# Neutron Scattering by Magnetic Crystals II.I: Neutron Scattering Theory

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Andrew T. Boothroyd "Principles of Neutron Scattering from Condensed Matter"

# Outline

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### III.II Neutron Reflectometer

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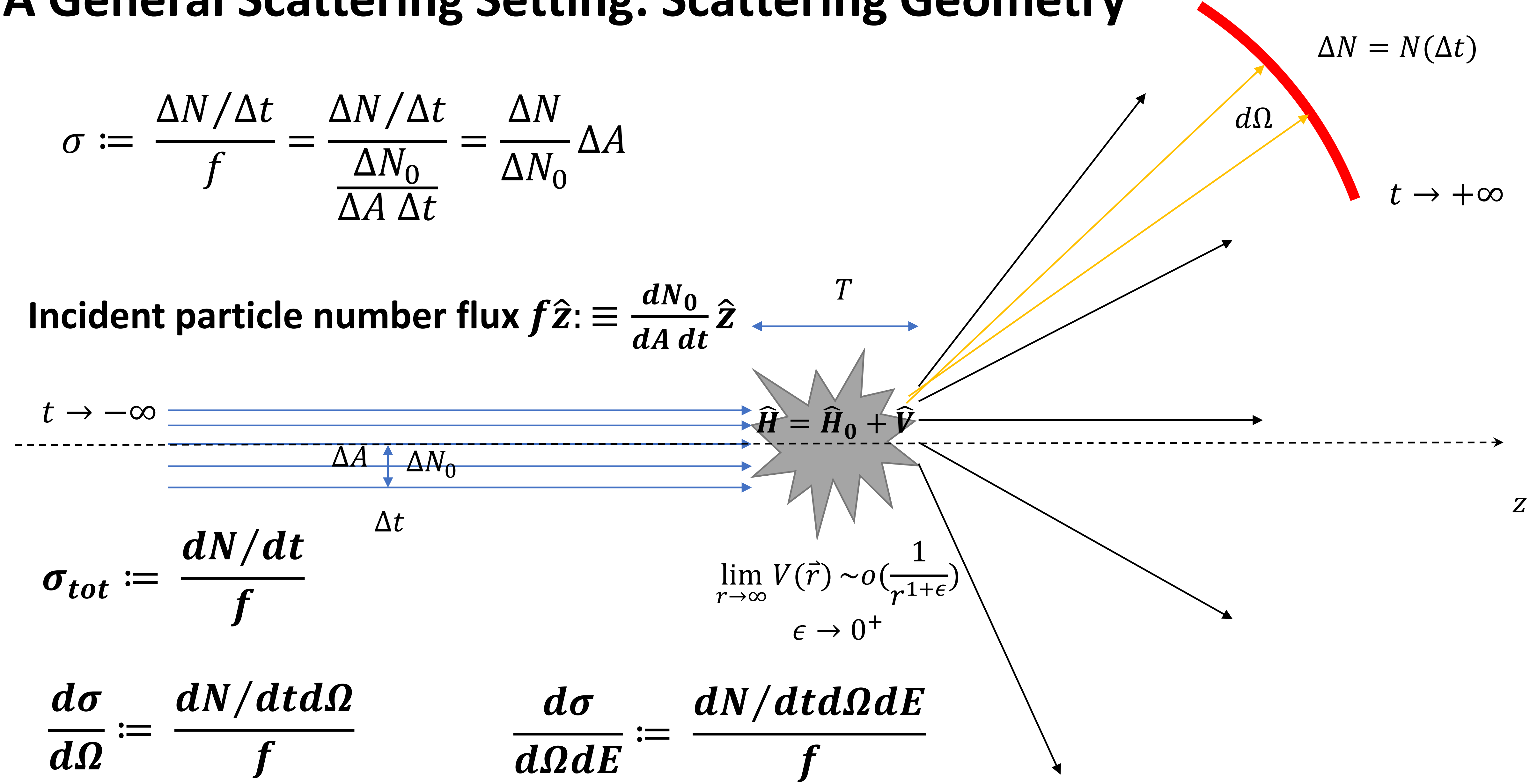
# General Scattering Theory

# A General Scattering Setting: Scattering Geometry

$$\sigma := \frac{\Delta N / \Delta t}{f} = \frac{\Delta N / \Delta t}{\frac{\Delta N_0}{\Delta A\ \Delta t}} = \frac{\Delta N}{\Delta N_0} \Delta A$$

**Incident particle number flux** $\boldsymbol{f\hat{z}} :\equiv \frac{\boldsymbol{dN_0}}{\boldsymbol{dA\ dt}} \boldsymbol{\hat{z}}$




$$\boldsymbol{\sigma_{tot}} := \frac{\boldsymbol{dN/dt}}{\boldsymbol{f}}$$

$$\frac{\boldsymbol{d\sigma}}{\boldsymbol{d\Omega}} := \frac{\boldsymbol{dN/dtd\Omega}}{\boldsymbol{f}} \qquad \frac{\boldsymbol{d\sigma}}{\boldsymbol{d\Omega dE}} := \frac{\boldsymbol{dN/dtd\Omega dE}}{\boldsymbol{f}}$$


[E. Koelink, Lectures on scattering theory, Delft the Netherlands 2006]

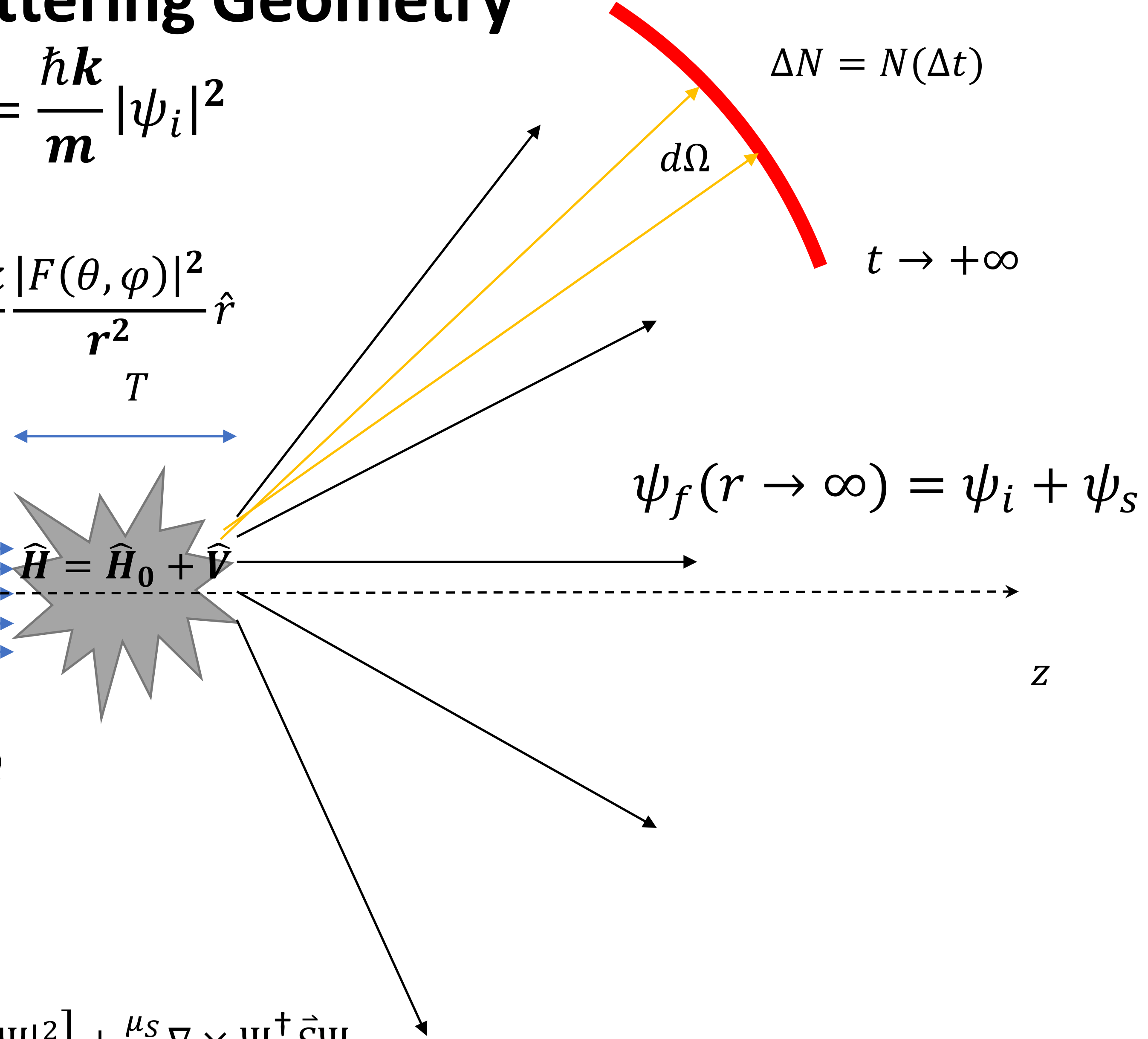
# A General Scattering Setting: Scattering Geometry

Plane wave $\psi_i = e^{ikz}$ $\qquad$ $\boldsymbol{f = \frac{dN_0}{dA\,dt} = \frac{\hbar k}{m}|\psi_i|^2}$

$$\psi_s = F(\theta,\varphi)\frac{e^{ikr}}{r} \qquad \vec{j}_s = \frac{-i\hbar}{2m}|\psi_s|^2 \nabla \ln\frac{\psi_s}{\psi_s^\dagger} = \frac{\hbar k}{m}\frac{|F(\theta,\varphi)|^2}{r^2}\hat{r}$$

**Incident particle number flux** $\boldsymbol{f\hat{z}} :\equiv \frac{dN_0}{dA\,dt}\hat{z}$

$t \to -\infty$




$$\boldsymbol{dN/dt = \vec{j}_s \cdot r^2 d\Omega \hat{r} = \frac{\hbar k}{m}|F(\theta,\varphi)|^2 d\Omega}$$

$$\boldsymbol{\frac{d\sigma}{d\Omega} = \frac{dN/dt d\Omega}{f} = |F(\theta,\varphi)|^2}$$

Non-relativistic flux: $\vec{j}[\Psi] = \frac{-i\hbar}{2m}\left[\Psi^\dagger\nabla\Psi - \Psi\nabla\Psi^\dagger - 2q\vec{A}|\Psi|^2\right] + \frac{\mu_S}{S}\nabla \times \Psi^\dagger\vec{S}\Psi$


Quantum mechanics, E. Zaarur, Y. Peleg, R. Pnini, Schaum's Easy Outlines Crash Course, Mc Graw Hill (USA), 2006

# A General Scattering Setting: S Matrix

$$f(\hat{A}) :\equiv \sum_{n=0}^{\infty} a_n \hat{A}^n$$

**Schrödinger picture:** $i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

$$\langle\Phi_\alpha|\Phi_\beta\rangle = \langle\Psi_\alpha|\Psi_\beta\rangle = \boldsymbol{\delta_{\alpha\beta}}$$

$t_0 = 0$

**Closed or isolated system:** $\partial_t\hat{H} = 0$ $\quad |\Psi(t)\rangle = e^{\frac{-i\hat{H}(t-t_0)}{\hbar}}|\Psi(t_0)\rangle = e^{\frac{-i\hat{H}t}{\hbar}}|\Psi(0)\rangle$

$$\int d\beta\, |\Phi_\beta\rangle\langle\Phi_\beta| = \int d\beta\, |\Psi_\beta\rangle\langle\Psi_\beta| = 1$$

$\hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle \quad \hat{H}_0|\Phi_\alpha\rangle = E_\alpha|\Phi_\alpha\rangle \qquad \boldsymbol{\hat{H} = \hat{H}_0 + \hat{V}}$

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots, |x| < 1$$

Lippmann-Schwinger equation $\qquad (E_\alpha - \hat{H}_0)|\Psi_\alpha\rangle = \hat{V}|\Psi_\alpha\rangle$

**Green Function Method:**

$$(E_\alpha - \hat{H}_0)\hat{G} = \hat{I} \qquad |\tilde{\Psi}_\alpha\rangle = \hat{G}\hat{V}|\Psi_\alpha\rangle$$

$$\boldsymbol{|\Psi_\alpha^\mp\rangle = |\Phi_\alpha\rangle + \frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)}\hat{V}|\Psi_\alpha^\mp\rangle = |\Phi_\alpha\rangle + \int d\beta \frac{\langle\Phi_\beta|\hat{V}|\Psi_\alpha^\mp\rangle}{(E_\alpha - E_\beta \pm i\epsilon)}|\Phi_\beta\rangle}$$

$$\boldsymbol{|\Psi_\alpha^\mp\rangle = |\Phi_\alpha\rangle + \frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)}\hat{V}|\Phi_\alpha\rangle + \frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)}\hat{V}\frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)}\hat{V}|\Phi_\alpha\rangle + \cdots = \frac{1}{1 - \frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)}\hat{V}}|\Phi_\alpha\rangle}$$

$$k_\alpha \equiv \frac{\sqrt{2mE_\alpha}}{\hbar} \qquad U(\vec{\boldsymbol{r}}) \equiv \frac{2m}{\hbar^2}V(\vec{\boldsymbol{r}})$$

If $\langle\vec{r}|\hat{H}_0|\vec{r}'\rangle = \frac{-\hbar^2}{2m}\delta(\vec{r} - \vec{r}')\nabla^2 \qquad (\nabla^2 + k_\alpha^2)\Psi_\alpha(\vec{r}) = U(\vec{r})\Psi_\alpha(\vec{r})$

$$(\nabla^2 + k_\alpha^2)G_\pm(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}') \qquad G_\pm(\vec{r} - \vec{r}') \equiv -\frac{1}{4\pi}\frac{e^{\pm ik_\alpha|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}$$

$$\Psi_\alpha^\pm(\vec{r}) = \Phi_\alpha(\vec{r}) + \int d\vec{r}' G_\pm(\vec{r} - \vec{r}')U(\vec{r}')\Psi_\alpha^\pm(\vec{r}') = \Phi_\alpha(\vec{r}) + \int d\vec{r}' G_\pm(\vec{r} - \vec{r}')U(\vec{r}')\Phi_\alpha(\vec{r}') + \int d\vec{r}' G_\pm(\vec{r} - \vec{r}')U(\vec{r}')\int d\vec{r}'' G_\pm(\vec{r}' - \vec{r}'')U(\vec{r}'')\Psi_\alpha^\pm(\vec{r}'')$$

**Far Field Approximation:** $|\vec{r}| \gg |\vec{r}'| \qquad |\vec{r} - \vec{r}'| \approx |\vec{r}| - (\vec{r}\cdot\vec{r}')\,/\,|\vec{r}|$

$$G_\pm(\vec{r} - \vec{r}') = -\frac{1}{4\pi}\frac{e^{\pm ik_\alpha|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|} \approx -\frac{1}{4\pi}\frac{e^{\pm ik_\alpha[|\vec{r}| - (\vec{r}\cdot\vec{r}')/|\vec{r}|]}}{|\vec{r}| - (\vec{r}\cdot\vec{r}')/|\vec{r}|} \approx -\frac{1}{4\pi}\frac{e^{\pm ik_\alpha|\vec{r}|}}{|\vec{r}|}e^{\mp i\vec{k}_\alpha\cdot\vec{r}'}$$

$$\lim_{r\to\infty}\Psi_\alpha^\pm(\vec{r}) = \Phi_\alpha(\vec{r}) + F(\theta,\varphi)\frac{e^{\pm ik_\alpha|\vec{r}|}}{|\vec{r}|}$$

$$F(\theta,\varphi) \equiv -\frac{1}{4\pi}\int e^{\mp i\vec{k}_\alpha\cdot\vec{r}'}d\vec{r}' U(\vec{r}')\Psi_\alpha^\pm(\vec{r}')$$


*Steven Weinberg, Ch.3: Scattering Theory; The Quantum Theory of Fields Volume I*

Lippmann, B. A.; Schwinger, J. (1950). "Variational Principles for Scattering Processes. I". *Phys. Rev. Lett.* **79** (3): 469–480.

# A General Scattering Setting: S Matrix

$g(\alpha) \equiv \langle \Psi_\alpha | \Psi(0) \rangle \qquad \|\varphi\| :\equiv \langle \varphi | \varphi \rangle$

$$\lim_{t\to\pm\infty} \|\Psi(t) - \Phi(t)\| = 0$$

$$|\Psi^\pm(t)\rangle = e^{\frac{-i\hat{H}t}{\hbar}} \int d\alpha\, g(\alpha) \left|\Psi_\alpha^\pm\right\rangle = \int d\alpha\, g(\alpha) e^{\frac{-iE_\alpha t}{\hbar}} \left|\Psi_\alpha^\pm\right\rangle;$$

$$\left|\Psi_\alpha^\mp\right\rangle = |\Phi_\alpha\rangle + \frac{1}{(E_\alpha - \hat{H}_0 \pm i\epsilon)} \hat{V} \left|\Psi_\alpha^\mp\right\rangle = |\Phi_\alpha\rangle + \int d\beta \frac{\langle \Phi_\beta | \hat{V} | \Psi_\alpha^\mp \rangle}{(E_\alpha - E_\beta \pm i\epsilon)} \left|\Phi_\beta\right\rangle$$

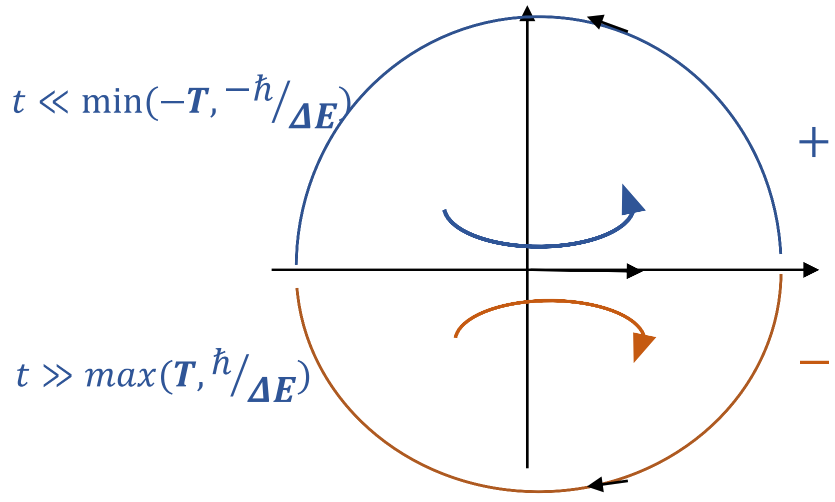
$$|\Phi(t)\rangle = e^{\frac{-i\hat{H}_0 t}{\hbar}} \int d\alpha\, g(\alpha) |\Phi_\alpha\rangle = \int d\alpha\, g(\alpha) e^{\frac{-iE_\alpha t}{\hbar}} |\Phi_\alpha\rangle$$

$$\wp_\beta^\pm(t) \equiv \int \boldsymbol{d\alpha\, g(\alpha) e^{\frac{-iE_\alpha t}{\hbar}} \frac{\langle \Phi_\beta | \hat{V} | \Psi_\alpha^\pm \rangle}{(E_\alpha - E_\beta \mp i\epsilon)}}$$

$$|\Psi^\pm(t)\rangle = |\Phi(t)\rangle + \int d\alpha\, g(\alpha) e^{\frac{-iE_\alpha t}{\hbar}} \int d\beta \frac{\langle \Phi_\beta | \hat{V} | \Psi_\alpha^\pm \rangle}{(E_\alpha - E_\beta \mp i\epsilon)} \left|\Phi_\beta\right\rangle = |\Phi(t)\rangle + \int d\beta\, \wp_\beta^\pm(t) \left|\Phi_\beta\right\rangle$$

$$\boldsymbol{-iE_\alpha t = -i\left(|E_\alpha| e^{i\theta}\right) t = -i|E_\alpha| t \cos\theta + |E_\alpha| t \sin\theta}$$

| $\wp_\beta(t)$ | $+\infty$ | $-\infty$ |
|---|---|---|
| + | 0 | $\boldsymbol{2\pi i e^{\frac{-iE_\beta t}{\hbar}} \int d\alpha \delta(E_\alpha - E_\beta)\, g(\alpha) \langle \Phi_\beta \| \hat{V} \| \Psi_\alpha^+ \rangle}$ |
| - | $\boldsymbol{-2\pi i e^{\frac{-iE_\beta t}{\hbar}} \int d\alpha \delta(E_\alpha - E_\beta)\, g(\alpha) \langle \Phi_\beta \| \hat{V} \| \Psi_\alpha^- \rangle}$ | 0 |




$$\lim_{t\to\pm\infty} |\Psi^\pm(t)\rangle = |\Phi(t)\rangle \qquad \left|\Psi_\alpha^\pm\right\rangle = W(\pm\infty) |\Phi_\alpha\rangle$$

**Wave Operator** $W(\pm\infty) :\equiv \lim_{t\to\pm\infty} W(t) = \lim_{t\to\pm\infty} e^{\frac{i\hat{H}t}{\hbar}} e^{\frac{-i\hat{H}_0 t}{\hbar}}$


*Steven Weinberg, Ch.3: Scattering Theory; The Quantum Theory of Fields Volume I*

Lippmann, B. A.; Schwinger, J. (1950). "Variational Principles for Scattering Processes. I". *Phys. Rev. Lett.* **79** (3): 469–480.

# A General Scattering Setting: S Matrix

$$\int d\beta \left|\Phi_\beta\right\rangle\left\langle\Phi_\beta\right| = \int d\beta \left|\Psi_\beta\right\rangle\left\langle\Psi_\beta\right| = 1$$

**Scattering matrix** $S_{\alpha\beta} = \langle\Psi_\alpha^+|\Psi_\beta^-\rangle = \langle\Phi_\alpha|\hat{S}|\Phi_\beta\rangle$

$$\hat{S} :\equiv W^\dagger(+\infty)W(-\infty) = \lim_{\substack{t\to-\infty,\\ \tau\to+\infty}} e^{\frac{i\hat{H}_0\tau}{\hbar}} e^{\frac{-i\hat{H}\tau}{\hbar}} e^{\frac{i\hat{H}t}{\hbar}} e^{\frac{-i\hat{H}_0 t}{\hbar}}$$

$$\lim_{t\to+\infty}|\Psi^-(t)\rangle = |\Phi(t)\rangle + \lim_{t\to+\infty}\int d\beta\, \wp_\beta^-(t)\left|\Phi_\beta\right\rangle = |\Phi(t)\rangle - \lim_{t\to+\infty}\int d\beta \left|\Phi_\beta\right\rangle 2\pi i e^{\frac{-iE_\beta t}{\hbar}}\int d\alpha\delta\left(E_\alpha - E_\beta\right) g(\alpha)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle$$

$$= \int d\alpha\, g(\alpha)e^{\frac{-iE_\alpha t}{\hbar}}|\Phi_\alpha\rangle - \lim_{t\to+\infty}\int d\beta\left|\Phi_\beta\right\rangle 2\pi i e^{\frac{-iE_\beta t}{\hbar}}\int d\alpha\delta\left(E_\alpha - E_\beta\right) g(\alpha)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle$$

$$= \lim_{t\to+\infty}\int d\beta e^{\frac{-iE_\beta t}{\hbar}}\left|\Phi_\beta\right\rangle\left[g(\beta) - 2\pi i\int d\alpha\delta\left(E_\alpha - E_\beta\right) g(\alpha)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle\right]$$

$$\lim_{t\to+\infty}|\Psi^-(t)\rangle = \lim_{t\to+\infty}\int d\beta g(\beta)e^{\frac{-iE_\beta t}{\hbar}}\left|\Psi_\beta^-\right\rangle = \lim_{t\to+\infty}\int d\beta g(\beta)e^{\frac{-iE_\beta t}{\hbar}}\int d\alpha|\Psi_\alpha^+\rangle\langle\Psi_\alpha^+|\Psi_\beta^-\rangle = \lim_{t\to+\infty}\int d\beta g(\beta)e^{\frac{-iE_\beta t}{\hbar}}\int d\alpha|\Psi_\alpha^+\rangle S_{\alpha\beta}$$

$$= \lim_{t\to+\infty}\int d\beta g(\beta)\int d\alpha|\Psi_\alpha^+\rangle e^{\frac{-iE_\alpha t}{\hbar}} S_{\alpha\beta} = \lim_{t\to+\infty}\int d\beta g(\beta)\int d\alpha|\Phi_\alpha\rangle e^{\frac{-iE_\alpha t}{\hbar}} S_{\alpha\beta}$$

$$\int d\alpha g(\alpha)\, S_{\beta\alpha} = g(\beta) - 2\pi i\int d\alpha\delta\left(E_\alpha - E_\beta\right) g(\alpha)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle \qquad \forall\, g(\alpha)$$

**Probability Amplitude**

$$\boldsymbol{S_{\beta\alpha} = \delta(\alpha-\beta) - 2\pi i\delta\left(E_\alpha - E_\beta\right)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle = \delta(\alpha-\beta) - 2\pi i\delta\left(E_\alpha - E_\beta\right)\delta^3\left(\vec{p}_\alpha - \vec{p}_\beta\right)M_{\beta\alpha}}$$

# A General Scattering Setting: Transition Rates and Cross Section

$$S_{\beta\alpha} = \delta(\alpha-\beta) - 2\pi i\delta(E_\alpha - E_\beta)\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle = \delta(\alpha-\beta) - 2\pi i\delta(E_\alpha - E_\beta)\delta^3(\vec{p}_\alpha - \vec{p}_\beta)M_{\beta\alpha}$$

$$\delta_T(E_\alpha - E_\beta) = \frac{1}{2\pi\hbar}\int_{-T/2}^{T/2} e^{i(E_\alpha - E_\beta)t/\hbar}\,dt \qquad [\delta_T(E_\alpha - E_\beta)]^2 = \delta_T(E_\alpha - E_\beta)\delta_T(0) = \delta_T(E_\alpha - E_\beta)\frac{T}{2\pi\hbar}$$

$$P(\alpha\to\beta) = |S_{\beta\alpha}|^2 = 4\pi^2|\delta_T(E_\alpha - E_\beta)|^2|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2$$

$$= 4\pi^2\delta_T(E_\alpha - E_\beta)\frac{T}{2\pi\hbar}|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2 = \frac{2\pi T}{\hbar}\delta_T(E_\alpha - E_\beta)|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2$$

$$dP(\alpha\to\beta) = |S_{\alpha\beta}|^2 d\mathcal{N}_\beta = \frac{2\pi T}{\hbar}\delta_T(E_\alpha - E_\beta)|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2 d\mathcal{N}_\beta$$

$d\mathcal{N}_\beta$: State Number in the range $(\beta, \beta + d\beta)$

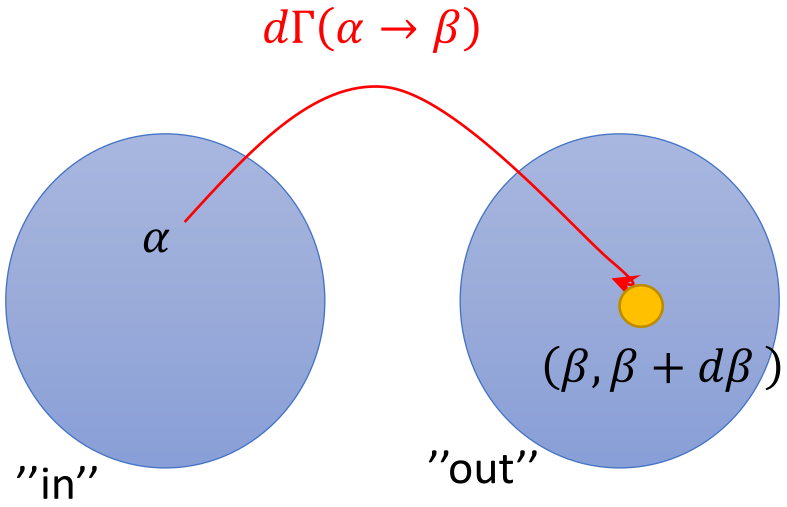
## Differential Transition Rate: Fermi's Golden Rule

$$d\boldsymbol{\Gamma}(\alpha\to\beta) = \frac{dP(\alpha\to\beta)}{T} = \frac{2\pi}{\hbar}\delta_T(E_\alpha - E_\beta)|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2 d\mathcal{N}_\beta$$

If $\alpha = \alpha_1 + \alpha_2$ Relative Velocity $u_\alpha E_1 E_2 = \sqrt{(p_1\cdot p_2)^2 - m_1^2 m_2^2}$

$$p_1\cdot p_2 \equiv E_1E_2 - \vec{p}_1\cdot\vec{p}_2$$

$$d\sigma(\alpha\to\beta) = \frac{d\Gamma(\alpha\to\beta)}{u_\alpha / V_0} = \frac{2\pi V_0}{\hbar u_\alpha}\delta_T(E_\alpha - E_\beta)|\langle\Phi_\beta|\hat{V}|\Psi_\alpha^-\rangle|^2 d\mathcal{N}_\beta$$



# Neutron Scattering

**Kinematical Theory** | **Neutron Diffraction and Spectroscopy**

Dynamical Theory | Neutron Optics: Reflection and Imaging

# Scattering Master Formula

$$\frac{\boldsymbol{d\sigma}\left(\left(\vec{\boldsymbol{k}}_i,\boldsymbol{\sigma}_i\right)\to\left(\vec{\boldsymbol{k}}_f+\boldsymbol{d}\vec{\boldsymbol{k}}_f,\boldsymbol{\sigma}_f\right)\right)}{\boldsymbol{d\Omega d}(\hbar\boldsymbol{\omega})}=\left(\frac{\boldsymbol{m}V_0}{\boldsymbol{2\pi}\hbar^2}\right)^2\frac{\boldsymbol{k}_f}{\boldsymbol{k}_i}\boldsymbol{\delta}\left(\boldsymbol{\varepsilon}_f-\boldsymbol{\varepsilon}_i-\hbar\boldsymbol{\omega}\right)\sum_{\boldsymbol{\varepsilon}_i,\boldsymbol{\varepsilon}_f}\boldsymbol{p}(\boldsymbol{\varepsilon}_i)\left|\left\langle\vec{\boldsymbol{k}}_f,\boldsymbol{\sigma}_f,\boldsymbol{\varepsilon}_f\middle|\widehat{\boldsymbol{V}}\middle|\vec{\boldsymbol{k}}_i,\boldsymbol{\sigma}_i,\boldsymbol{\varepsilon}_i\right\rangle\right|^2$$

$$\frac{\boldsymbol{d\sigma}}{\boldsymbol{d\Omega d}(\hbar\boldsymbol{\omega})}=\frac{\boldsymbol{k}_f}{\boldsymbol{k}_i}\frac{\mathbf{1}}{\boldsymbol{2\pi}\hbar}\int_{-\infty}^{\infty}\boldsymbol{dte}^{-\boldsymbol{i\omega t}}\left\langle\boldsymbol{A}^{\dagger}(\vec{\boldsymbol{q}})\boldsymbol{A}(\vec{\boldsymbol{q}},\boldsymbol{t})\right\rangle$$

$$A(\vec{q},t)\equiv\frac{m}{2\pi\hbar^2}\left\langle\sigma_f\left|V(\vec{q},t)\right|\sigma_i\right\rangle$$

$$V(\vec{q},t)\equiv e^{iH_St/\hbar}V(\vec{q})e^{i-H_St/\hbar}$$

$$V(\vec{q})\equiv\int d\vec{r}_nV(\vec{r}_n)e^{i\vec{q}\cdot\vec{r}_n}\qquad\vec{q}\equiv\vec{k}_i-\vec{k}_f$$

# Neutron Scattering Setting: Lab Frame

$$d\boldsymbol{\sigma}(\boldsymbol{\alpha} \to \boldsymbol{\beta}) = \frac{2\pi V_0}{\hbar u_\alpha} \delta_T(E_\alpha - E_\beta) \left| \langle \boldsymbol{\Phi}_\beta | \hat{V} | \boldsymbol{\Psi}_\alpha^- \rangle \right|^2 d\mathcal{N}_\beta$$

Born Approximation: Weak interaction, High Energy

$$d\boldsymbol{\sigma}(\boldsymbol{\alpha} \to \boldsymbol{\beta}) = \frac{2\pi V_0}{\hbar u_\alpha} \delta_T(E_\alpha - E_\beta) \left| \langle \boldsymbol{\Phi}_\beta | \hat{V} | \boldsymbol{\Phi}_\alpha \rangle \right|^2 d\mathcal{N}_\beta$$

$$d\Omega \equiv \sin\theta \, d\theta d\phi \qquad \boldsymbol{\beta} = \boldsymbol{f}$$

$$\hbar\omega \coloneqq \frac{(\hbar k_i)^2}{2m} - \frac{(\hbar k_f)^2}{2m}$$

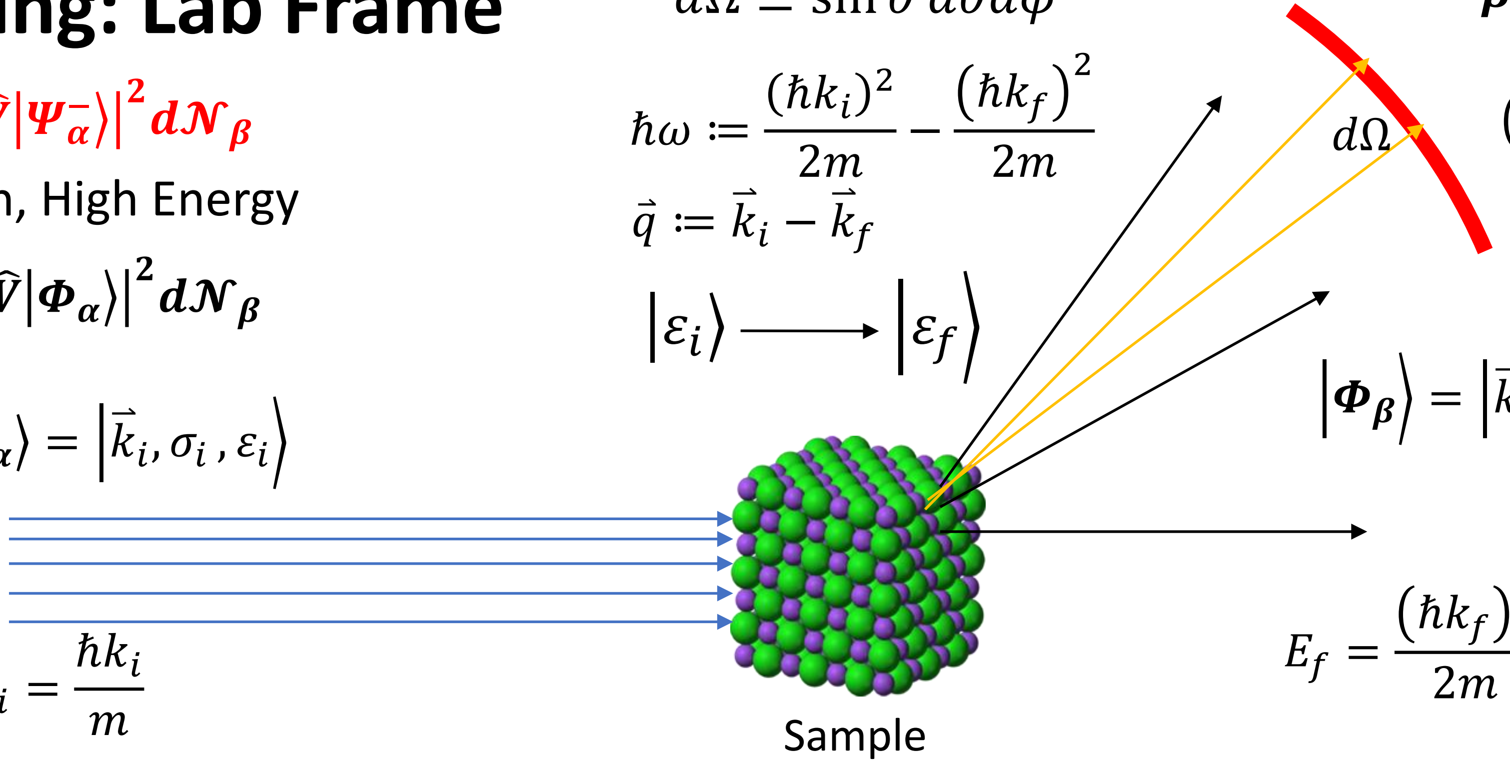
$$\vec{q} \coloneqq \vec{k}_i - \vec{k}_f$$

$$|\varepsilon_i\rangle \longrightarrow |\varepsilon_f\rangle$$

$$|\boldsymbol{\Phi}_\beta\rangle = |\vec{k}_f, \sigma_f, \varepsilon_f\rangle \qquad |\boldsymbol{\Phi}_\alpha\rangle = |\vec{k}_i, \sigma_i, \varepsilon_i\rangle$$

$$\boldsymbol{\alpha} = \boldsymbol{i} \qquad (\vec{k}_i, \sigma_i)$$

$$E_i = \frac{(\hbar k_i)^2}{2m} + \varepsilon_i \qquad u_i = \frac{\hbar k_i}{m} \qquad E_f = \frac{(\hbar k_f)^2}{2m} + \varepsilon_f$$



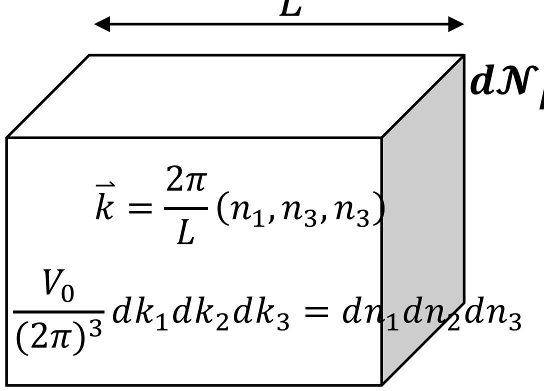

$$d\sigma\left((\vec{k}_i, \sigma_i, \varepsilon_i) \to (\vec{k}_f + d\vec{k}_f, \sigma_f, \varepsilon_f)\right) = \frac{2\pi m V_0}{\hbar^2 k_i} \delta(\varepsilon_f - \varepsilon_i - \hbar\omega) \left| \langle \vec{k}_f, \sigma_f, \varepsilon_f | \hat{V} | \vec{k}_i, \sigma_i, \varepsilon_i \rangle \right|^2 \frac{m k_f V_0}{(2\pi)^3 \hbar^2} d(\hbar\omega) d\Omega$$

$$= \left(\frac{m V_0}{2\pi\hbar^2}\right)^2 \frac{k_f}{k_i} \delta(\varepsilon_f - \varepsilon_i - \hbar\omega) \left| \langle \vec{k}_f, \sigma_f, \varepsilon_f | \hat{V} | \vec{k}_i, \sigma_i, \varepsilon_i \rangle \right|^2 d(\hbar\omega) d\Omega$$

$$\boldsymbol{d\sigma}\left((\vec{\boldsymbol{k}}_i, \boldsymbol{\sigma}_i) \to (\vec{\boldsymbol{k}}_f + \boldsymbol{d}\vec{\boldsymbol{k}}_f, \boldsymbol{\sigma}_f)\right) = \sum_{\varepsilon_i, \varepsilon_f} p(\varepsilon_i) d\sigma\left((\vec{k}_i, \sigma_i, \varepsilon_i) \to (\vec{k}_f, \sigma_f, \varepsilon_f)\right)$$

$$= \left(\frac{m V_0}{2\pi\hbar^2}\right)^2 \frac{k_f}{k_i} \delta(\varepsilon_f - \varepsilon_i - \hbar\omega) \sum_{\varepsilon_i, \varepsilon_f} p(\varepsilon_i) \left| \langle \vec{k}_f, \sigma_f, \varepsilon_f | \hat{V} | \vec{k}_i, \sigma_i, \varepsilon_i \rangle \right|^2 d(\hbar\omega) d\Omega$$

$p(\varepsilon_i)$: Statistical Probability of Sample Initial State Being $|\varepsilon_i\rangle$




$$\boldsymbol{d\mathcal{N}_\beta} = \frac{V_0}{(2\pi)^3} (k_f)^2 d(k_f) d\Omega$$

$$= \frac{V_0}{(2\pi)^3} \frac{m k_f}{\hbar^2} d(\hbar\omega) d\Omega$$

# Master Formula : Scattering Function and Intermediate Function

$$\frac{d\sigma\left((\vec{k}_i,\sigma_i)\rightarrow(\vec{k}_f+d\vec{k}_f,\sigma_f)\right)}{d\Omega d(\hbar\omega)}=\left(\frac{mV_0}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)\sum_{\varepsilon_i,\varepsilon_f}p(\varepsilon_i)\left|\langle\vec{k}_f,\sigma_f,\varepsilon_f|\hat{V}|\vec{k}_i,\sigma_i,\varepsilon_i\rangle\right|^2$$

$$\int d\vec{r}_n\,|\vec{r}_n\rangle\langle\vec{r}_n|=1$$

$$\langle\vec{k}_f,\sigma_f,\varepsilon_f|\hat{V}|\vec{k}_i,\sigma_i,\varepsilon_i\rangle=\int d\vec{r}_n d\vec{r}_n'\langle\vec{k}_f,\sigma_f,\varepsilon_f|\vec{r}_n\rangle\langle\vec{r}_n|\hat{V}|\vec{r}_n'\rangle\langle\vec{r}_n'|\vec{k}_i,\sigma_i,\varepsilon_i\rangle=\int d\vec{r}_n d\vec{r}_n'\langle\vec{k}_f,\sigma_f,\varepsilon_f|\vec{r}_n\rangle V(\vec{r}_n)\delta(\vec{r}_n-\vec{r}_n')\langle\vec{r}_n'|\vec{k}_i,\sigma_i,\varepsilon_i\rangle$$

$$=\int d\vec{r}_n\langle\vec{k}_f,\sigma_f,\varepsilon_f|\vec{r}_n\rangle V(\vec{r}_n)\langle\vec{r}_n|\vec{k}_i,\sigma_i,\varepsilon_i\rangle=\frac{1}{V_0}\int d\vec{r}_n\left\langle\sigma_f,\varepsilon_f\middle|V(\vec{r}_n)e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{r}_n}\middle|\sigma_i,\varepsilon_i\right\rangle$$

$$\langle\vec{r}_n|\vec{k}_i\rangle=\frac{1}{\sqrt{V_0}}e^{i\vec{k}_i\cdot\vec{r}_n}$$

$$=\frac{1}{V_0}\langle\sigma_f,\varepsilon_f|V(\vec{q})|\sigma_i,\varepsilon_i\rangle\qquad V(\vec{q})\equiv\int d\vec{r}_n V(\vec{r}_n)e^{i\vec{q}\cdot\vec{r}_n}\qquad\vec{q}\equiv\vec{k}_i-\vec{k}_f$$

$$\frac{d\sigma}{d\Omega d(\hbar\omega)}=\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)\sum_{\varepsilon_i,\varepsilon_f}p(\varepsilon_i)\left|\langle\sigma_f,\varepsilon_f|V(\vec{q})|\sigma_i,\varepsilon_i\rangle\right|^2$$

$$\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{i(\varepsilon_f-\varepsilon_i)t/\hbar}e^{-i\omega t}\,dt$$

$$\frac{d\sigma}{d\Omega d(\hbar\omega)}=\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{i(\varepsilon_f-\varepsilon_i)t/\hbar}e^{-i\omega t}\,dt\sum_{\varepsilon_i,\varepsilon_f}p(\varepsilon_i)\left\langle\sigma_i,\varepsilon_i\middle|V^\dagger(\vec{q})\middle|\sigma_f,\varepsilon_f\right\rangle\langle\sigma_f,\varepsilon_f|V(\vec{q})|\sigma_i,\varepsilon_i\rangle$$

$$\sum_{\varepsilon_f}|\varepsilon_f\rangle\langle\varepsilon_f|=1$$

$$=\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dte^{-i\omega t}\sum_{\varepsilon_i,\varepsilon_f}p(\varepsilon_i)\left\langle\sigma_i,\varepsilon_i\middle|V^\dagger(\vec{q})\middle|\sigma_f,\varepsilon_f\right\rangle\langle\sigma_f,\varepsilon_f|e^{iH_St/\hbar}V(\vec{q})e^{i-H_St/\hbar}|\sigma_i,\varepsilon_i\rangle$$

$$\langle O\rangle\equiv\sum_{\varepsilon_i}p(\varepsilon_i)\langle\varepsilon_i|\bar{O}|\varepsilon_i\rangle$$

$$=\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dte^{-i\omega t}\sum_{\varepsilon_i}p(\varepsilon_i)\left\langle\sigma_i,\varepsilon_i\middle|V^\dagger(\vec{q})\middle|\sigma_f\right\rangle\langle\sigma_f|e^{iH_St/\hbar}V(\vec{q})e^{i-H_St/\hbar}|\sigma_i,\varepsilon_i\rangle$$

$$V(\vec{q},t)\equiv e^{iH_St/\hbar}V(\vec{q})e^{i-H_St/\hbar}$$

$$=\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dte^{-i\omega t}\left\langle\left\langle\sigma_i\middle|V^\dagger(\vec{q})\middle|\sigma_f\right\rangle\langle\sigma_f|V(\vec{q},t)|\sigma_i\rangle\right\rangle$$

$H_S$: Sample Hamiltonian $\quad H_S|\varepsilon\rangle=\varepsilon|\varepsilon\rangle$

# Master Formula: Scattering Function and Intermediate Function

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\left\langle\left\langle\sigma_i\left|V^\dagger(\vec{q})\right|\sigma_f\right\rangle\left\langle\sigma_f\left|V(\vec{q},t)\right|\sigma_i\right\rangle\right\rangle$$

$$V(\vec{q},t) \equiv e^{iH_S t/\hbar}V(\vec{q})e^{i-H_S t/\hbar}$$

$$p(\varepsilon_i) = \frac{e^{-\frac{\varepsilon_i}{k_B T}}}{\sum_{\varepsilon_i} e^{-\frac{\varepsilon_i}{k_B T}}}$$

$$A(\vec{q},t) \equiv \frac{m}{2\pi\hbar^2}\left\langle\sigma_f\left|V(\vec{q},t)\right|\sigma_i\right\rangle \qquad A^\dagger(\vec{q},t) \equiv \frac{m}{2\pi\hbar^2}\left\langle\sigma_i\left|V^\dagger(\vec{q},t)\right|\sigma_f\right\rangle \qquad A^\dagger(\vec{q},0) \equiv A^\dagger(\vec{q})$$

$$\boldsymbol{\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i}S(\vec{q},\omega)}$$

**Scattering Function** $\boldsymbol{S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t)}$

**Intermediate Scattering Function** $\boldsymbol{I(\vec{q},t) \equiv \left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle}$

Correlation function

Thermal Equilibrium

$$\left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle = \left\langle A^\dagger(\vec{q},t_0)A(\vec{q},t+t_0)\right\rangle$$

$$\left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle = \left\langle A(\vec{q})\, A^\dagger(\vec{q},-t+\frac{i\hbar}{k_B T})\right\rangle$$

$$\left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle^* = \left\langle A^\dagger(\vec{q},t)A(\vec{q})\right\rangle$$

$$V(\vec{r}_n) = V^\dagger(\vec{r}_n) \qquad V(-\vec{q}) = V^\dagger(\vec{q}) \qquad A(-\vec{q},t)_{\sigma_f\to\sigma_i} = A^\dagger(\vec{q},t)_{\sigma_i\to\sigma_f}$$

$$\left\langle A^\dagger(-\vec{q})A(-\vec{q},t)\right\rangle_{\sigma_f\to\sigma_i} = \left\langle A(\vec{q})A^\dagger(\vec{q},t)\right\rangle_{\sigma_i\to\sigma_f}$$

$$\left\langle A^\dagger(\vec{q})A(\vec{q},\infty)\right\rangle = \left\langle A^\dagger(\vec{q})\right\rangle\langle A(\vec{q},\infty)\rangle = \left\langle A^\dagger(\vec{q})\right\rangle\langle A(\vec{q})\rangle = |\langle A(\vec{q})\rangle|^2$$

$$\left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle = |\langle A(\vec{q})\rangle|^2 + \left[\left\langle A^\dagger(\vec{q})A(\vec{q},t)\right\rangle - |\langle A(\vec{q})\rangle|^2\right]$$

Static Dynamic

$$\boldsymbol{S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t) = |\langle A(\vec{q})\rangle|^2\delta(\hbar\omega) + \widetilde{S}(\vec{q},\omega)}$$

Static, Elastic Inelastic, Dynamic

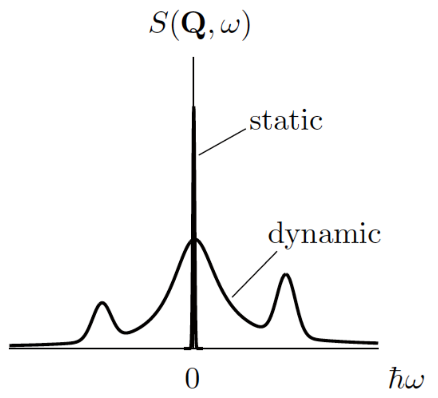



**Fig. 3.4** Schematic of the response function $S(\mathbf{Q},\omega)$. The elastic component arises from static correlations, and the inelastic component arises from dynamic correlations.

# Master Formula: Scattering Function and Intermediate Function

## The Principle of Detailed Balance

$$S(\vec{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle$$

$$S(-\vec{q},-\omega)_{\sigma_f\to\sigma_i} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle A^{\dagger}(-\vec{q})A(-\vec{q},t)\right\rangle$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle A(\vec{q})A^{\dagger}(\vec{q},t)\right\rangle_{\sigma_i\to\sigma_f}$$

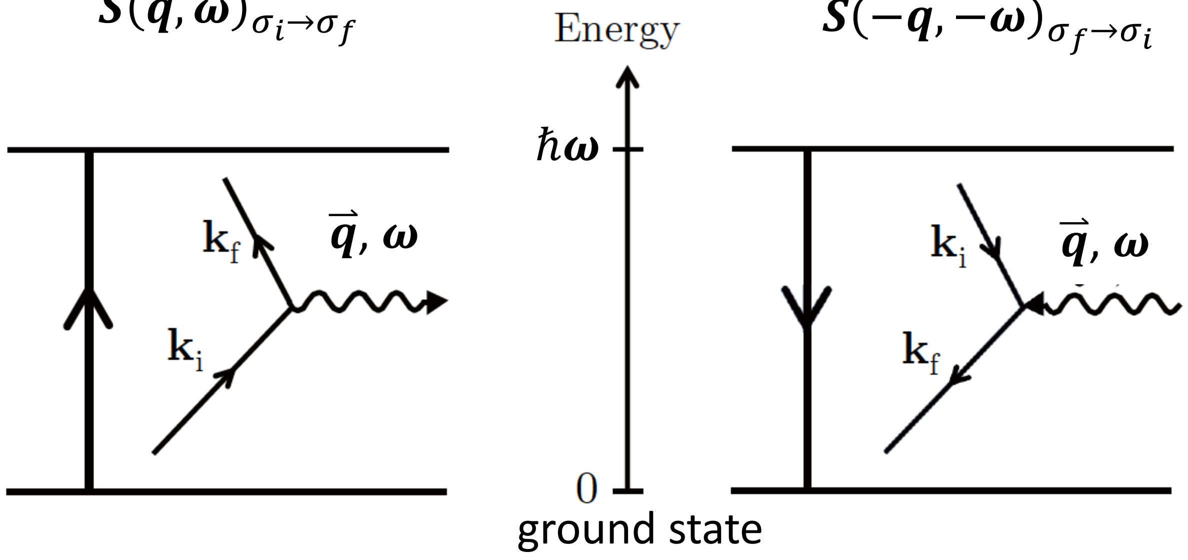
$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle A^{\dagger}(\vec{q})A(\vec{q},-t+\frac{i\hbar}{k_BT})\right\rangle_{\sigma_i\to\sigma_f}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}e^{-\frac{\hbar\omega}{k_BT}}\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle_{\sigma_i\to\sigma_f}$$

$$= e^{-\frac{\hbar\omega}{k_BT}}S(\vec{q},\omega)_{\sigma_i\to\sigma_f}$$

(a) Neutron energy-loss $S(\vec{q},\omega)_{\sigma_i\to\sigma_f}$

(b) Neutron energy-gain $S(-\vec{q},-\omega)_{\sigma_f\to\sigma_i}$




$$\left\langle A^{\dagger}(-\vec{q})A(-\vec{q},t)\right\rangle_{\sigma_f\to\sigma_i} = \left\langle A(\vec{q})A^{\dagger}(\vec{q},t)\right\rangle_{\sigma_i\to\sigma_f}$$

$$\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle = \left\langle A(\vec{q})\, A^{\dagger}(\vec{q},-t+\frac{i\hbar}{k_BT})\right\rangle$$

(1) The population of states with energy $\hbar\omega$ above the ground state is proportional to $e^{-\frac{\hbar\omega}{k_BT}}$

(2) Scattering probability is proportional to the population of initial states

# Master Formula : Structure Factor $S(\vec{q})$

$$S(\vec{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle$$

$$S(\vec{q}) = \int_{-\infty}^{\infty} S(\vec{q},\omega)d(\hbar\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} e^{-i\omega t} d(\hbar\omega)\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle$$

$$= \int_{-\infty}^{\infty} dt\delta(t)\left\langle A^{\dagger}(\vec{q})A(\vec{q},t)\right\rangle = \left\langle A^{\dagger}(\vec{q})A(\vec{q},0)\right\rangle = \left\langle A^{\dagger}(\vec{q})A(\vec{q})\right\rangle = \langle |A(\vec{q})|^2 \rangle$$

If thermal equilibrium,

$$\left\langle A^{\dagger}(\vec{q},t)A(\vec{q},t)\right\rangle = \left\langle A^{\dagger}(\vec{q})A(\vec{q})\right\rangle$$

**Structure Factor** $S(\vec{q})$ (1)represents both static and dynamic correlations

(2) measures equal-time, or instantaneous correlation

$$S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t) = S_{el}(\vec{q},\omega) + \widetilde{S}(\vec{q},\omega)$$

$$S_{el}(\vec{q},\omega) = |\langle A(\vec{q})\rangle|^2\delta(\hbar\omega)$$

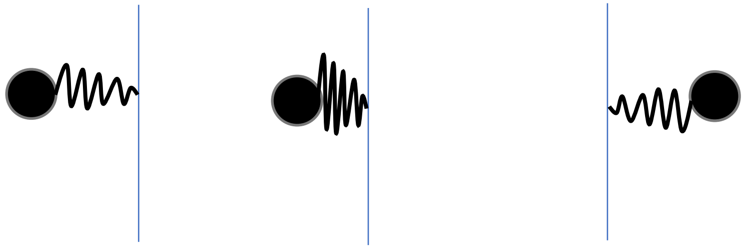
Elastic structure factor $S_{el}(\vec{q}) = |\langle A(\vec{q})\rangle|^2$

$$S(\vec{q}) = S_{el}(\vec{q}) + \widetilde{S}(\vec{q})$$

Dynamic structure factor $\widetilde{S}(\vec{q}) = \left\langle |A(\vec{q})|^2\right\rangle - |\langle A(\vec{q})\rangle|^2$

*e.l. Scattering from nuclei*

$S(\vec{q})$: instantaneous position of nuclei;
$S_{el}(\vec{q})$: time-averaged position of nuclei;



# Neutron-Nuclei Interaction

# Neutron-Nuclei Interaction: Short-Range Neutron-Nuclei Strong Interaction

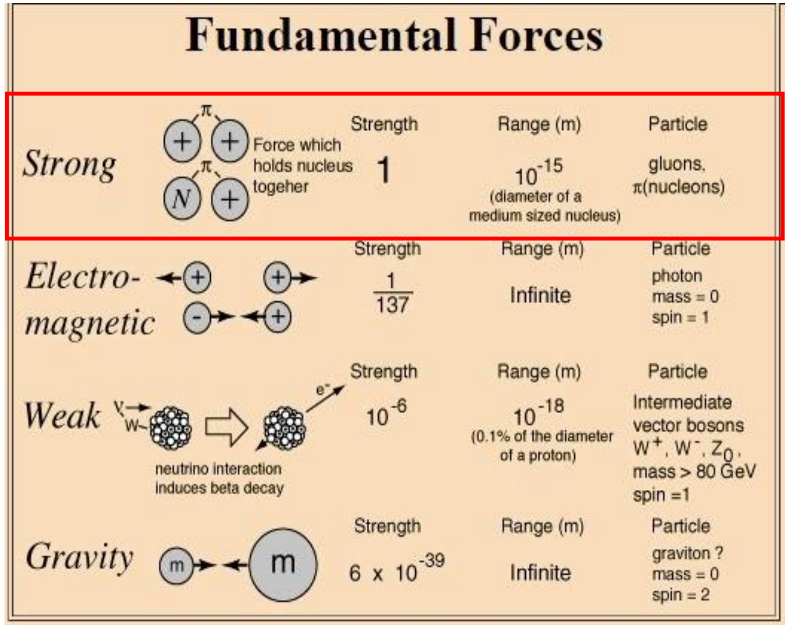
## What we know:

(1) The accurate neutron-nuclei interaction unknow: Many-body interaction

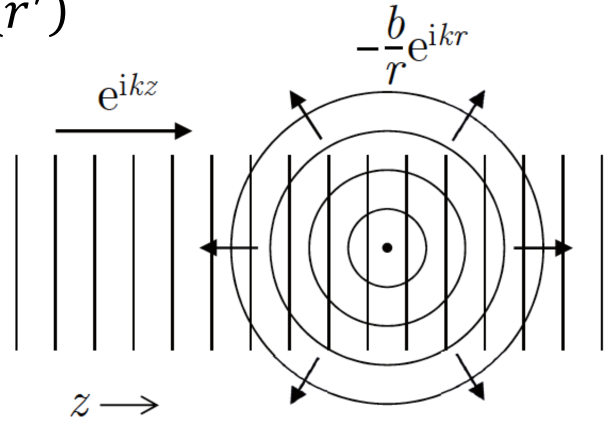
(2) The neutron-nuclei interaction depends both on the number of nucleons in the nuclei and the total spin of this neutron-nuclei system

(3) Strong nuclear force is isotropic

(4) $1\ fm \ll 1\ \text{Å}$, so that intra-nucleus interference ignored and neutron's penetration depth ($10^{-2}m$) in samples is much larger than that of x-ray ($10^{-4} - 10^{-7}m$)




$$\lim_{r\to\infty} \Psi_\alpha^+(\vec{r}) = \Phi_\alpha(\vec{r}) + F(\theta,\varphi)\frac{e^{+ik_\alpha|\vec{r}|}}{|\vec{r}|} \qquad F(\theta,\varphi) \equiv -\frac{1}{4\pi}\int d\vec{r}' e^{-i\vec{k}_\alpha\cdot\vec{r}'}U(\vec{r}')\Psi_\alpha^\pm(\vec{r}')$$




$$\frac{d\sigma}{d\Omega} = |F(\theta,\varphi)|^2$$ $S$-wave dominated $$\lim_{|\vec{k}_\alpha|\to 0}|F(\theta,\varphi)|^2 = b^2 \qquad \sigma = 4\pi b^2$$

Scattering length $b \coloneqq -\lim_{|\vec{k}_\alpha|\to 0} F(\theta,\varphi) = \lim_{|\vec{k}_\alpha|\to 0}\frac{1}{4\pi}\int d\vec{r}' U(\vec{r}')\Psi_\alpha^+(\vec{r}')$

# Neutron-Nuclei Interaction: Fermi Pseudopotential

## Born Approximation???

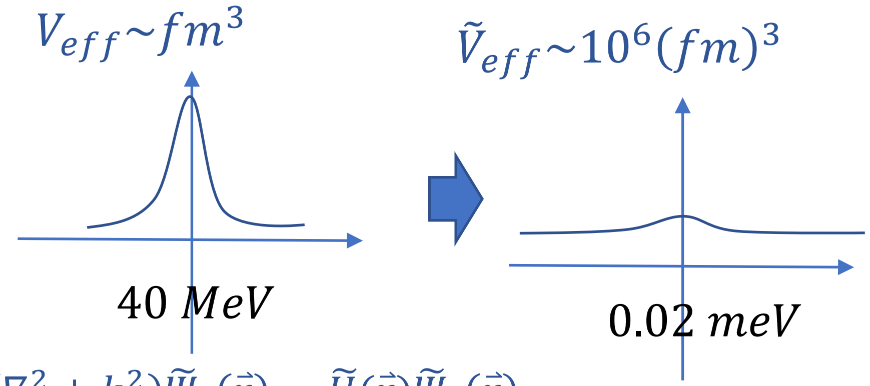
$$b_c = \lim_{|\vec{k}_\alpha| \to 0} \frac{1}{4\pi} \int d\vec{r}' U(\vec{r}') \Psi_\alpha^+(\vec{r}')$$

$$U(\boldsymbol{r}) \equiv \frac{2m}{\hbar^2} V(\boldsymbol{r})$$

| | Energy (meV) | Temp (K) | Wavelength (nm) |
|---|---|---|---|
| Cold | 0.1 – 10 | 1 – 120 | 0.4 – 3 |
| Thermal | 5 – 100 | 60 – 1000 | 0.1 – 0.4 |
| Hot | 100 – 500 | 1000 – 6000 | 0.04 – 0.1 |

$$\frac{\int_{V_{eff}} V(\vec{r}') d\vec{r}'}{V_{eff}} \sim 40\ MeV \gg E_n$$

Born Approximation does not work!




**Fermi Approximation** $\tilde{U}(\boldsymbol{r}) \coloneqq 10^{-6} U(10^{-2} \boldsymbol{r})$ $\Psi_\alpha^+(\boldsymbol{r}) \to \tilde{\Psi}_\alpha^+(\boldsymbol{r})$

$$b_c = \lim_{|\vec{k}_\alpha| \to 0} \frac{1}{4\pi} \int d\vec{r}' U(\vec{r}') \Psi_\alpha^+(\vec{r}') = \lim_{|\vec{k}_\alpha| \to 0} \frac{1}{4\pi} \int d\vec{r}'\ \tilde{U}(\vec{r}') \tilde{\Psi}_\alpha^+(\vec{r}')$$

$$(\nabla^2 + k_\alpha^2) \tilde{\Psi}_\alpha(\vec{r}) = \tilde{U}(\vec{r}) \tilde{\Psi}_\alpha(\vec{r})$$

Born Approximation! $\tilde{\Psi}_\alpha^\pm(\vec{r}) \approx \Phi_\alpha(\vec{r}) = e^{i\vec{k}_\alpha \cdot \vec{r}}$

$$\tilde{\Psi}_\alpha^\pm(\vec{r}) = \Phi_\alpha(\vec{r}) + \int d\vec{r}' G_\pm(\vec{r} - \vec{r}')\ \tilde{U}(\vec{r}') \tilde{\Psi}_\alpha^\pm(\vec{r}')$$

$$b_c = \lim_{|\vec{k}_\alpha| \to 0} \frac{1}{4\pi} \int d\vec{r}'\ \tilde{U}(\vec{r}') \tilde{\Psi}_\alpha^+(\vec{r}') \approx \lim_{|\vec{k}_\alpha| \to 0} \frac{1}{4\pi} \int d\vec{r}'\ \tilde{U}(\vec{r}') e^{i\vec{k}_\alpha \cdot \vec{r}'} = \frac{1}{4\pi} \int d\vec{r}'\ \tilde{U}(\vec{r}')$$

Since still $100\ fm \ll 1\ \text{Å}$, $\tilde{U}(\vec{r}) \approx a\delta(\vec{r})$ $b_c = \frac{1}{4\pi} \int d\vec{r}' a\delta(\vec{r}) = \frac{a}{4\pi}$ $\tilde{U}(\vec{r}) = 4\pi b_c \delta(\vec{r}) = \frac{2m}{\hbar^2} V(\boldsymbol{r})$

**Fermi Pseudopotential** $\boldsymbol{V(\vec{r}) = \frac{2\pi\hbar^2}{m} b_c \delta(\vec{r})}$

*X.-L. Zhou, S.-H. Chen, Physics Reports 257 (1995) 223-348*

# Neutron-Nuclei Interaction: Fermi Contact Interaction

$$V(\vec{r}) = \frac{2\pi\hbar^2}{m} b_c \delta(\vec{r}) + 2\Delta \vec{I} \cdot \vec{s}\delta(\vec{r}) = \frac{2\pi\hbar^2}{m}\hat{b}_r \delta(\vec{r}) \qquad \hat{b}_r = b_c + 2\Delta \vec{I} \cdot \vec{s}$$

$\Delta$ is a certain constant

$b_c$: coherent scattering length

$\hat{\vec{J}} = \hat{\vec{I}} + \hat{\vec{s}} \qquad \hat{J}^2 = \hat{I}^2 + \hat{s}^2 + 2\hat{\vec{I}} \cdot \hat{\vec{s}} \qquad \hat{J}^2, \hat{J}_z, \hat{I}^2, \hat{s}^2$ commute with each other and share common eigenstates $\{|J, J_z, I, s\rangle\}$

$$[\hat{J}^2, \hat{J}_z, \hat{I}^2, \hat{s}^2]|J, J_z, I, s\rangle = [J(J+1)\hbar, J_z\hbar, I(I+1)\hbar, s(s+1)\hbar]|J, J_z, I, s\rangle$$

$s = \frac{1}{2} \qquad J = I + \frac{1}{2}, I - \frac{1}{2} \qquad J_z = -J, -J+1, \ldots J$

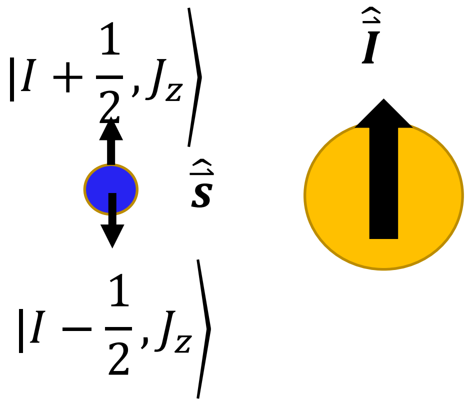
$\left|I - \frac{1}{2}, J_z\right\rangle \equiv \left|I - \frac{1}{2}, J_z, I, s = \frac{1}{2}\right\rangle$

$\left|I + \frac{1}{2}, J_z\right\rangle \equiv \left|I + \frac{1}{2}, J_z, I, s = \frac{1}{2}\right\rangle$

$$2\hat{\vec{I}} \cdot \hat{\vec{s}} = \hat{J}^2 - \hat{I}^2 - \hat{s}^2 = J(J+1)\hbar - I(I+1)\hbar - s(s+1)\hbar$$

$2\hat{\vec{I}} \cdot \hat{\vec{s}}\left|I + \frac{1}{2}, J_z\right\rangle = I\left|I + \frac{1}{2}, J_z\right\rangle \qquad 2\left(I + \frac{1}{2}\right) + 1 = 2I + 2$-fold degenerate

$2\hat{\vec{I}} \cdot \hat{\vec{s}}\left|I - \frac{1}{2}, J_z\right\rangle = -(I+1)\left|I - \frac{1}{2}, J_z\right\rangle \qquad 2\left(I - \frac{1}{2}\right) + 1 = 2I$–fold degenerate




Define $b_{r+}$, $b_{r-}$, $b_i$ Incoherent scattering length $b_i := \sqrt{\langle \hat{b}_r^{\,2}\rangle - \langle \hat{b}_r\rangle^2}$

$\hat{b}_r\left|I + \frac{1}{2}, J_z\right\rangle = b_{r+}\left|I + \frac{1}{2}, J_z\right\rangle$

$\hat{b}_r\left|I - \frac{1}{2}, J_z\right\rangle = b_{r-}\left|I - \frac{1}{2}, J_z\right\rangle$

$\Rightarrow$

$$b_c = \frac{1}{2I+1}[(I+1)b_{r+} + I b_{r-}] \qquad \Delta = \frac{1}{2I+1}[b_{r+} - b_{r-}]$$

$$\langle \hat{b}_r \rangle := b_{r+} \cdot \frac{2I+2}{4I+2} + b_{r-} \cdot \frac{2I}{4I+2} = b_c$$

$$b_i = \sqrt{b_{r+}^2 \cdot \frac{2I+2}{4I+2} + b_{r-}^2 \cdot \frac{2I}{4I+2} - b_c^2} = \frac{\sqrt{I(I+1)}\,|b_{r+} - b_{r-}|}{2I+1}$$

$$\hat{b}_r = b_c - \frac{b_i}{\sqrt{I(I+1)}} 2\vec{I} \cdot \vec{s}$$

# Neutron-Nuclei Interaction: Neutron Absorption and Absorption Cross Section

(1) Absorption mechanism: four types of nuclear reaction $(n,\gamma),(n,fission),(n,p)\ and(n,\alpha)$

(2) Only $^4He$ and $^3H$ has no neutron absorption; many light nuclides have very weak thermal absorption

(3) Heavy nuclides tend to have more significant neutron absorption than light ones.

(4) $(n,\gamma)$ is the dominant mechanism for thermal neutron absorption

$$U(\vec{\boldsymbol{r}})=U_r(\vec{\boldsymbol{r}})+\boldsymbol{i}U_i(\vec{\boldsymbol{r}}) \qquad V_r(\vec{\boldsymbol{r}})\approx \mathbf{42MeV},\ V_i(\vec{\boldsymbol{r}})\approx \mathbf{2MeV} \qquad U(\vec{\boldsymbol{r}})\equiv\frac{2m}{\hbar^2}(V_r(\vec{\boldsymbol{r}})+\boldsymbol{i}V_i(\vec{\boldsymbol{r}}))$$

$$b=b_r-ib_a \qquad b=\lim_{|\vec{k}_\alpha|\to 0}\frac{1}{4\pi}\int d\vec{r}'U_r(\vec{r}')\Psi_\alpha^+(\vec{r}') \qquad b_a=-\lim_{|\vec{k}_\alpha|\to 0}\frac{1}{4\pi}\int d\vec{r}'U_i(\vec{r}')\Psi_\alpha^+(\vec{r}')$$

$$(\nabla^2+k_\alpha^2)\Psi_\alpha(\vec{r})=U(\vec{r})\Psi_\alpha(\vec{r}) \qquad \int d\vec{r}\,\Psi_\alpha^\dagger(\vec{r})(\nabla^2+k_\alpha^2)\Psi_\alpha(\vec{r})=\int d\vec{r}\,\Psi_\alpha^\dagger(\vec{r})U(\vec{r})\Psi_\alpha(\vec{r})$$

$$\int d\vec{r}\,\Psi_\alpha^\dagger(\vec{r})\nabla^2\Psi_\alpha(\vec{r})=\int d\vec{r}\,U(\vec{r})|\Psi_\alpha(\vec{r})|^2-\int d\vec{r}\,k_\alpha^2|\Psi_\alpha(\vec{r})|^2$$

$$\Psi_\alpha^\dagger(\vec{r})\nabla^2\Psi_\alpha(\vec{r})=\nabla\cdot\left(\Psi_\alpha^\dagger(\vec{r})\nabla\Psi_\alpha(\vec{r})\right)-\left(\nabla\cdot\Psi_\alpha^\dagger(\vec{r})\right)\left(\nabla\Psi_\alpha(\vec{r})\right)$$

$$\int d\vec{r}\left[\nabla\cdot\left(\Psi_\alpha^\dagger(\vec{r})\nabla\Psi_\alpha(\vec{r})\right)-\left(\nabla\cdot\Psi_\alpha^\dagger(\vec{r})\right)\left(\nabla\Psi_\alpha(\vec{r})\right)\right]=\int d\vec{r}\,U(\vec{r})|\Psi_\alpha(\vec{r})|^2-\int d\vec{r}\,k_\alpha^2|\Psi_\alpha(\vec{r})|^2$$

$$\vec{j}[\Psi]=\frac{-i\hbar}{2m}\left[\Psi^\dagger\nabla\Psi-\Psi\nabla\Psi^\dagger\right]$$

$$\int d\vec{S}\cdot\Psi_\alpha^\dagger(\vec{r})\nabla\Psi_\alpha(\vec{r})=\int d\vec{r}\,U(\vec{r})|\Psi_\alpha(\vec{r})|^2+\int d\vec{r}\,[|\nabla\Psi_\alpha(\vec{r})|^2-k_\alpha^2|\Psi_\alpha(\vec{r})|^2]$$

$$\Phi_\alpha(\vec{r})=e^{i\vec{k}_\alpha\cdot\vec{r}}$$

$$\int d\vec{S}\cdot\vec{j}[\Psi]=\frac{-i\hbar}{2m}\int d\vec{r}\left[U(\vec{r})-U^\dagger(\vec{r})\right]|\Psi_\alpha(\vec{r})|^2=\frac{\hbar}{m}\int d\vec{r}\,U_i(\vec{\boldsymbol{r}})|\Psi_\alpha(\vec{r})|^2$$

$$\vec{j}[\Phi_\alpha(\vec{r})]=\frac{-i\hbar}{2m}\left[\Phi_\alpha(\vec{r})^\dagger\nabla\Phi_\alpha(\vec{r})-\Phi_\alpha(\vec{r})\nabla\Phi_\alpha(\vec{r})^\dagger\right]=\frac{\hbar\vec{k}_\alpha}{m}$$

$$\boldsymbol{\sigma_a}=\frac{-\int d\vec{S}\cdot\vec{j}[\Psi]}{|\vec{j}[\Phi_\alpha(\vec{r})]|}=-\frac{1}{k_\alpha}\int d\vec{r}\,U_i(\vec{\boldsymbol{r}})|\Psi_\alpha(\vec{r})|^2\approx-\frac{1}{k_\alpha}\int d\vec{r}\,U_i(\vec{\boldsymbol{r}})|\Phi_\alpha(\vec{r})|^2=-\frac{1}{k_\alpha}\int d\vec{r}\,U_i(\vec{\boldsymbol{r}})=\frac{4\pi b_a}{k_\alpha}$$

# Neutron-Nuclei Interaction: Material Medium

$$V(\vec{q}) \equiv \int d\vec{r} V(\vec{r}) e^{i\vec{q}\cdot\vec{r}}$$

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k_f}{k_i} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle \left\langle \sigma_i \left| V^\dagger(\vec{q}) \right| \sigma_f \right\rangle \left\langle \sigma_f \left| V(\vec{q},t) \right| \sigma_i \right\rangle \right\rangle$$

$$V(\vec{q},t) \equiv e^{iH_S t/\hbar} V(\vec{q}) e^{-iH_S t/\hbar}$$

$$\boldsymbol{V(\vec{r}) = \frac{2\pi\hbar^2}{m} \sum_j \hat{b}_j \delta(\vec{r} - \vec{r}_j)}$$

$$\boldsymbol{\hat{b}_j \equiv \hat{b}_{j;r} + i\hat{b}_{j;a} = b_{j;c} - \frac{b_{j;i}}{\sqrt{I_j(I_j+1)}} 2\vec{I}_j \cdot \vec{s} + ib_{j;a}}$$

$$\hat{A}(t) \equiv e^{\frac{iH_S t}{\hbar}} \hat{A} e^{\frac{-iH_S t}{\hbar}}$$

**Scattering Length Density** $\boldsymbol{\rho_{SL}(\vec{r}) = \sum_j \hat{b}_j \delta(\vec{r} - \vec{r}_j)}$

$$e^{\frac{iH_S t}{\hbar}} \hat{A}^n e^{\frac{-iH_S t}{\hbar}} = e^{\frac{iH_S t}{\hbar}} \hat{A} e^{\frac{-iH_S t}{\hbar}} e^{\frac{iH_S t}{\hbar}} \hat{A} e^{\frac{-iH_S t}{\hbar}} \ldots e^{\frac{iH_S t}{\hbar}} \hat{A} e^{\frac{-iH_S t}{\hbar}} = \left[\hat{A}(t)\right]^n$$

$\boldsymbol{\rho_{SL}(\vec{r}) = \sum_M \hat{b}_M \rho_M(\vec{r})}$; $\boldsymbol{\rho_M(\vec{r})}$**: density of type M nucleus**

$$e^{\frac{iH_S t}{\hbar}} e^{i\vec{q}\cdot\vec{r}_j} e^{\frac{-iH_S t}{\hbar}} = \sum_{n=0}^{\infty} e^{\frac{iH_S t}{\hbar}} \frac{(i\vec{q}\cdot\vec{r}_j)^n}{n!} e^{\frac{-iH_S t}{\hbar}} = \sum_{n=0}^{\infty} \frac{(i\vec{q}\cdot\vec{r}_j(t))^n}{n!} = e^{i\vec{q}\cdot\vec{r}_j(t)}$$

$$V(\vec{q}) \equiv \int d\vec{r} V(\vec{r}) e^{i\vec{q}\cdot\vec{r}} = \frac{2\pi\hbar^2}{m} \sum_j \hat{b}_j e^{i\vec{q}\cdot\vec{r}_j}$$

$$V(\vec{q},t) \equiv e^{\frac{iH_S t}{\hbar}} V(\vec{q}) e^{\frac{-iH_S t}{\hbar}} = \frac{2\pi\hbar^2}{m} \sum_j e^{\frac{iH_S t}{\hbar}} \hat{b}_j e^{i\vec{q}\cdot\vec{r}_j} e^{\frac{-iH_S t}{\hbar}} = \frac{2\pi\hbar^2}{m} \sum_j e^{\frac{iH_S t}{\hbar}} \hat{b}_j e^{\frac{-iH_S t}{\hbar}} e^{\frac{iH_S t}{\hbar}} e^{i\vec{q}\cdot\vec{r}_j} e^{\frac{-iH_S t}{\hbar}} = \frac{2\pi\hbar^2}{m} \sum_j \hat{b}_j(t) e^{i\vec{q}\cdot\vec{r}_j(t)}$$

$$\boldsymbol{\vec{r}_j = \vec{r}_j(0)}$$

$$\hat{\beta}_j = \hat{\beta}_j(0)$$

Define $\hat{\beta}_j(t) \coloneqq \left\langle \sigma_f \left| \hat{b}_j(t) \right| \sigma_i \right\rangle$

$$\left\langle \sigma_f \left| V(\vec{q},t) \right| \sigma_i \right\rangle = \frac{2\pi\hbar^2}{m} \sum_j \hat{\beta}_j(t) e^{i\vec{q}\cdot\vec{r}_j(t)}$$

$$\boldsymbol{I(\vec{q},t) = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left\langle \left\langle \sigma_i \left| V^\dagger(\vec{q}) \right| \sigma_f \right\rangle \left\langle \sigma_f \left| V(\vec{q},t) \right| \sigma_i \right\rangle \right\rangle = \sum_{j,l} \left\langle e^{-i\vec{q}\cdot\vec{r}_j} \hat{\beta}_j^\dagger \hat{\beta}_l(t) e^{i\vec{q}\cdot\vec{r}_l(t)} \right\rangle}$$

$$\boldsymbol{\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i} S(\vec{q},\omega)} \qquad \boldsymbol{S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t)}$$

# Neutron-Nuclei Interaction: Coherent and Incoherent Cross Section

**Assumptions:**

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i} S(\vec{q},\omega) \qquad S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t) \qquad I(\vec{q},t) = \sum_{j,l}\left\langle e^{-i\vec{q}\cdot\vec{r}_j}\hat{\beta}_j^\dagger \hat{\beta}_l(t) e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle$$

$$\hat{\beta}_j(t) \coloneqq \langle \sigma_f | \hat{b}_j(t) | \sigma_i \rangle; \; \hat{b}_j(t) \equiv e^{\frac{iH_S t}{\hbar}} \hat{b}_j e^{\frac{-iH_S t}{\hbar}}$$

$$\hat{b}_j \equiv \hat{b}_{j;r} + i\hat{b}_{j;a} = b_{j;c} - \frac{b_{j;i}}{\sqrt{I_j(I_j+1)}} 2\vec{I}_j \cdot \vec{s} + i b_{j;a}$$

$$\langle O \rangle \equiv \sum_{\varepsilon_i} p(\varepsilon_i)\langle \varepsilon_i | \bar{O} | \varepsilon_i \rangle \qquad p(\varepsilon_i) = \frac{e^{-\frac{\varepsilon_i}{k_B T}}}{\sum_{\varepsilon_i} e^{-\frac{\varepsilon_i}{k_B T}}}$$

$\bar{O}$: averaged over different isotopes and nuclear spin states

(1) The motion of atoms is decoupled from the internal states of nuclei(**characterized by scattering length**)

$$I(\vec{q},t) = \sum_{j,l}\left\langle e^{-i\vec{q}\cdot\vec{r}_j}\hat{\beta}_j^\dagger \hat{\beta}_l(t) e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle = \sum_{j,l}\left\langle \hat{\beta}_j^\dagger \hat{\beta}_l(t)\right\rangle \left\langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle$$

**Counterexamples**: strong nuclei-nuclei exchange interactions; large isotopic difference

(2) Nuclear spin dynamics are sufficiently slow relative to the neutron-nuclei interaction

$$\left\langle \hat{\beta}_j^\dagger \hat{\beta}_l(t)\right\rangle = \left\langle \hat{\beta}_j^\dagger \hat{\beta}_l(0)\right\rangle = \left\langle \hat{\beta}_j^\dagger \hat{\beta}_l\right\rangle$$

(3) Different isotopes and/or spin states are distributed **randomly** among the sites for a given atomic species

$$\left\langle \hat{\beta}_j^\dagger \hat{\beta}_l\right\rangle = \overline{\hat{\beta}_j^\dagger \hat{\beta}_l} = \begin{cases} \overline{|\hat{\beta}_l|^2} & j = l \\ \bar{\hat{\beta}}_j^\dagger \bar{\hat{\beta}}_l & j \neq l \end{cases}$$

$$I(\vec{q},t) = \sum_{j\neq l} \bar{\hat{\beta}}_j^\dagger \bar{\hat{\beta}}_l \left\langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle + \sum_l \overline{|\hat{\beta}_l|^2}\left\langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle$$

$$= \sum_{j,l} \bar{\hat{\beta}}_j^\dagger \bar{\hat{\beta}}_l \left\langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle + \sum_l \left[\overline{|\hat{\beta}_l|^2} - |\bar{\hat{\beta}}_l|^2\right]\left\langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_l(t)}\right\rangle$$

$$I_{coh}(\vec{q},t) \qquad I_{inc}(\vec{q},t)$$

**Counterexamples**: isotopically labelled systems; strong nuclei-nuclei exchange interactions; nuclear spin-ordered system

# Neutron-Nuclei Interaction: Unpolarized Neutron Case

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i} S(\vec{q},\omega) \qquad S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t)$$

$$I(\vec{q},t) = \sum_{j,l} \bar{\hat{\beta}}_j^{\dagger} \bar{\hat{\beta}}_l \langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)} \rangle + \sum_l \left[ \overline{|\hat{\beta}_l|^2} - |\bar{\hat{\beta}}_l|^2 \right] \langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_l(t)} \rangle$$

$$\left[\frac{d\sigma}{d\Omega d(\hbar\omega)}\right]_{unpol} = \sum_{\sigma_i\sigma_f} \frac{d\sigma}{d\Omega d(\hbar\omega)}$$

$$\hat{\beta}_j = \langle \sigma_f | \hat{b}_j | \sigma_i \rangle \rightarrow \hat{b}_j \rightarrow \langle \hat{b}_j \rangle_{iso;spin} = \bar{b}_j$$

$$\left[\frac{d\sigma}{d\Omega d(\hbar\omega)}\right]_{unpol;coh} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{j,l} \bar{b}_j^* \bar{b}_l \int_{-\infty}^{\infty} dt e^{-i\omega t} \langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)} \rangle$$

$$\left[\frac{d\sigma}{d\Omega d(\hbar\omega)}\right]_{unpol;inc} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l} \frac{(\sigma_{inc})_l}{4\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} \langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_l(t)} \rangle$$

$$(\sigma_{inc})_l \equiv \left[ \overline{|b_l|^2} - |\bar{b}_l|^2 \right]$$

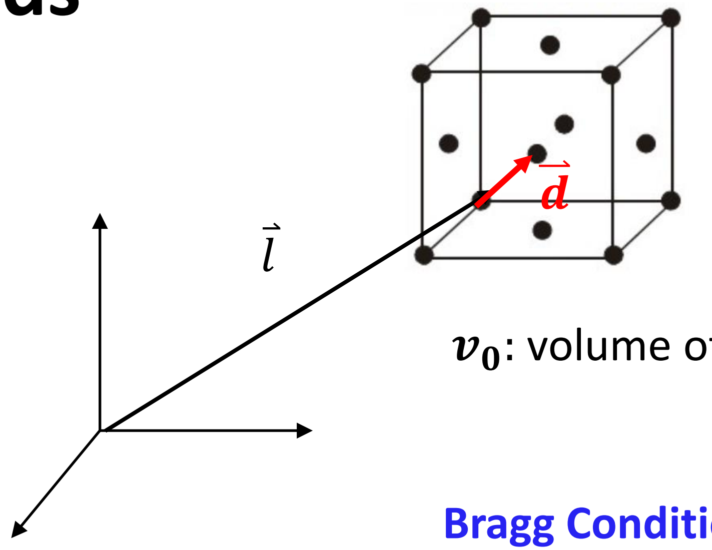
# Neutron-Nuclei Interaction: Crystalline Solids

$$\vec{r}_{ld}(t) = \vec{l} + \vec{d} + \vec{u}_{ld}(t)$$

$$\sum_{j,l} \overline{b}_j^* \overline{b}_l \langle e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)} \rangle = \left\langle \sum_{j,l} \overline{b}_j^* \overline{b}_l e^{-i\vec{q}\cdot\vec{r}_j} e^{i\vec{q}\cdot\vec{r}_l(t)} \right\rangle$$

$$= \left\langle \sum_{\vec{l},\vec{d},\vec{l}',\vec{d}'} \overline{b}_{\vec{d}'}^* \overline{b}_{\vec{d}} e^{-i\vec{q}\cdot(\vec{l}'+\vec{d}')} e^{i\vec{q}\cdot\vec{l}+\vec{d}+\vec{u}_{ld}(t)} \right\rangle$$

$$= N \sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} \sum_{\vec{d},\vec{d}'} \overline{b}_{\vec{d}'}^* \overline{b}_{\vec{d}} e^{i\vec{q}\cdot(\vec{d}-\vec{d}')} \left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)} \right\rangle$$




$v_0$: volume of unit cell

**Bragg Condition**

$$\sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} = \frac{(2\pi)^3}{v_0} \sum_{\vec{G}} \delta(\vec{q} - \vec{G})$$

$$\left[\frac{d\sigma}{d\Omega d(\hbar\omega)}\right]_{unpol;coh} = \frac{k_f}{k_i} \frac{N}{2\pi\hbar} \sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} \sum_{\vec{d},\vec{d}'} \overline{b}_{\vec{d}'}^* \overline{b}_{\vec{d}} e^{i\vec{q}\cdot(\vec{d}-\vec{d}')} \int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)} \right\rangle$$

$$V = e^{i\vec{q}\cdot\vec{u}_{ld}(t)}$$

$$U = -i\vec{q}\cdot\vec{u}_{0\vec{d}'}$$

$$\left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)} \right\rangle = \langle e^U e^V \rangle = e^{-W_d - W_{d'}} e^{\langle UV \rangle} = e^{-W_d - W_{d'}} \left[ 1 + \langle UV \rangle + \frac{1}{2!} \langle UV \rangle^2 \right]$$

elastic One-phonon two-phonon

$$W_d = \frac{1}{2} \left\langle (\vec{q}\cdot\vec{u}_d)^2 \right\rangle$$

$$\left[\frac{d\sigma}{d\Omega d(\hbar\omega)}\right]_{unpol;inc} = \frac{k_f}{k_i} \frac{N}{2\pi\hbar} \sum_{d} \frac{(\sigma_{inc})_d}{4\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle e^{-i\vec{q}\cdot\vec{u}_{\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_d(t)} \right\rangle$$

$$(\sigma_{inc})_d \equiv \left[ \overline{|b_d|^2} - \left|\overline{b}_d\right|^2 \right]$$

# Magnetic Interaction

# Magnetic Interaction : Dipole-Dipole Interaction

$$v_M(\vec{R}) = -\vec{\mu}_n \cdot \vec{B}(\vec{R}) \qquad \vec{\mu}_n \equiv -2\gamma_n\mu_N\vec{s}_n$$

Neutron gyromagetic ratio $\gamma_n = 1.913$

Nuclear magneton: $\mu_N = \frac{e\hbar}{2m_p}$ $\qquad m_p$: mass of proton

Bohr magneton $\mu_B = \frac{e\hbar}{2m_e}$

$$\vec{B}(\vec{r}) = \vec{B}_S(\vec{R}) + \vec{B}_L(\vec{R}) \qquad \vec{R} = \vec{r}_n - \vec{r}_e \qquad \vec{\mu}_e \equiv -2\mu_B\vec{s}$$

$$\vec{B}_S(\vec{R}) = \frac{\mu_0}{4\pi}\nabla\times\left(\frac{\vec{\mu}_e\times\vec{R}}{r^3}\right) = -2\mu_B\frac{\mu_0}{4\pi}\nabla\times\left(\frac{\vec{s}\times\vec{R}}{r^3}\right) \qquad \vec{B}_L(\vec{R}) = \frac{\mu_0}{4\pi}\frac{e\vec{v}_e\times\vec{R}}{r^3} = -2\mu_B\frac{\mu_0}{4\pi}\frac{1}{\hbar}\frac{\vec{p}\times\vec{R}}{r^3}$$

$$\boldsymbol{V_M(\vec{r}) = \sum_j v_{M;j} = 2\gamma_n\mu_N\vec{s}_n\cdot\sum_j \vec{B}_j(\vec{r})}$$

$$\boldsymbol{= -\frac{\mu_0}{\pi}\gamma_n\mu_B\mu_N\vec{s}_n\cdot\sum_j\left[\nabla\times\left(\frac{\vec{s}_j\times\vec{R}_j}{R_j^{\,3}}\right)+\frac{1}{\hbar}\frac{\vec{p}_j\times\vec{R}_j}{R_j^{\,3}}\right]} \qquad \vec{R}_j = \vec{r}-\vec{r}_j$$

$$\vec{B}_{S;j}(\vec{q}) \equiv -2\mu_B\frac{\mu_0}{4\pi}\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\nabla\times\left(\frac{\vec{s}_j\times\vec{R}_j}{R_j^{\,3}}\right) = -2\mu_B\mu_0\{\hat{q}\times(\vec{s}_j\times\hat{q})\}e^{i\vec{q}\cdot\vec{r}_j}$$

$$\vec{B}_{L;j}(\vec{q}) \equiv -2\mu_B\frac{\mu_0}{4\pi}\int d\vec{r}\frac{1}{\hbar}\frac{\vec{p}_j\times\vec{R}_j}{R_j^{\,3}}e^{i\vec{q}\cdot\vec{r}} = -2\mu_B\mu_0\frac{i}{\hbar q}e^{i\vec{q}\cdot\vec{r}_j}(\vec{p}_j\times\hat{q})$$

$$V_M(\vec{q}) \equiv \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}V_M(\vec{r}) = 2\gamma_n\mu_N\vec{s}_n\cdot\sum_j\left[\vec{B}_{S;j}(\vec{q})+\vec{B}_{L;j}(\vec{q})\right]$$

$$= -4\gamma_n\mu_0\mu_B\mu_N\vec{s}_n\cdot\sum_j e^{i\vec{q}\cdot\vec{r}_j}\left[\hat{q}\times(\vec{s}_j\times\hat{q})+\frac{i}{\hbar q}(\vec{p}_j\times\hat{q})\right]$$

$$V(\vec{q}) \equiv \int d\vec{r}V(\vec{r})e^{i\vec{q}\cdot\vec{r}} = \frac{2\pi\hbar^2}{m}\sum_j\hat{b}_je^{i\vec{q}\cdot\vec{r}_j}$$

$$|V_M(\vec{q})| \propto 2\gamma_n\mu_0\mu_B\mu_N = 2\gamma_n\mu_0\frac{e\hbar}{2m_e}\frac{e\hbar}{2m_p} = \frac{\gamma_n\mu_0e^2\hbar^2}{2m_em_p} \qquad |V_N(\vec{q})| \propto \frac{2\pi\hbar^2}{m}b_c$$

$$\boldsymbol{\frac{|V_M(\vec{q})|}{|V_N(\vec{q})|} \sim \frac{3.075fm}{b_c} \sim 1}$$

# Magnetic Interaction : Dipole-Dipole Interaction

$$[\vec{q}\cdot\vec{r}_j, \vec{p}_j \times \hat{q}] = 0$$

$$V_M(\vec{q}) = -4\gamma_n\mu_0\mu_B\mu_N\vec{s}_n \cdot \sum_j e^{i\vec{q}\cdot\vec{r}_j}\left[\hat{q}\times(\vec{s}_j\times\hat{q}) + \frac{i}{\hbar q}(\vec{p}_j\times\hat{q})\right]$$

Define Spin Magnetization Density $M_S(\vec{r}) = -2\mu_B\sum_j \vec{s}_j\delta(\vec{r}-\vec{r}_j)$

$$\vec{M}_S(\vec{q}) := \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{M}_S(\vec{r}) = -2\mu_B\sum_j e^{i\vec{q}\cdot\vec{r}_j}\vec{s}_j$$

$$\sum_j e^{i\vec{q}\cdot\vec{r}_j}\frac{i}{\hbar q}(\vec{p}_j\times\hat{q}) = \frac{i}{2\hbar q}\sum_j[e^{i\vec{q}\cdot\vec{r}_j}(\vec{p}_j\times\hat{q}) + (\vec{p}_j\times\hat{q})e^{i\vec{q}\cdot\vec{r}_j}] = \frac{-i}{2\hbar q}\hat{q}\times\sum_j[e^{i\vec{q}\cdot\vec{r}_j}\vec{p}_j + \vec{p}_j e^{i\vec{q}\cdot\vec{r}_j}] = \frac{-i}{2\hbar q}\hat{q}\times\frac{2m_e}{e}\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{J}_L(\vec{r})$$

Orbital electric current-density operator $\vec{J}_L(\vec{r}) \equiv \frac{e}{2m_e}\sum_j[\vec{p}_j\delta(\vec{r}-\vec{r}_j) + \delta(\vec{r}-\vec{r}_j)\vec{p}_j]$

$$\vec{J}_L(\vec{r}) = \nabla\times\vec{M}_L(\vec{r}) + \nabla\phi$$

Transverse molecular current | Longitudinal conduction current

$$\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{J}_L(\vec{r}) = \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}[\nabla\times\vec{M}_L(\vec{r}) + \nabla\phi] = -i\vec{q}\times\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{M}_L(\vec{r}) - i\vec{q}\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\phi$$

Surface terms ignored

$$\sum_j e^{i\vec{q}\cdot\vec{r}_j}\frac{i}{\hbar q}(\vec{p}_j\times\hat{q}) = \frac{-i}{2q\mu_B}\hat{q}\times\left[-i\vec{q}\times\int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{M}_L(\vec{r})\right] = \frac{-1}{2\mu_B}\hat{q}\times[\hat{q}\times\vec{M}_L(\vec{q})]$$

$$\vec{M}_L(\vec{q}) := \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{M}_L(\vec{r}) \quad \vec{M}(\vec{q}) \equiv \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}\vec{M}(\vec{r})$$

$$V_M(\vec{q}) = 2\gamma_n\mu_0\mu_N\vec{s}_n\cdot[\hat{q}\times(\vec{M}_S(\vec{q})\times\hat{q}) + \hat{q}\times(\vec{M}_L(\vec{q})\times\hat{q})]$$

$$\vec{M}(\vec{r}) = \vec{M}_S(\vec{r}) + \vec{M}_L(\vec{r}) \qquad \vec{M}_\perp(\vec{q}) \equiv \vec{M}(\vec{q}) - (\vec{M}(\vec{q})\cdot\hat{q})\hat{q}$$

$$= 2\gamma_n\mu_0\mu_N\vec{s}_n\cdot\hat{q}\times(\vec{M}(\vec{q})\times\hat{q}) = -\vec{\mu}_n\cdot\mu_0\vec{M}_\perp(\vec{q})$$

$$\vec{M}_L(\vec{r}) = \frac{1}{4\pi}\nabla\times\int\frac{\vec{J}_L(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}' - \frac{1}{8\pi}\nabla\nabla\cdot\int\frac{\vec{r}'\times\vec{J}_L(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'$$

*O. Steinsvoll, et al. Phys. Rev. 161, 499 (1967)*

# Magnetic Interaction : Magnetic Pair Correlation Function and Cross Section

$$V_M(\vec{q}) = -\vec{\mu}_n \cdot \mu_0 \vec{M}_\perp(\vec{q}) \qquad I_M(\vec{q},t) = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left\langle \left\langle \sigma_i \left| V_M^\dagger(\vec{q}) \right| \sigma_f \right\rangle \langle \sigma_f | V_M(\vec{q},t) | \sigma_i \rangle \right\rangle$$

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i} S(\vec{q},\omega)$$

$$S(\vec{q},\omega) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} I(\vec{q},t)$$

$$\langle \sigma_f | V_M(\vec{q},t) | \sigma_i \rangle = -\langle \sigma_f | \vec{\mu}_n | \sigma_i \rangle \cdot \mu_0 \vec{M}_\perp(\vec{q},t) \qquad \left\langle \sigma_i \left| V_M^\dagger(\vec{q}) \right| \sigma_f \right\rangle = -\langle \sigma_i | \vec{\mu}_n | \sigma_f \rangle \cdot \mu_0 \vec{M}_\perp^\dagger(\vec{q})$$

$$I_M(\vec{q},t) = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle \sigma_i | \vec{\mu}_n | \sigma_f \rangle|^2 \left\langle \mu_0 \vec{M}_\perp^\dagger(\vec{q}) \mu_0 \vec{M}_\perp(\vec{q},t) \right\rangle = \mu_0{}^2 \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle \sigma_i | \vec{\mu}_n | \sigma_f \rangle|^2 \left\langle \vec{M}_\perp^\dagger(\vec{q}) \vec{M}_\perp(\vec{q},t) \right\rangle$$

$$= \left(2\gamma_n \mu_N \mu_0 \mu_B \frac{m}{2\pi\hbar^2}\right)^2 \frac{1}{(2\mu_B)^2} |2\langle \sigma_i | \vec{s}_n | \sigma_f \rangle|^2 \left\langle \vec{M}_\perp^\dagger(\vec{q}) \vec{M}_\perp(\vec{q},t) \right\rangle = \left(\frac{3.075 fm}{2\mu_B}\right)^2 |2\langle \sigma_i | \vec{s}_n | \sigma_f \rangle|^2 \left\langle \vec{M}_\perp^\dagger(\vec{q}) \vec{M}_\perp(\vec{q},t) \right\rangle$$

**Define** $S_M(\vec{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle \vec{M}_\perp^\dagger(\vec{q}) \vec{M}_\perp(\vec{q},t) \right\rangle$

$$S(\vec{q},\omega) = \left(\frac{3.075 fm}{2\mu_B}\right)^2 |2\langle \sigma_i | \vec{s}_n | \sigma_f \rangle|^2 S_M(\vec{q},\omega) \qquad \frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i}\left(\frac{3.075 fm}{2\mu_B}\right)^2 |2\langle \sigma_i | \vec{s}_n | \sigma_f \rangle|^2 S_M(\vec{q},\omega)$$

**Define Magnetic pair correlation function:** $\Gamma_{ij}(\vec{r},t) := \frac{1}{N}\int \langle M_i(\vec{r}',0) M_j(\vec{r}'+\vec{r},t)\rangle d\vec{r}'$

$$S_M(\vec{q},\omega) = \frac{N}{2\pi\hbar}\sum_{ij}\int_{-\infty}^{\infty} dt d\vec{r} e^{i(\vec{q}\cdot\vec{r}-\omega t)} \Gamma_{ij}(\vec{r},t)[\delta_{ij} - \hat{q}_i \hat{q}_j]$$

$\Gamma_{ij}(\vec{r},t)$:measures correlations between two magnetization at different place and different time

# Magnetic Interaction : Magnetic Static and Dynamic Correlation

$$S_M(\vec{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\left\langle \vec{M}_\perp^\dagger(\vec{q})\vec{M}_\perp(\vec{q},t)\right\rangle$$

$$S_M(\vec{q},\omega) = \frac{N}{2\pi\hbar}\sum_{ij}\int_{-\infty}^{\infty} dt d\vec{r} e^{i(\vec{q}\cdot\vec{r}-\omega t)}\Gamma_{ij}(\vec{r},t)\left[\delta_{ij} - \hat{q}_i\hat{q}_j\right]$$

$$\Gamma_{ij}(\vec{r},t) := \frac{1}{N}\int \left\langle M_i(\vec{r}',0)M_j(\vec{r}'+\vec{r},t)\right\rangle d\vec{r}'$$

**Static Correlation:** $\left\langle \vec{M}_\perp^\dagger(\vec{q})\vec{M}_\perp(\vec{q},+\infty)\right\rangle = \left\langle \vec{M}_\perp^\dagger(\vec{q})\right\rangle \langle \vec{M}_\perp(\vec{q},\infty)\rangle = \left\langle \vec{M}_\perp^\dagger(\vec{q})\right\rangle \langle \vec{M}_\perp(\vec{q})\rangle$

$$S_M(\vec{q},\omega) = \left|\langle \vec{M}_\perp(\vec{q})\rangle\right|^2 \delta(\hbar\omega) + \tilde{S}_M(\vec{q},\omega)$$

**Static** **Dynamic**

# Magnetic Interaction : Magnetic and Structure Correlation

Assumptions

1. Localized Magnetizations $\vec{M}(\boldsymbol{\vec{r}}) = \sum_{j} \vec{M}_{j}(\boldsymbol{\vec{r}} - \boldsymbol{\vec{r}}_{j})$

$$\vec{M}(\vec{q}) \equiv \int d\vec{r} e^{i\vec{q}\cdot\vec{r}} \vec{M}(\vec{r}) = \sum_{j} \int d\vec{r} e^{i\vec{q}\cdot\vec{r}} \vec{M}_{j}(\vec{r} - \vec{r}_{j})$$

$$= \sum_{j} \int d\vec{r} e^{i\vec{q}\cdot\vec{r}'} \vec{M}_{j}(\vec{r}')\, e^{i\vec{q}\cdot\vec{r}_{j}} = \sum_{j} \vec{M}_{j}(\vec{q}) e^{i\vec{q}\cdot\vec{r}_{j}}$$

2. Magnetic correlations are decoupled with the structure correlations

$$\left\langle e^{-i\vec{q}\cdot\vec{r}_{l}} \vec{M}_{l\perp}^{\dagger}(\vec{q}) \vec{M}_{j\perp}(\vec{q},t) e^{i\vec{q}\cdot\vec{r}_{j}(t)} \right\rangle = \left\langle e^{-i\vec{q}\cdot\vec{r}_{l}} e^{i\vec{q}\cdot\vec{r}_{j}(t)} \right\rangle \left\langle \vec{M}_{l\perp}^{\dagger}(\vec{q}) \vec{M}_{j\perp}(\vec{q},t) \right\rangle$$

$$S_{M}(\vec{q},\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jl} \left\langle e^{-i\vec{q}\cdot\vec{r}_{l}} e^{i\vec{q}\cdot\vec{r}_{j}(t)} \right\rangle \left\langle \vec{M}_{l\perp}^{\dagger}(\vec{q}) \vec{M}_{j\perp}(\vec{q},t) \right\rangle$$

**Counterexamples: Dynamic Jahn-Teller Effect—the coupling between lattice vibrations and the orbital fluctuations of an ion with an orbitally-degenerate ground state.**

$$\boldsymbol{S_{M}(\vec{q},\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle \vec{M}_{\perp}^{\dagger}(\vec{q}) \vec{M}_{\perp}(\vec{q},t) \right\rangle}$$

$$\vec{M}_{j}(\vec{q}) \equiv \int d\vec{r} e^{i\vec{q}\cdot\vec{r}'} \vec{M}_{j}(\boldsymbol{\vec{r}}')$$

$$\boldsymbol{S_{M}(\vec{q},\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jl} \left\langle e^{-i\vec{q}\cdot\vec{r}_{l}} \vec{M}_{l\perp}^{\dagger}(\vec{q}) \vec{M}_{j\perp}(\vec{q},t) e^{i\vec{q}\cdot\vec{r}_{j}(t)} \right\rangle}$$

**a. Magnetic scattering and elastic in structure**

$(static)(static)$ $(static)(dynamic)$

**b. Magnetovibrational scattering: magnetically ordered systems**

$(dynamic)(static)$

Neutron destroy and create phonons through magnetic interaction but without change to magnetic part

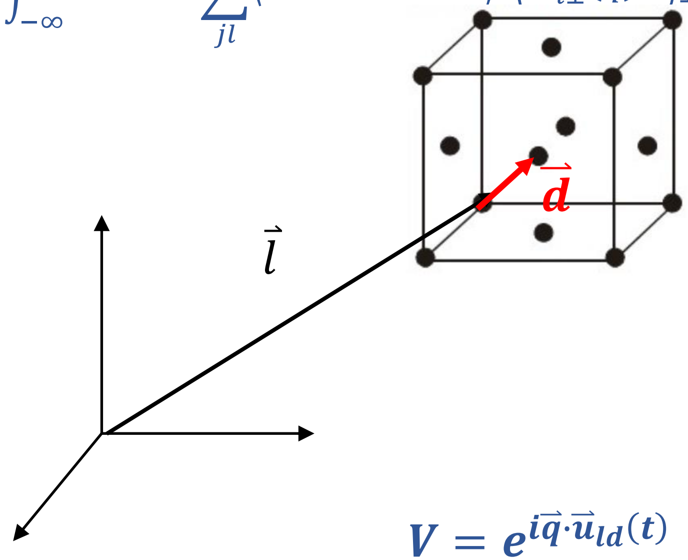
**c. Inelastic Scattering in both magnetic and structural systems**

$(dynamic)(dynamic)$

# Magnetic Interaction : Crystalline Solids and Static Lattice Approximation

$$S_M(\vec{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jl} \langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_j(t)}\rangle \left\langle \vec{M}^{\dagger}_{l\perp}(\vec{q})\vec{M}_{j\perp}(\vec{q},t)\right\rangle$$

$$\vec{r}_{ld}(t) = \vec{l} + \vec{d} + \vec{u}_{ld}(t)$$




$$\sum_{jl} \langle e^{-i\vec{q}\cdot\vec{r}_l} e^{i\vec{q}\cdot\vec{r}_j(t)}\rangle \left\langle \vec{M}^{\dagger}_{l\perp}(\vec{q})\vec{M}_{j\perp}(\vec{q},t)\right\rangle$$

$$= N \sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} \sum_{\vec{d},\vec{d}'} e^{i\vec{q}\cdot(\vec{d}-\vec{d}')} \left\langle \vec{M}^{\dagger}_{\vec{d}'\perp}(\vec{q})\vec{M}_{\vec{d}\perp}(\vec{q},t)\right\rangle \left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)}\right\rangle$$

$$V = e^{i\vec{q}\cdot\vec{u}_{ld}(t)}$$

$$U = -i\vec{q}\cdot\vec{u}_{0\vec{d}'}$$

$$W_d = \frac{1}{2}\langle(\vec{q}\cdot\vec{u}_d)^2\rangle$$

$$\left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)}\right\rangle = \langle e^U e^V\rangle = e^{-W_d - W_{d'}} e^{\langle UV\rangle} = e^{-W_d-W_{d'}}\left[1 + \langle UV\rangle + \frac{1}{2!}\langle UV\rangle^2\right]$$

elastic One-phonon two-phonon

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{Nk_f}{k_i}\left(\frac{3.075fm}{2\mu_B}\right)^2 \left|2\langle\sigma_i\left|\vec{s}_n\right|\sigma_f\rangle\right|^2 \sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} \sum_{\vec{d},\vec{d}'} e^{i\vec{q}\cdot(\vec{d}-\vec{d}')} \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} \left\langle \vec{M}^{\dagger}_{\vec{d}'\perp}(\vec{q})\vec{M}_{\vec{d}\perp}(\vec{q},t)\right\rangle \left\langle e^{-i\vec{q}\cdot\vec{u}_{0\vec{d}'}} e^{i\vec{q}\cdot\vec{u}_{ld}(t)}\right\rangle$$

**Bragg Condition**

$$\sum_{\vec{l}} e^{i\vec{q}\cdot\vec{l}} = \frac{(2\pi)^3}{v_0}\sum_{\vec{G}} \delta(\vec{q}-\vec{G})$$

# Supplementary

# Lippmann-Schwinger equation

$\hat{H}|\Psi\rangle = E|\Psi\rangle$ (1) $\quad \hat{H}_0|\Phi\rangle = E|\Phi\rangle$ (2) $\quad \hat{H} = \hat{H}_0 + \hat{V}$

Solution??? $\quad (E - \hat{H}_0)|\Psi\rangle = \hat{V}|\Psi\rangle$

Step 1 / Step 2

**Complete** $|\boldsymbol{\Psi}\rangle = \boldsymbol{General\ Solution\ of\ }(2) + \boldsymbol{A\ \ Special\ Solution\ of\ \ }(1)$

Step 3 $\quad |\boldsymbol{\Psi}\rangle = |\boldsymbol{\Psi}\rangle|_{\boldsymbol{Boundary\ Conditions}}$

**Step1 :** $\boldsymbol{General\ Solution\ of\ }(2)\text{: } \int d\boldsymbol{\alpha}\ \boldsymbol{c}(\boldsymbol{\alpha})|\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\rangle$

**Step2 :Green Function Method**

If Operator $\hat{G}$ satisfies $(E_\alpha - \hat{H}_0)\hat{G} = \hat{I}$ $\quad \hat{I}$: Unit Operator $\quad \hat{\boldsymbol{G}}_{\pm} = \dfrac{\mathbf{1}}{(\boldsymbol{E}_{\boldsymbol{\alpha}} - \hat{\boldsymbol{H}}_{\mathbf{0}} \mp \boldsymbol{i\epsilon})}\hat{\boldsymbol{I}}$ $\quad \epsilon \to 0^+$

Then corresponding special solutions of (1) are $\left|\tilde{\boldsymbol{\Psi}}^{\pm}\right\rangle = \hat{\boldsymbol{G}}_{\pm}\hat{\boldsymbol{V}}|\boldsymbol{\Psi}\rangle$

Then the complete solution of (1) is $\left|\boldsymbol{\Psi}^{\pm}\right\rangle = \int d\boldsymbol{\alpha}\ \boldsymbol{c}(\boldsymbol{\alpha})|\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\rangle + \hat{\boldsymbol{G}}_{\pm}\hat{\boldsymbol{V}}|\boldsymbol{\Psi}\rangle$

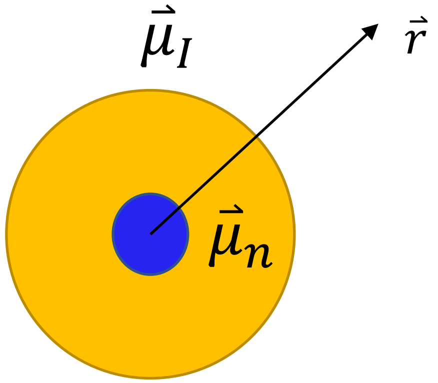
**Step 3: Boundary Conditions** $\quad \lim_{\|\hat{V}\| \to 0} |\boldsymbol{\Psi}\rangle = |\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\rangle \quad \lim_{t \to \pm\infty} e^{\frac{-i\hat{H}t}{\hbar}} \left|\boldsymbol{\Psi}^{\pm}\right\rangle = \lim_{t \to \pm\infty} e^{\frac{-i\hat{H}_0 t}{\hbar}} |\boldsymbol{\Phi}\rangle$ **(note that this condition also restricts $\hat{V}$)**

➡ $|\boldsymbol{\Psi}^{-}\rangle$: "in" state ; $|\boldsymbol{\Psi}^{+}\rangle$: "out" state ;
$\mathbf{t} \to -\infty \qquad \mathbf{t} \to +\infty$

$$\left|\boldsymbol{\Psi}_{\boldsymbol{\alpha}}^{\mp}\right\rangle = |\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\rangle + \frac{\mathbf{1}}{(\boldsymbol{E}_{\boldsymbol{\alpha}} - \hat{\boldsymbol{H}}_{\mathbf{0}} \pm \boldsymbol{i\epsilon})}\hat{\boldsymbol{V}}\left|\boldsymbol{\Psi}_{\boldsymbol{\alpha}}^{\mp}\right\rangle$$

# Fermi Contact Interaction

Interaction between neutron magnetic moment $\vec{\mu}_n$ and nucleus magnetic moment $\vec{\mu}_I$ is




$$\hat{U} = -\vec{\mu}_n \cdot \vec{B}(\vec{r})$$

Magnetic field $\vec{B}(\vec{r})$ is produced by $\vec{\mu}_I$

$$\vec{B}(\vec{r}) = \nabla \times \frac{\vec{\mu}_I \times \vec{r}}{r^3} = \frac{3\vec{r}(\vec{\mu}_I \cdot \vec{r}) - \vec{\mu}_I r^2}{r^5} - 4\pi\vec{\mu}_I \delta(\vec{r})$$

Outside nucleus Inside nucleus

Inside nucleus $\hat{U} = -\vec{\mu}_n \cdot \vec{B}(\vec{r}) = \vec{\mu}_n \cdot 4\pi\vec{\mu}_I \delta(\vec{r}) = 2\Delta\vec{I} \cdot \vec{s}\delta(\vec{r})$ $\Delta = 2\pi\gamma_n\gamma_I$

https://en.wikipedia.org/wiki/Magnetic_dipole