$\frac{E^2}{mc^2} = \epsilon$

central field of potential

potential energy

$\frac{E^2}{2m}$ $\quad \hbar^2 k^2$

$\frac{\hbar^2 k^2}{2m}$

$\vec{F} = -\vec{\nabla}\varphi_0$

$E_n = \int_c \vec{F}\, d\vec{r} = \int \vec{\nabla}\varphi_0$

$$\left(\frac{\hbar^2 \nabla^2}{2m} + V(r)\right)\psi = E\psi$$

$V_0 \cdot \varphi(r)$

strength $\quad$ potential field

$p = \hbar k = \frac{E}{c}$

$\vec{E} = \frac{\vec{\nabla}\varphi}{q}$

field

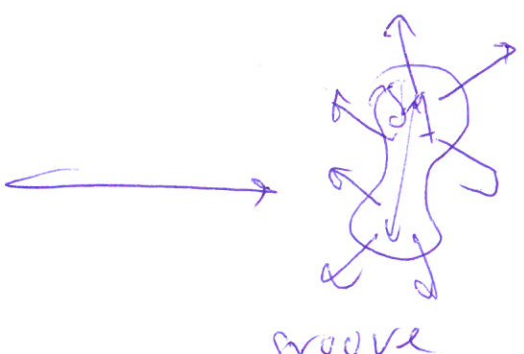
$\vec{E} = \frac{\vec{F}}{q}$

$\vec{C} \propto \vec{\nabla}\varphi_c$

$k^2 \quad V$

$E_k \quad E_p$

$H_0 + \delta H = \hat{H}$



groove

$$\Psi_{\text{scat}}(\boldsymbol{r}) = C \int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} \phi(\boldsymbol{r}')\Psi(\boldsymbol{r}')\, d\boldsymbol{r}'^3 \tag{2.10}$$

where C is the so-called *scattering length*. If the detection position $\boldsymbol{r}$ is at distance much larger than the scattering object size, as outlined in figure 2.3, the Fraunhofer approximation applies and $|\boldsymbol{r}-\boldsymbol{r}'| \simeq r$ (Feigin & Svergun, 1987), resulting in

$$\Psi_{\text{scat}}(\boldsymbol{r}) = C\frac{e^{ikr}}{r} \int e^{-ik\boldsymbol{r}'} \phi(\boldsymbol{r}')\Psi(\boldsymbol{r}')\, d\boldsymbol{r}'^3 \tag{2.11}$$

Assuming that there are no multiple scattering events due to the low concentration of scatterers and that the potential field is weak, the first Born approximation can be employed ($\Psi(\boldsymbol{r}) \simeq \Psi_0(\boldsymbol{r})$) (Cowley, 1995), leading to

$$\Psi_{\text{scat}}(\boldsymbol{r}) = CA_0\frac{e^{ikr}}{r} \int e^{i\boldsymbol{q}\boldsymbol{r}'} \phi(\boldsymbol{r}')d\boldsymbol{r}'^3 \tag{2.12}$$

where $\boldsymbol{q} = \boldsymbol{k}_s - \boldsymbol{k}$ is the momentum transfer vector and $\boldsymbol{k}_s$ the scattered wavevector. Analogously to equation 2.8, the differential scattering cross-section is:

$$\frac{d\sigma}{d\Omega} = \frac{|\Psi_{\text{scat}}|^2 \cdot \left(r^2 \Delta\Omega\right)}{|\Psi_0|^2 \Delta\Omega} = r_e^2 |f(\boldsymbol{q})|^2 \tag{2.13}$$

where $f(\boldsymbol{q}) = \int e^{i\boldsymbol{q}\boldsymbol{r}'} \phi(\boldsymbol{r}')d\boldsymbol{r}'^3$ is the scattering amplitude and the scattering length is the classical electron radius r_e. The scattering amplitude $f(\boldsymbol{q})$ is simply the Fourier transform of the scattering potential field $\phi(\boldsymbol{r})$.

This type of scattering mechanism is named Rayleigh-Gans-Debye when the refractive index of the object n_{obj} is close to unity and the condition $2\pi/\lambda \cdot D \cdot \left|n_{\text{med}} - n_{\text{obj}}\right| \ll 1$ is fulfilled, being D the size of the object and n_{med} the refractive index of the suspending medium. For X-ray photons with wavelenghts λ around 0.1 nm and nanoscaled objects, this approximation can be applied and it can be safely assumed that the same electromagnetic wave impinges each part of the object (van de Hulst, 1957; Barber & Wang, 1978). In the case of optical radiation scattered by colloids, the Mie scattering framework is used, while the Rayleigh scattering corresponds to light wavelengths much larger than the scattering object.

Anomalous scattering

In X-ray scattering experiments, the scattering centres are the electrons of the atom and the scattering field is the electron charge density about the nucleous, so $\phi(\boldsymbol{r}) = \rho_e(\boldsymbol{r})$. The electron density is related to the atomic properties as introduced in equation 2.5 and therefore the scattering amplitude increases with the atomic number Z as can be shown by calculating equation 2.13 at the limit $\boldsymbol{q} \to 0$

$$f(\boldsymbol{q} \to 0) = \int \rho_e(\boldsymbol{r}')d\boldsymbol{r}'^3 = Z \tag{2.14}$$

This is valid when the incident radiation energy is much larger than the energy corresponding to a resonant excitation. When the X-ray energy is close to an absorption edge, the anomalous dispersion becomes relevant and the scattering amplitude depends on the energy of the X-ray by adding the anomalous corrections (Als-Nielsen & McMorrow, 2011):

1) $-\frac{\hbar^2}{2m}\nabla^2\psi + e\varphi(r)\psi = i\hbar\partial_t\psi$

$e\varphi(r)$: potential energy // potential

$\varphi(r)$: electrostatic potential function // potential field

2) $e\varphi(r) \Rightarrow \mu\varphi(r)$

μ: strength of the interaction with the potential field

$\varphi(r)$: potential field

$\Rightarrow \left(\nabla^2 + 4\pi^2 k_0^2 + \mu\varphi(r)\right)\psi = 0$

(1)+(2) $\rightarrow \mu = \frac{2me}{\hbar^2}$

$\mu\varphi(r) = \frac{2m}{\hbar^2}V(r)$

$\left(\frac{\hbar^2}{2m}\nabla^2 + E\right)\psi_0 = V(r)\psi_0 \longrightarrow \psi' = \psi_0 + \int G_0(r,r'|E)V(r')\psi_K'(r')$

$V(r)$: interaction potential / potential

$G_0 = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{iK\cdot|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$

$\frac{2m}{\hbar^2}\cdot\mu = r_e$

$r_e = \frac{\mu_0}{4\pi} = \frac{2m_e e}{4\pi\hbar^2} = \frac{e}{4\pi}\cdot\frac{2m_e}{\hbar^2}$

$r_e = \frac{e^2}{4\pi\varepsilon_0 m_e c^2} = \frac{e}{4\pi}\cdot\frac{e}{\varepsilon_0 m_e c^2}$

$\left\{\begin{array}{l} \frac{2m}{\hbar^2} = \frac{e}{\varepsilon_0 mc^2} \\ mc^2 = \frac{e\hbar^2}{2m} \end{array}\right.$

$\mu = \frac{r_e}{2m}\cdot\hbar^2 = \frac{e^2\hbar^2}{24\pi\varepsilon_0 m^2 c^2} = \frac{1}{4\pi\varepsilon_0 2}\left(\frac{e\hbar}{mc}\right)^2$

$\left(\mu\varphi(r) + \nabla^2 + 4\pi k_0^2\right)\psi = 0 \longleftrightarrow \left(\frac{2m}{\hbar^2}V(r) + \nabla^2 + 4\pi k_0^2\right)\psi = 0$

$\frac{\mu}{4\pi} = r_e \Rightarrow \mu = r_e 4\pi \rightarrow r_e 4\pi\varphi(r) = V(r)\frac{2m}{\hbar^2}$

$\hookrightarrow \varphi(r) = V(r)\frac{2m}{\hbar^2 r_e 4\pi} = \frac{4\pi\varepsilon_0 mc^2 2m}{e^2\hbar^2 4\pi}$

$\boxed{\varphi(r) = 2\varepsilon_0\left(\frac{mc}{e\hbar}\right)^2 V(r)}$