Momentum Representation (chap. 5).

The momentum representation is similar to the coordinate representation in that a continuous state vector is used as a set of basis states for an expansion:

$$\hat{P}_\alpha |\vec{p}\rangle = p_\alpha |\vec{p}\rangle \qquad \alpha = 1, 2, 3.$$

$$\langle \vec{p} \,|\, \vec{p}\,' \rangle = \delta^3(\vec{p} - \vec{p}\,').$$

Often we replace $\vec{p} = \hbar\vec{k}$ just to remove some $\hbar$'s from expressions. Now, lets see how to transform between representations. We need to evaluate $\langle \vec{x} | \vec{p} \rangle = \langle \vec{x} | \hbar\vec{k} \rangle$.

$$\hat{\vec{P}} \langle \vec{x} | \hbar\vec{k} \rangle = \underline{-i\hbar \vec{\nabla} \langle \vec{x} | \hbar\vec{k} \rangle} = \langle \vec{x} | \hat{\vec{P}} | \hbar k \rangle = \underline{\hbar\vec{k} \langle \vec{x} | \hbar\vec{k} \rangle}$$

This has the solution $\langle \vec{x} | \hbar\vec{k} \rangle = \underbrace{c(\vec{k})}_{\text{constant}} e^{i\vec{k}\cdot\vec{x}}$

Now, the normalization constant $c(\vec{k})$ can be obtained from

$$\delta^3(\hbar\vec{k} - \hbar\vec{k}') = \langle \hbar\vec{k} | \hbar\vec{k}' \rangle = \int \langle \hbar\vec{k} | \vec{x} \rangle \langle \vec{x} | \hbar\vec{k}' \rangle d^3x$$

$$= c^*(k)\, c(k') \underbrace{\int e^{i(\vec{k}' - \vec{k})\cdot\vec{x}} d^3x}_{= (2\pi)^3 \delta^3(\vec{k} - \vec{k}')}.$$

$$\therefore \quad |c(k)|^2 = \frac{1}{\hbar^3} \frac{1}{(2\pi)^3} \text{"}\left(\frac{\delta}{\delta}\right)\text{"}$$

or $c = \dfrac{1}{(2\pi\hbar)^{3/2}}$ $\Rightarrow$ $\langle \vec{x} | \hbar\vec{k} \rangle = \dfrac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{x}}$

Suppose we call $\varphi(k)$ the momentum space equivalent of $\psi(x)$:

$$\varphi(k) = \langle \hbar \vec{k} | \psi \rangle = \int \langle \hbar\vec{k} | \vec{x} \rangle \langle \vec{x} | \psi \rangle d^3x$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\vec{k}\cdot\vec{x}} \psi(x) d^3x$$

The momentum representation of the operators is simple.

$$\hat{\vec{P}} \varphi(k) = \hbar\vec{k}\, \varphi(k)$$

$$\hat{Q}_\alpha \varphi(\vec{k}) = \langle \hbar\vec{k} | Q_\alpha | \psi \rangle \qquad \alpha = 1,2,3$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\vec{k}\cdot\vec{x}} Q_\alpha \psi(\vec{x}) d^3x$$

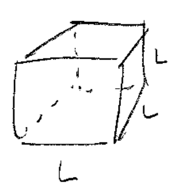
$$= \frac{1}{(2\pi\hbar)^{3/2}} \int x_\alpha e^{-i\vec{k}\cdot\vec{x}} \psi(\vec{x}) d^3x$$

$$= \left(\frac{1}{-i}\right) \frac{\partial}{\partial k_\alpha} \varphi(\vec{k})$$

$\Rightarrow$ The momentum representation for $\hat{Q}$ is then $\hat{Q}_\alpha = i \dfrac{\partial}{\partial k_\alpha} = i\hbar \dfrac{\partial}{\partial p_\alpha}$

Box Normalization

For those who are uncomfortable with δ-function normalization, there is an alternative. Suppose we consider a cubic box of length L to each side



If we impose periodic boundary conditions on the box, then the wavevector k must be an integer multiple of $2\pi/L$

[or, λ must be given by $\frac{1}{n}L$, $n = 1, 2, 3 \cdots \infty$

$$\Rightarrow k = \frac{p}{\hbar} = \frac{1}{\hbar}\left(\frac{h}{\lambda}\right) = \frac{2\pi}{L} \cdot n \;]$$

Note that there is a *minimum* value of k for a given L, but no maximum. Now, the states corresponding to these k's will be of the form

$$\langle \vec{x} | \hbar \vec{k} \rangle_L = N e^{i\vec{k}\vec{x}}$$

since they satisfy the usual Schrodinger Equation. If we normalize the states via

$$\langle \hbar \vec{k}' | \hbar \vec{k} \rangle_L = \delta_{kk'}$$

(instead of $\delta(\vec{k} - \vec{k}')$, because now the k's are discrete rather than continuous)

$$\Rightarrow \int_{V=L^3} \langle \hbar \vec{k}' | \vec{x} \rangle \langle \vec{x} | \hbar \vec{k} \rangle d\vec{x} = \delta_{kk'}$$

$$\Rightarrow |N|^2 \int_{V=L^3} d\vec{x} = 1. \quad \text{or } N = \frac{1}{L^{3/2}}.$$

Suppose we wish to look at the continuum limit for this problem. In the discrete k situation, we insert a set of states via

$$\sum_k |\hbar \vec{k} \rangle \langle \hbar \vec{k} |.$$

In the continuum situation $\sum_k \rightarrow \int \left(\begin{matrix}\text{density of}\\ \text{states}\end{matrix}\right) d^3k$.

The density of states is the number of states per unit volume in k space. But $k = \left(\frac{2\pi}{L}\right) n \Rightarrow$ one new state ~~#~~ increases k-space volume $\left(\frac{2\pi}{L}\right)^3$.

So the density of states is $\left(\frac{L}{2\pi}\right)^3$, and

$$\sum_k \rightarrow \int \left(\frac{L}{2\pi}\right)^3 d^3k = \left(\frac{L}{2\pi\hbar}\right)^3 \int d^3p.$$

The expectation of a quantity f becomes

$$\langle f(p)\rangle = \sum_k f(\hbar k)\,|\langle \hbar \vec{k} | \psi\rangle_L|^2 \rightarrow \int f(\hbar k)\left(\frac{L}{2\pi}\right)^3 d^3k \cdot |\langle \hbar k|\psi\rangle_L|^2$$

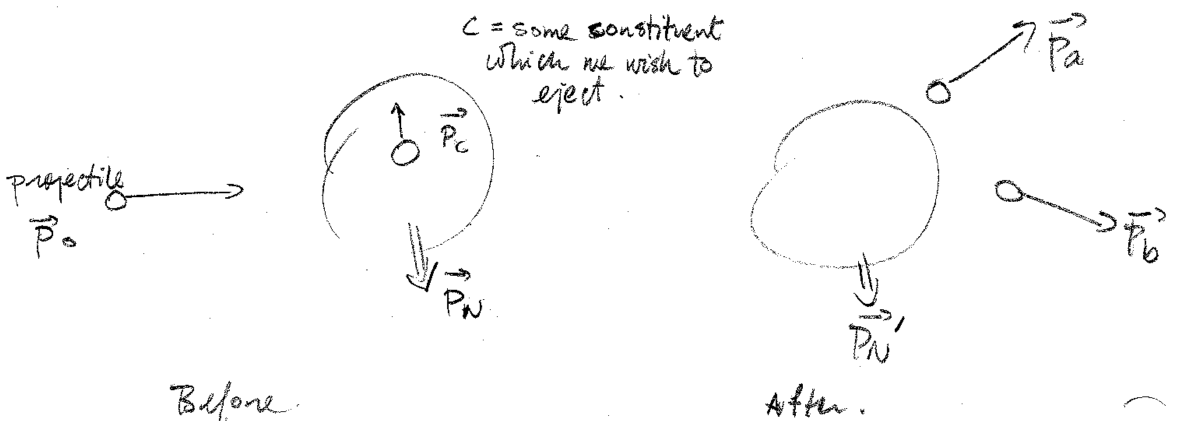
$$= \int f(\hbar k)\, d^3k \left(\frac{L}{2\pi}\right)^3 \cdot \int \langle \hbar k|x\rangle\langle x|\psi\rangle d^3x \cdot \int \langle \psi|x'\rangle\langle x'|\hbar k\rangle d^3x'$$

$$= \int f(\hbar k)\, d^3k \, \frac{L^3}{(2\pi)^3}\frac{1}{(L^{3/2})^2}\int e^{-ikx}\psi(x)\, d^3x \cdot \int e^{+ikx'}\psi^*(x')\, d^3x'$$

$$= \int f(\hbar k)\, d^3k \cdot \hbar^3 \varphi(k)\varphi^*(k) = \int f(p)|\varphi(p)|^2 d^3p \text{ as expected.}$$

Momentum Distributions

The momentum state representation has its largest applications in scattering experiments. There are a number of experiments performed on atoms, nuclei and particles, which are of the following general form:

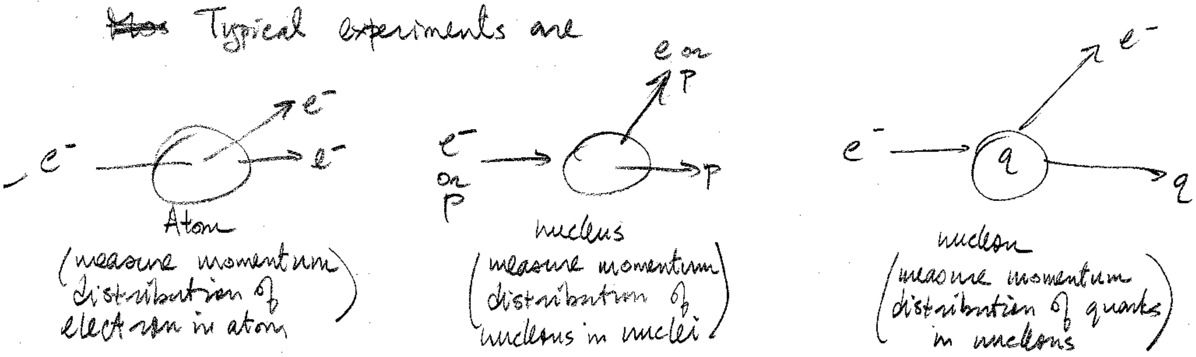


In general, the experiment is done with high energy projectiles ~~&~~ so that the collision process is fast compared to the "rearrangement time" of the residual system. In this approximate situation, $\vec{p}_N = \vec{p}_N{}'$. Then, by conservation of momentum,

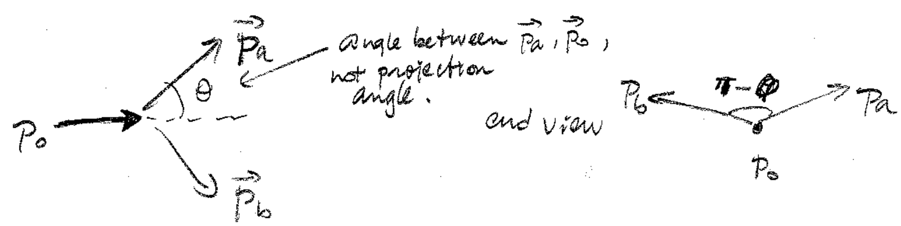
$$\vec{p}_o + \vec{p}_c = \vec{p}_a + \vec{p}_b .$$

(In the experiment, $\vec{p}_c \cong -\vec{p}_N$. Why not measure $\vec{p}_N{}'$ directly to find p_N and p_c? The answer is that most detectors are not sensitive to low energy particles like N, they are most sensitive to fast particles like a & b.)

~~Mos~~ Typical experiments are



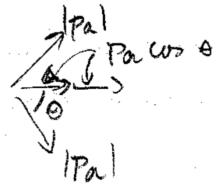
For atomic and nuclear studies, the socalled "symmetric" geometry is measured. In any given reaction, the final state is a three-body one so that the momenta $\vec{p}_a$, $\vec{p}_b$, $\vec{p}_N$ are neither equal nor coplanar. In the symmetric geometry, events are selected which satisfy.



Since $|\vec{p}_a| = |\vec{p}_b| = p_a$, the electron momentum can be solved by conservation of momentum:

x - direction

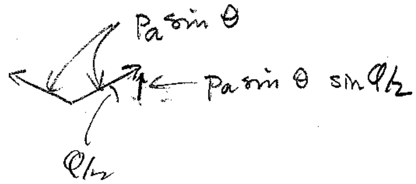
$p_o \longrightarrow \vec{p}_{e_x}$



$$p_{e_x} = 2 p_a \cos\theta - p_o$$

y - direction

p_o ⊙ $\uparrow p_{e_y}$



$$p_{e_y} = 2\ p_a \sin\theta \sin\varphi/2$$

Now, one typically measures a <u>rate</u> of events, so many events per second. This is given by

$$\text{rate} = \text{cross section} \left(\overset{\text{area}}{\equiv \sigma}\right) \times \underbrace{\text{flux}}_{\text{given by experimental conditions.}} \left(\frac{\#\ \text{per}}{cm^2\ \text{per sec}}\right).$$

The cross section for the event to occur is

$$\sigma(p_a, p_b) = \underbrace{\sigma_{ee}}_{\text{electron-electron elementary cross section}} \times \text{Probability to find atomic electron with momentum } p_e.$$

$$\Rightarrow \quad \underbrace{\sigma(p_a, p_b)}_{\text{Measure this}} = \underbrace{\sigma_{ee}}_{\text{Try to keep this as constant as possible, fix } p_o, |p_a|, |p_b|.} \underbrace{|\langle p_e | \psi \rangle|^2}_{\text{deduce this.}}$$

What should $|\langle p|\psi\rangle|^2$ look like? From undergraduate quantum mechanics, $\psi(r) \sim e^{-r/a_0}$ for the hydrogen atom ground state with $a_0 = \hbar^2/me^2$. Then

$$I = \int e^{-i\vec{k}\cdot\vec{x}} e^{-r/a_0} d^3x$$

$$= 2\pi \int e^{-ikr\cos\theta} e^{-r/a_0} r^2 dr\, d\cos\theta = 2\pi \int r^2 e^{-r/a_0} \frac{dr}{(-ikr)} \int_{+ikr}^{-ikr} e^{z} dz \qquad \leftarrow \int_1^{-1} d\cos\theta$$

$$= \frac{2\pi}{ik} \int r e^{-r/a_0} dr \left(e^{ikr} - e^{-ikr}\right)$$

$$= \frac{2\pi}{ik} \left[\int_0^\infty r\, e^{-r\left(\frac{1}{a_0} + ik\right)} dr - \int_0^\infty r\, e^{-r\left(\frac{1}{a_0} - ik\right)} dr \right]$$

$$= \frac{2\pi}{ik} \left[\frac{1}{\left(\frac{1}{a_0} + ik\right)^2} - \frac{1}{\left(\frac{1}{a_0} - ik\right)^2} \right] \int_0^\infty z e^{-z} dz$$

$$\int_0^\infty z^n e^{-z} dz = n!$$

$$= \frac{2\pi a_0^2}{ik} \underbrace{\left[\frac{1}{(1+ia_0k)^2} - \frac{1}{(1-ia_0k)^2} \right]}_{\frac{1 - 2ia_0k - a_0^2k^2 - (1 + 2ia_0k - a_0^2k^2)}{[(1+ia_0k)(1-ia_0k)]^2}} \qquad \underbrace{\int_0^\infty z e^{-z} dz}_{= 1}$$

(Reif, 607.)

$$= \frac{-4ia_0k}{(1+a_0^2k^2)^2}$$

$$\Rightarrow I = \frac{2\pi a_0^2}{ik} \frac{(-4ia_0k)}{(1+a_0^2k^2)^2}$$

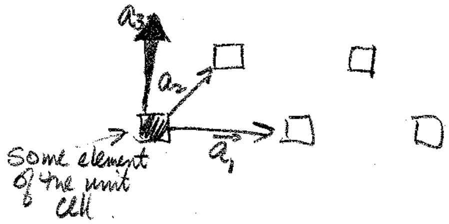
$$= \frac{-8\pi a_0^3}{(1+a_0^2k^2)^2}$$

Hence $$|\langle p|\psi\rangle|^2 \sim \frac{1}{(1+a_0^2k^2)^4}$$

For hydrogen spectra, this form has been verified by Weigold (AIP proceedings, 1982.) Other forms have been found for nuclei, reflecting the Fermi gas spectra.

Bloch's Theorem

In a crystal, there is a translational symmetry associated with the crystal lattice



The crystal is unchanged by a displacement of the form

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 \text{ are integers}$$

Corresponding to this translation there is a unitary operator $\hat{U}(\vec{R}_n)$ of the form $\hat{U}(\vec{R}_n) = \exp(-i\hat{\vec{P}}\cdot\vec{R}_n/\hbar)$ which leaves the crystal Hamiltonian invariant

$$\hat{U}(\vec{R}_n)\hat{H}\hat{U}^{-1}(R_n) = H.$$

Since the generators $\hat{\vec{P}}$ in $\hat{U}$ commute, then the $\hat{U}$'s commute among each other. $\hat{U}$ also leaves $\hat{H}$ unchanged. Hence, both $\hat{U}$ & $\hat{H}$ share a set of eigenvectors $|\psi\rangle$

$$H|\psi\rangle = E|\psi\rangle$$

$$\hat{U}(\vec{R}_n)|\psi\rangle = c(\vec{R}_n)|\psi\rangle$$

c is an eigenvalue which is a function of R_n.

To determine the form of the eigenvalues c, we use the property of the $\hat{U}$'s that $\hat{U}(\vec{R}_a)\hat{U}(\vec{R}_b) = \hat{U}(\vec{R}_a+\vec{R}_b)$

$$\Rightarrow c(\vec{R}_a)c(\vec{R}_b) = c(\vec{R}_a+\vec{R}_b)$$

$$\Rightarrow c(R_n) = e^{-i\vec{k}\cdot\vec{R}_n}$$

If $|c| = 1$, then $\vec{k}$ must be real. [Otherwise, < 1 by $e^{-k_I R}\, e^{ik_R R}$].
required by $\hat{U}\hat{U}^\dagger = 1$

Now, suppose that we take the coordinate representation $\psi(\vec{x}) = \langle \vec{x} | \psi \rangle$.

Then
$$\hat{U}(\vec{R}_n)\psi(\vec{x}) = \langle \vec{x} | \hat{U}(R_n) | \psi \rangle$$
$$= \left(\langle \psi | \hat{U}^{+}(R_n) | \vec{x} \rangle \right)^*$$
$$= \left(\langle \psi | e^{+i\frac{\hat{P}}{\hbar}R_n} | \vec{x} \rangle \right)^*$$
$$= \left(\langle \psi | \vec{x} - \vec{R}_n \rangle \right)^*$$
$$= \psi(\vec{x} - \vec{R}_n)$$

[which is also what we expect from the old functional argument]

but this is
$$e^{-i\frac{\vec{P}}{\hbar}\cdot\vec{R}_n}\psi(\vec{x})$$

So
$$\psi(\vec{x} - \vec{R}_n) = e^{-i\vec{k}\vec{R}_n}\psi(\vec{x}) \qquad (1)$$

[This symmetry demand determines k]

This is a constraint on the form of ψ and shows its periodicity in $\frac{\vec{k}}{k^2}$.

Suppose now that we choose to expand $\psi(x)$ as
$$\psi(\vec{x}) = \sum_{\vec{k}'} a(\vec{k}')e^{i\vec{k}'\cdot\vec{x}} \qquad (2)$$

Then, substituting into the condition (1) gives
$$\sum_{\vec{k}'} a(\vec{k}')e^{i\vec{k}'\cdot(\vec{x}-\vec{R}_n)} = e^{-i\vec{k}\cdot\vec{R}_n}\sum_{\vec{k}'} a(\vec{k}')e^{i\vec{k}'\vec{x}}$$

$$\Rightarrow \sum_{\vec{k}'} a(\vec{k}')\,\underline{\underline{e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_n}}}\,e^{i\vec{k}'\vec{x}} = \sum_{\vec{k}'} a(k')e^{i\vec{k}'\cdot\vec{x}}$$

In order for these two expressions on l.h.s. and r.h.s to be equivalent, then all $a(k)$ must vanish except those for which $e^{i(\vec{k}-\vec{k}')\vec{R}_n} = 1$.

This implies that the only allowed values of $\vec{k}-\vec{k}'$ are $\vec{k}'-\vec{k} = \vec{G}$ where $G_\alpha \perp \vec{a}_\beta \times \vec{a}_\gamma$ The vectors $\vec{G}$ are the reciprocal lattice of $\vec{R}_n$.

(5-10) So, if we write $\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$\vec{G}_m = m_1\vec{A}_1 + m_2\vec{A}_2 + m_3\vec{A}_3$

then $\vec{a}_1 \cdot \vec{A}_1 = 2\pi$

$\vec{a}_2 \cdot \vec{A}_1 = 0$ etc. So $\vec{A}_1$ is perpendicular to $\vec{a}_2 \times \vec{a}_3$ etc.

$\vec{a}_3 \cdot \vec{A}_1 = 0$

$$\Rightarrow \vec{A}_1 = \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

With this convention for $\vec{k}' = \vec{k} + \vec{G}_m$

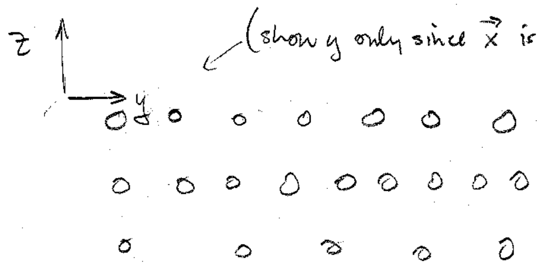
$$\Rightarrow \psi(\vec{x}) = \sum_{\vec{G}_m} a(\vec{k} + \vec{G}_m)\, e^{i(\vec{k} + \vec{G}_m)\cdot\vec{x}}$$

This implies that the momentum values of a state described by are quantized.

Diffraction Scattering

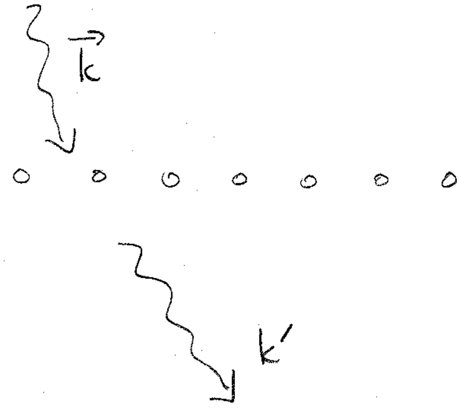
One common problem in solid state physics is scattering from a crystal. Suppose that we have a coordinate system defined by

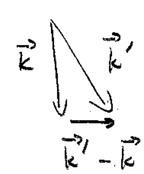
(showing y only since $\vec{x}$ is the position vector).



← periodic in x and y, arbitrary in −z direction

Then a scattering experiment might be of the form





Bloch Theorem: The eigenfunctions of the wave equation for a periodic potential are of the form

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_k(\vec{r})$$

where $u_k(\vec{r})$ is periodic ...

The incident "particle" has a wavefunction of the form

$$e^{i\vec{k}\cdot\vec{x}}$$

with $k_z < 0$ since the wave is travelling in the $-$ve z direction.

Once the incident particle has scattered and passed outside of the crystal, there is no potential W and the wavefunction again has a solution $e^{i\vec{k}\cdot\vec{x}}$ plus another piece associated with the scattering

$$\psi(x) = e^{i\vec{k}\cdot\vec{x}} + \sum_{\vec{k}'} \underbrace{r(\vec{k}')}_{\text{function to be determined later.}} e^{i\vec{k}'\cdot\vec{x}}$$

(Ballentine restricts the free part of the Hamiltonian W to lie in $z > 0$, and hence deals with backscattering.)

The magnitude of k is determined by the energy of the incident particle $\epsilon = (\hbar k)^2/2m$. After scattering, we have only $|\vec{k}'| = |\vec{k}|$ at this point.

The wavefunction in the crystal can be written in the form

$$\varphi_{\vec{q}}(\vec{x}) = \sum_{n=0}^{\infty} e^{i(\vec{q}+\vec{g}_n)\cdot\vec{x}} \underbrace{b_n(\vec{q}, z)}_{\text{all the } z\text{-dependence is in here.}}$$

$\vec{q}$ is a two-dimensional vector in the x,y plane.

$\vec{g}_n$ is a reciprocal lattice vector, also lying in the x,y plane.

The $n=0$ term in $\varphi_{\vec{q}}$ is of the form $e^{i\vec{q}\cdot\vec{x}} b_0(\vec{q}, z)$, and hence we identify $\vec{q}$ with the xy components of the incident momentum $\vec{k}$: $\vec{q} = \vec{k}_{xy}$. Upon scattering, the $n \neq 0$ components contribute, and we identify

$$\vec{q} + \vec{g}_n = \vec{k}'_{xy} \quad \text{or} \quad (\vec{k}' - \vec{k})_{xy} = \vec{g}_n$$

In other words, the momentum transferred to and from a periodic object is quantized, and the transfer has a direction which is that of the reciprocal lattice $\vec{g}_n$.

For example, scattering from a line of atoms in the y direction with spacing a. The reciprocal lattice is $g_n = \frac{2\pi n}{a}$,

$$\Rightarrow \quad k_y' - k_y = \frac{2\pi n}{a}$$

[This approach is different from the usual deBroglie wavelength approach with emphasizes Huygens-like construction. Here, it is the property of the lattice which directly results in quantization]

Diffraction scattering: experiment ← skipped, but preliminary discussion useful in emphasizing that deBroglie wavelength not needed to describe diffraction.

Motion in a Uniform Force Field

We finish off this section with a few simple examples of the usefulness of the momentum representation. First, we consider the force-free situation in 1 dimension

coord. rep. $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$ ← 2nd order equation; separation of variables problem.

momentum rep. $\frac{\hbar^2 k^2}{2M}\varphi(k,t) = i\hbar\frac{\partial}{\partial t}\varphi(k,t)$ ← 1st order in 1 variable, t.

$$\Rightarrow \varphi(\vec{k},t) = e^{-\frac{it\hbar k^2}{2M}}\varphi(\vec{k},0)$$

To find $\psi(x,t)$ once we have $\varphi(\vec{k},t)$, just take the Fourier transform:

$$\psi(\vec{x},t) = \frac{1}{(2\pi\hbar)^{3/2}}\int \exp\left(i\vec{k}\cdot\vec{x} - \frac{it\hbar k^2}{2M}\right)\varphi(\vec{k},0)\, d^3(\hbar\vec{k})$$

Suppose that we make the force constant in the x-direction, so that

$$W = -Fx \qquad \left(F = -\frac{dW}{dx} \right).$$

Then the mom. space. schrodinger equation separates into a ~~po~~ time-piece and momentum piece:

$$i\hbar \frac{\partial}{\partial t} f(t) = E\, f(t)$$

$$\frac{\hbar^2 k^2}{2M} \varphi(k) - F \frac{i\partial}{\underline{\underline{\partial k}}} \varphi(k) = E\, \varphi(k)$$

$$\text{or } \hat{x} = i\hbar \frac{\partial}{\partial p}$$

$$= i\hbar \frac{\partial}{\partial \hbar k} = i\hbar \frac{\partial}{\partial k}$$

$$\frac{\partial}{\partial k} \varphi(k) = i \left(\frac{E}{F} - \frac{\hbar^2 k^2}{2MF} \right) \varphi(k)$$

Which has the solution $\varphi(k) = \underset{\text{normalization constant}}{\underline{\underline{A}}}\, e^{-i\left(\frac{kE}{F} - \frac{\hbar^2 k^3}{6MF} \right)}$

The corresponding coordinate representation is an Airy function, which does not have a closed form. The asymptotic forms $(x \to \pm\infty)$ are discussed in Ballentine.