now write,

$$\begin{aligned} \langle E \rangle &= (1/2m) \cdot (\hbar/2L_0)^2 + \langle kL_0^2 \rangle \\ \langle E \rangle &= (\hbar^2/8m) \cdot (1/L_0^2) + \langle kL_0^2 \rangle \end{aligned}$$

$$y = a_1(1/x^2) + a_2(x^2)$$

Finding the minimum of this gives the lowest value gives,

$$\langle E \rangle = (\hbar/2) \cdot (k/m)^{1/4} = (\hbar \omega / 2)$$

However,

$$\hbar \omega / 2 = \hbar \nu / 2$$

This is the ZERO POINT ENERGY.

10/11/98

Normalising the wave function

$$\begin{aligned} H \Psi &= E \Psi \\ \int \Psi^* \Psi dT &= N \\ \int (\Psi^*/N) (\Psi/N) dT &= 1 \end{aligned}$$

$$\begin{aligned} \text{Now let,} \\ \Psi_1 &= \Psi/N, \text{ so that now,} \\ \int \Psi_1^* \Psi_1 dT &= 1 \end{aligned}$$

You can always choose Ψ 's so that the integral always is equal to one. Without loss of generality we can always choose the eigen functions such that the integral is always one. The function Ψ is said to be **normalised**

$$\begin{aligned} \int \Psi dT &= 1 \\ \text{but by analogy} \\ \int \Psi_1 dT &= 1 \end{aligned}$$

Suppose

$$\begin{aligned} H \Psi &= E \Psi \\ \text{(with } E \text{ unknown)} \end{aligned}$$

then,

$$\int H \Psi dT = E \int \Psi dT$$

So,

$$E = \int H \Psi dT$$

This is an expectation value or average. This also implies that E is a real number.

So,

$$E^* = \int \Psi^* (H \Psi) dT$$

E must be equal to E^* because E is a real number.

So,

$$\int H \Psi dT = \int \Psi^* (H \Psi) dT$$

In general,

$$\int (A^* \Psi) dT = \int (B \Psi) dT$$

For any Ψ and any Ψ and any operator A , you can always find an operator B such that the equation is valid. B is said to be the hermitian conjugate of A . IFF $B=A$, A is said to be Hermitian. If A is hermitian, then,

$$\int (A^* \Psi) dT = \int (A \Psi) dT$$

But it can also be shown that (by the reason that the energy operator E is a real number),

$$\int (H^* \Psi) dT = \int (H \Psi) dT$$

(when $\Psi = \Psi$)

So, the operator H is hermitian. All quantum operators which represent real quantities are (and have to be) hermitian.

Now,

$$\begin{aligned} H \psi_i &= E_i \psi_i \\ H \psi_j &= E_j \psi_j \\ \int (\psi_j^*) (H \psi_i) dT &= 0 \end{aligned}$$

then,

$$\begin{aligned} \int (\psi_i^*) (H \psi_j) dT &= E_j \int (\psi_i^*) \psi_j dT \\ \int (\psi_i^*) (H \psi_j) dT &= E_i \int (\psi_i^*) \psi_j dT \end{aligned}$$

Since H is hermitian.

But,

$$\begin{aligned} H \psi_i &= E_i \psi_i \\ E_i \int (\psi_i^*) \psi_j dT &= E_j \int (\psi_i^*) \psi_j dT \end{aligned}$$

If $A \psi = n \psi$, then ψ is an eigen function of A with eigenvalue n

Now if we rearrange the above,

$$(E_i - E_j) \int (\psi_i^*) \psi_j dT = 0$$

But,

$$E_i - E_j \neq 0$$

Therefore,

$$\int \psi_i \psi_j dT = 0$$

ψ_i is orthogonal to ψ_j .

A strong analogy can be drawn between vector analysis and Quantum mechanics, as it may have already become apparent. Here are the analogies in a more explicit presentation,

In 3 dimensional vectors we have the unit vectors i, j , and k . In Quantum Mechanics we have ψ_1 to ψ_N

In vector analysis we can say,

$$\underline{i} \cdot \underline{i} = \underline{j} \cdot \underline{j} = \underline{k} \cdot \underline{k} = 1$$

In Quantum mechanics the same principal exists simply under a different operation,

$$\int \psi_i \psi_i dT = 1$$

(The states are normalised)
(where $i=1..N$)

In vector analysis the relations exist,

$$\underline{i} \cdot \underline{j} = \underline{j} \cdot \underline{k} = \underline{i} \cdot \underline{k} = 0$$

In Quantum mechanics we write,

$$\int \psi_i \psi_j dT = 0$$

if $i <> j$. The states are orthogonal

The above two Quantum mechanical sets are known together as an **OrthoNormal set**

For an arbitrary vector in vector analysis we can express it as,

$$\underline{R} = a_i \underline{i} + a_j \underline{j} + a_k \underline{k}$$

In Quantum mechanics we write a wave function Psi in a similar, summing all the present dimensions,

$$\langle \Psi | = \text{Sum } (i=1..N) \{ a_i \}$$

The latter Quantum mechanical statement is not proven. It is only argued for by analogy, it is one of Quantum mechanics largest assumptions. These analogies lead us to this final statement,

Quantum Mechanics is an N dimensional linear vector space theory.

17/11/98

(prove that a real number is a hermitian operator)

$$p_x x - x p_x = i \hbar$$

$$AB - BA = C \text{ (all ops)}$$

$$\begin{aligned} \text{put } (A - \langle A \rangle) \Psi \text{bar} &= \Psi \\ \text{put } (B - \langle B \rangle) \Psi \text{bar} &= \Psi \\ \Delta A \cdot \Delta B &= \text{Im} \int (\Psi \cdot dT) \end{aligned}$$

$$\begin{aligned} \text{For a complex number,} \\ Z &= X + iY \\ |\text{Im } Z| &= |Y| = \ll |Z - Z| \end{aligned}$$

$$\begin{aligned} \text{Now let } Z &= \int (\Psi \cdot dT) \\ Z^* &= \int (\Psi \cdot dT) \end{aligned}$$

$$Z - Z^* = \int ((\Psi \cdot) \cdot \Psi) \cdot dT$$

$$\begin{aligned} \text{Now,} \\ \Psi &= (A - \langle A \rangle) \Psi \text{bar} \\ \Psi &= (B - \langle B \rangle) \Psi \text{bar} \end{aligned}$$

$$\begin{aligned} \int (\Psi \cdot dT) &= \int ((A - \langle A \rangle) \Psi \text{bar} \Psi = (B - \langle B \rangle) \Psi \text{bar}) \\ &= \int (\Psi [A - \langle A \rangle] [B - \langle B \rangle] \Psi) \end{aligned}$$

now show that

$$\begin{aligned} \int (\Psi \cdot dT) &= \int (\Psi \cdot dT) \\ \Psi^* [B - \langle B \rangle] [A - \langle A \rangle] \Psi \end{aligned}$$

Now also show that,

$$\Delta A \cdot \Delta B = \ll \left| \int (\Psi (AB - BA) \Psi \cdot dT) \right|$$

But $AB - BA = C$

$$\Delta A \cdot \Delta B = \ll \left| \int (\Psi C \Psi \cdot dT) \right|$$

$$\begin{aligned} \text{If } C &= \tilde{n} - i \hbar \\ \Delta A \cdot \Delta B &= \hbar / 2 \\ \Delta p_x \cdot \Delta x &= \hbar / 2 \end{aligned}$$

Likewise for energy and time, where $E = \hbar \cdot \partial / \partial t$

$$E \cdot t - \hbar = \text{ihbar}$$

$$\Delta E \cdot \Delta t \geq \hbar/2$$

24/11/98

Angular Momentum

This is not required for the exam of this module, but is required knowledge for later modules .

Consider the vector relation,

$$\underline{J} = \underline{r} \times \underline{p}$$

\underline{J} is a spatial operator, from vector analysis we can say,

$$J_x = y \cdot p_z - z \cdot p_y, \quad J_y = z \cdot p_x - x \cdot p_z, \quad J_z = x \cdot p_y - y \cdot p_x$$

Therefore, the commutators can be written as,

$$\begin{aligned} [J_x, J_y] &= [y \cdot p_z - z \cdot p_y, z \cdot p_x - x \cdot p_z] \\ &= [y \cdot p_z, z \cdot p_x] + [z \cdot p_y, x \cdot p_z] \\ &= -i \cdot \hbar \cdot y \cdot p_x + i \cdot \hbar \cdot x \cdot p_y = i \cdot \hbar \cdot J_z \end{aligned}$$

The spatial components of J are cyclically related, so we can write the following,

$$\begin{aligned} [J_y, J_z] &= i \cdot \hbar \cdot J_x \\ [J_z, J_x] &= i \cdot \hbar \cdot J_y \end{aligned}$$

We can readily show that,

$$[J_y, J_x] = [J_x, J_y] = [J_z, J_z] = 0$$

Where,

$$\begin{aligned} J_y &= J_x \hat{y} + J_y \hat{y} + J_z \hat{y} \\ J_y - J_z \hat{y} &= J_x \hat{y} + J_y \hat{y} \end{aligned}$$

Since J_y and J_z commute they have a simultaneous eigen function, $\Psi(J_i, M)$ say, where,

$$\begin{aligned} J_y \Psi(J, M) &= \hbar \cdot M \cdot \Psi(J, M), \\ J_z \Psi(J, M) &= \hbar \cdot M \cdot \Psi(J, M) \end{aligned} \quad (1)$$

Consider the eigen function, $\chi_+ = J + \Psi$ and $\chi_- = J - \Psi$ (2). Where,

$$J_{\bar{n}} = J_x \bar{n} i J_y \quad (3)$$

One can readily show that,

$$[J_z, J_{\bar{n}}] = \bar{n} \hbar J_x \quad (4)$$

Consider,

$$\begin{aligned} J_z \psi_+ &= J_z J_+ \Psi = (J_z J_+ + \hbar J_x) \Psi \\ &\quad \text{(using (4))} \\ &= \hbar (M+1) J_+ \Psi \\ &\quad \text{(Using (1))} \\ &= \hbar (M+1) \psi_+ \end{aligned}$$

i.e. ψ_+ is an eigen function of J_z with eigen value $(M+1)\hbar$. Similarly we can show that ψ_- is an eigen function of J_z with eigen value $(M-1)\hbar$. Thus, starting from $\Psi(J_i, M)$ we can by successively applying J_+ (or J_-) keep stepping the eigen value of M up (or down) by one unit, suppose $\Psi(J_i, M_{\max})$ is the eigen function with the maximum value of J_z . It then follows that $J_+ \Psi(J_i, M_{\max}) = 0$ and hence that,

$$\begin{aligned} 0 &= J_+ J_+ \Psi(J_i, M_{\max}) = \{J_x \hat{y} + J_y \hat{y} + i(J_x J_y - J_y J_x)\} \Psi \\ &= \{J_y \hat{y} - J_x \hat{y} - \hbar J_z\} \Psi \\ &= \{\hbar \hat{y} J_x - \hbar \hat{y} J_x - \hbar M_{\max} \hat{y} - \hbar M_{\max}\} \Psi \quad (5) \end{aligned}$$

i.e.

$$J_x = M_{\max} (M_{\max} + 1)$$

(note, J_y commutes with $J_{\bar{n}}$ hence applying the latter leaves eigen value if J_y unchanged. Similarly if $\psi_-(J_i, M_{\min})$ is the eigen function with the minimum value of J_z , we have $J_- \psi_- = 0$ from which we obtain,

$$J_x = M_{\min} (M_{\min} - 1) \quad (6)$$

Equating the two values of J_x , gives either $M_{\min} = -M_{\max}$ or $M_{\min} = M_{\max} + 1$. We reject the latter as absurd. Putting $J = \text{Max}$ gives $J_x = J(J+1)$. Also starting from $\text{max} = J$ and stepping down N times gives $M_{\min} = -J = M_{\max} - N = J - N$. i.e. $2J = N$. Therefore $J = N/2$

01/12/98

Perturbation Theory

The act of measurement always "Disturbs" ("Perturbs") the system being measured. The standard notion used here is H_0 for the unperturbed system. A small perturbation is switched onto the system, it is represented by V . The hamiltonian for such a system is,

$$\mathbf{H}=\mathbf{H}_0+\mathbf{V}$$

We assume that we have all the solutions to,

$$\mathbf{H}_0|\psi_i\rangle=\mathbf{E}_i|\psi_i\rangle$$

$$i=0,1,2,\dots,N$$

This is called **Dirac notation**. The actual solution we want is,

$$(\mathbf{H}_0+\mathbf{V})|\psi_0\rangle=\mathbf{E}_0|\psi_0\rangle$$

Which leads us to **Second Order Perturbation Theory**. We now express the energy of the perturbed system as follows,

$$\mathbf{E}_0=\mathbf{E}_0+\langle\psi_0|\mathbf{V}|\psi_0\rangle+\text{Sum } (i\neq 0) \{(\langle\psi_0|\mathbf{V}|\psi_i\rangle\langle\psi_i|\mathbf{V}|\psi_0\rangle)/(\mathbf{E}_0-\mathbf{E}_i)\}$$

Dirac Notation

to be done !!!

Effective Mass Theory k.p perturbation theory.

k.p is a quantity from perturbation theory that is used in Effective Mass Theory.

When we consider a solid and its quantum level properties, it is a useful tool to consider an *infinite* solid, in which there are no boundaries or edges. At a particular point in such a solid we consider the inter atomic spacing to be constant, **a** say. Any electron in transit from one atom's space to another sees the potentials in whether it goes left or right (in a one dimensional system). This is known as *cyclic boundary conditions* because having identical points going as far as one likes in any direction (left or right) is as if a group of such atoms are linked in a loop.

In digression, if an electron moving from atom to atom sees the same potential, there is an equal probability of find the electron anywhere in the system of atoms, hence we can state,

$$|\Psi(x)|^2 = |\Psi(x+a)|^2$$

Expanding this formalism,

$$\Psi(x) = \exp(i\theta) \cdot \Psi(x+a)$$

$$\Psi(x) = \exp(ikx) \cdot u(x)$$

$$\Psi(x+a) = \exp(ik(x+a)) \cdot u(x+a)$$

Therefore,

$$\begin{aligned}\Psi(\mathbf{x}) &= \Psi(\mathbf{x}+\mathbf{a}) \\ u(\mathbf{x}) &= u(\mathbf{x}+\mathbf{a})\end{aligned}$$

This is the form is the **Bloch theory (for an infinite solid)**

$$\begin{aligned}\Psi(\mathbf{x}) &= \exp(i\mathbf{k}\cdot\mathbf{x}) \cdot u_{\mathbf{k}}(\mathbf{x}), \text{ where...} \\ \dots u_{\mathbf{k}}(\mathbf{x}+\mathbf{a}) &= u_{\mathbf{k}}(\mathbf{x})\end{aligned}$$

Now consider the Hamiltonian of such an electron,

$$\begin{aligned}H_0 &= KE + PE \\ \text{or} \\ H_0 &= (\mathbf{p}_x^2/2m) + V(\mathbf{x}), \\ \text{where,} \\ V(\mathbf{x}+\mathbf{a}) &= V(\mathbf{x})\end{aligned}$$

From the above Bloch equations, suppose $k=0$, then,

$$H_0 \cdot u_a = E_a u_a$$

Considering the above Bloch equations again, we wish now to get rid of the $\exp(i\mathbf{k}\cdot\mathbf{x})$,

$$((\mathbf{p}_x^2/2m) + (\hbar \cdot \mathbf{k} \cdot \mathbf{p}_x/m) + \hbar \cdot \mathbf{p}_x \cdot \mathbf{a} + V) u_{\mathbf{k}} = E_{\mathbf{k}} \cdot u_{\mathbf{k}}$$

$$\begin{aligned}\text{Which gives us,} \\ (((\mathbf{p}_x^2/2m) + V)/\hbar) \cdot u_0 &= E_0 u_0(\mathbf{x})\end{aligned}$$

Therefore,

$$H = H_0 + (\hbar \cdot \mathbf{p}_x \cdot \mathbf{a}/2m) + (\hbar \cdot \mathbf{k} \cdot \mathbf{p}_x/m)$$

Where V is the perturbation energy, in full, $V_{\text{per}}(\mathbf{x}+\mathbf{a}) = V_{\text{per}}(\mathbf{x})$.

If we consider the previous equation,

$$E_0 = E_0 + \langle u_0 | V | u_0 \rangle + \text{Sum } (i=\hat{n}0) \{ (\langle u_i | V | u_1 \rangle \langle u_1 | V | u_0 \rangle) / (E_0 - E_i) \}$$

Which leads to, $a \cdot k_x \cdot \hbar$. So we then write,

$$\begin{aligned}E_0 &= E_0 + (\hbar \cdot k_x \cdot \hbar / 2m) + a \cdot k_x \cdot \hbar \\ &= E_0 + k_x \cdot \hbar \cdot ((\hbar / 2m) + a) \\ &= E_0 + k_x \cdot \hbar \cdot (2m^*)\end{aligned}$$

$$\begin{aligned}\text{Where,} \\ \hbar / 2m^* &= (\hbar / 2m) + a\end{aligned}$$

m^* is not actually the real mass or an altered mass, it is simply a mathematical factor giving an *effective mass* of the electron.

The energy can also be expressed as a polynomial in k_x .

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_0 + a k_x \dot{y} + b k_x \ddot{u} + c k_x^4 \\ &= \mathbf{E}_0 + (\hbar \dot{y} \cdot k_x / 2m^*) \end{aligned}$$

So,

$$1/m^* = a \cdot (1 + (b k_x / a) + (c/a) k_x^3)$$

Hence, m^* is energy dependant, and *non-parabolic effects are noted*.

**End of course
bye bye !
:-)**