## 2. Quantum Mechanics of Particles in a Box

M. App: B1 and B2; B\&S Chapter 7.1-7.3, K\&K p72

Imagine a cubic box of side L .

### 2.1 Single Particle Energy Eigenvalues

## TISE

$-\frac{\hbar^{2}}{2 M} \nabla^{2} \psi+V \psi=E \psi$
$V=0$ inside the box. $V=\infty$ outside the box.
$\Rightarrow \psi=0$ on the walls.
For a 1D well of width L;
$\psi=\sqrt{\frac{2}{L}} \sin k x$
where $k=\frac{\ell \pi}{L}, \ell=1,2,3, \ldots$
$E=\frac{\hbar^{2} k^{2}}{2 M}$

$\psi$ has an integral number of half-wavelengths in the box.
For 3D "cubic" well;
$\psi(x, y, z)=\left(\sqrt{\frac{2}{L}}\right)^{3} \sin k_{x} x \sin k_{y} y \sin k_{z} z$
$k_{x}=\frac{\ell \pi}{L}, k_{y}=\frac{m \pi}{L}, k_{z}=\frac{n \pi}{L}$
$\ell, m, n$ are positive integers.
NB: integer values are forced by the boundary condition $\psi(x=0, y, z)=(x=L, y, z)=0$.
$E=\frac{\hbar^{2} k^{2}}{2 M}$ where $k^{2}=k_{x}^{2}+k_{y}^{2}+k_{z}^{2}($ confirm this -+ or x ? $)$
$\ell=0 \rightarrow \psi=0$ so zero is not allowed.
Negative integers $\rightarrow[\psi \rightarrow-\psi] \rightarrow$ this is not a distinct state.

### 2.2 The concept of Reciprocal Space (also called momentum space or $k$-space)

Very important concept. Used in particle, nuclear, atomic and solid state physics. It allows the plotting of the eigenstates.

The $\underline{k}$-vector has components $\left(k_{x}, k_{y}, k_{z}\right)=\frac{\pi}{L}(\ell, m, n)$.

(supposed to be a 3D box with a vector pointing to the point...)
The point represents the state $\ell, m, n$ with energy $\frac{\hbar^{2} k^{2}}{2 M}$ and distance squared from the origin in k-space.
The states of the particle in the box are referred to as k -states.
Why reciprocal space? Because k has dimensions of $1 /$ length .
Why k-space? $k$ is universally used for wave numbers.
Why momentum space? Because $\hbar k$ has dimensions of momentum.
$\ell \rightarrow \ell+1$ would be equivalent to a displacement $\frac{\pi}{L}$ along $k_{x}$.
$m \rightarrow m+1$ would be equivalent to a displacement $\frac{\pi}{L}$ along $k_{y}$.
$n \rightarrow n+1$ would be equilavent to a displacement $\frac{\pi}{L}$ along $k_{z}$.
The totality of states corresponds to all positive values of $\ell, n, m$.
The points representing these states map out a simple cubic lattice in k space of side $\frac{\pi}{L}$.


### 2.3 The density of states

(This will definitely be on the exam.)
Say we have a $1 \mathrm{~cm}^{3}$ box of Helium atoms at $T=300 \mathrm{k}$.
The energy $k_{0} T=\frac{\hbar^{2} \pi^{2}}{2 M L^{2}}\left(\ell^{2}+m^{2}+n^{2}\right)$.
$\ell^{2}+m^{2}+n^{2} \approx 5 \times 10^{16}$.
We are usually interested in states far from the origin i.e. large $\ell, m, n$ (except for the important case of Bose-Einstein condensation).

One state occupies a volume $\left(\frac{\pi}{L}\right)^{3}$ of k -space. Therefore the density of states $=\left(\frac{L}{\pi}\right)^{3}=\frac{V}{\pi^{2}}$ states per unit volume of k -space.

How many states in a spherical shell of $k$-space?
Shell between $k$ and $k+d k$. Assume $d k \gg \frac{\pi}{2}$.


3D case:
The number of states in the shell is:
$\frac{1}{8} 4 \pi k^{2} d k \times \frac{V}{\pi^{3}}$
where $1 / 8$ is the positive octant $k_{x}, k_{y}, k_{z}>0$ only, the second part is the spherical shell volume, and the last part is the density of state.
$=\frac{V k^{2}}{2 \pi^{2}} d x=\rho(k) d k$
where $\rho(k)=\frac{V k^{2}}{2 \pi^{2}}$. This is also called the density of states. It is the rate at which the number of states increases per unit increase in the magnitude of k .
$\rho(k) d x$ is the number of states between $k$ and $k+d k$.
Let $g(\varepsilon) d \varepsilon$ equal the number of stases whose energies lie between $\varepsilon$ and $\varepsilon+d \varepsilon$. $g(\varepsilon) d \varepsilon=\rho(k) d k$.
$\varepsilon=\frac{\hbar \hat{k}}{2 M}$ for non-relativistic particles.
For photons:
$\varepsilon=p c=\hbar c k$
Now:
$g(\varepsilon)=\rho(k) \frac{d k}{d \varepsilon}$
For non-relativistic particles
$\frac{d \varepsilon}{d k}=\frac{\hbar^{2} k}{M}$
Therefore:
$g(\varepsilon)=\frac{V k^{2}}{2 \pi^{2}} \frac{M}{\hbar^{2} k}=\frac{V M k}{2 \pi^{2} \hbar^{2}}$
$k=\left(\frac{2 M \varepsilon}{\hbar^{2}}\right)^{1 / 2}$
So:
$g(\varepsilon)=\frac{V}{4 \pi^{2}}\left(\frac{2 M}{\hbar^{2}}\right)^{3 / 2} \varepsilon^{1 / 2}$
For photons $\varepsilon=\hbar c k$ :
$\frac{d \varepsilon}{d k}=\hbar c$
$g(\varepsilon)=\rho(k) \frac{d k}{d \varepsilon}=\frac{V k^{2}}{2 \pi^{2}} \frac{1}{\hbar c}=\frac{V}{2 \pi^{2} \hbar c} k^{2}=\frac{V}{2 \pi^{2}}\left(\frac{\varepsilon}{\hbar c}\right)^{2}$

$\mathrm{a}=$ non-relativistic particles
$\mathrm{b}=$ photons
Allow for spin degeneracy:
$g(\varepsilon)=(2 s+1) \frac{V}{4 \pi^{2}}\left(\frac{2 M}{\hbar^{2}}\right)^{3 / 2} \varepsilon^{1 / 2}$
$(2 s+1)$ is the spin degeneracy. Each state might be occupied (say for electrons) by $\uparrow$ or $\downarrow$ electron.

### 2.4 Two dimensional density of state

Density of states:

$k(x)=\frac{m \pi}{L} k_{y}=\frac{n \pi}{L}(\mathrm{~m}, \mathrm{n}$ are positive integers)
Area of one box $=\left(\frac{\pi}{L}\right)^{2}=\frac{\pi^{2}}{A}$
$L^{2}=A$ the area of the box.
Density of states $=\frac{1}{(\pi / L)^{2}}=\frac{A}{\pi^{2}}$
No. of states between $k$ and $k+d k\left(k, d k \gg \frac{\pi}{2}\right)=\frac{1}{4} 2 \pi k d k \frac{A}{\pi^{2}}$
Where $\frac{1}{4} 2 \pi k d k$ is the area between the curved lines, and $\frac{A}{\pi^{2}}$ the density of states in two dimensions.
$\frac{A}{2 \pi} k=\rho(k)$
$g(\varepsilon) d \varepsilon=\rho(k) d k$
$g(\varepsilon)=\rho(k) \frac{d k}{d \varepsilon}$
$\varepsilon=\frac{\hbar^{2} k^{2}}{2 M}$
$\frac{d \varepsilon}{d k}=\frac{\hbar^{2} k}{M}$
$g(\varepsilon)=\frac{A}{2 \pi} k \frac{M}{\hbar^{2} k}=\frac{A}{2 \pi} \frac{M}{\hbar^{2}}$


