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Лекция 6. Основы теории ядерного рассеяния нейтронов.

- *Сечение рассеяния нейтронов и корреляционные функции*
- *Статическое приближение*

Случай когерентного рассеяния. Определения

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{j,n}\int_{-\infty}^{\infty}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(t)}\right\rangle e^{-i\omega t}dt$$

$$I(\mathbf{Q},t) = \frac{1}{N}\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(t)}\right\rangle$$

$$G(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int I(\mathbf{Q},t)e^{-i\mathbf{Qr}}d\mathbf{Q}$$

Парная корреляционная функция

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int I(\mathbf{Q},t)e^{-i\omega t}dt$$

Функция рассеяния. Динамический структурный фактор (dynamical structure factor)

Свойства

$$I(\mathbf{Q},t)=\int G(\mathbf{r},t)e^{i\mathbf{Qr}}d\mathbf{r}$$

$$S(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar}\int G(\mathbf{r},t)e^{-i\omega t}e^{i\mathbf{Qr}}dtd\mathbf{r}$$

$$G(\mathbf{r},t)=\frac{\hbar}{(2\pi)^3}\int S(\mathbf{Q},\omega)e^{i\omega t}e^{-i\mathbf{Qr}}d\omega d\mathbf{Q}$$

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\mathrm{coh}}=\frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k_f}{k_i}NS(\mathbf{Q},\omega)$$

Случай некогерентного рассеяния. Определения

$$I_s(\mathbf{Q},t) = \frac{1}{N}\sum_j \left\langle e^{-i\mathbf{Q}\mathbf{R}_j(0)} e^{i\mathbf{Q}\mathbf{R}_j(t)} \right\rangle$$

$$G_s(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int I_s(\mathbf{Q},t) e^{-i\mathbf{Q}\mathbf{r}} d\mathbf{Q}$$

Автокорреляционная функция

$$S_i(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int I_s(\mathbf{Q},t) e^{-i\omega t} dt$$

Функция некогерентного рассеяния

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\text{inc}} = \frac{\sigma_{\text{inc}}}{4\pi}\frac{k_f}{k_i} N S_i(\mathbf{Q},\omega)$$

Выражения для G(**r**,t) и G_s(**r**,t)

$$G(\mathbf{r},t)=\frac{1}{(2\pi)^3}\int\frac{1}{N}\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(t)}\right\rangle e^{-i\mathbf{Qr}}d\mathbf{Q}$$

$$\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(t)}\right\rangle=\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))e^{-i\mathbf{Qr}'}e^{i\mathbf{QR}_n(t)}\right\rangle d\mathbf{r}'$$

$$G(\mathbf{r},t)=\frac{1}{(2\pi)^3}\frac{1}{N}\sum_{j,n}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))\int e^{-i\mathbf{Qr}'}e^{i\mathbf{QR}_n(t)}e^{-i\mathbf{Qr}}d\mathbf{Q}\right\rangle d\mathbf{r}'$$

$$=\frac{1}{(2\pi)^3}\frac{1}{N}\sum_{j,n}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))(2\pi)^3\,\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_n(t))\right\rangle d\mathbf{r}'$$

$$G(\mathbf{r},t)=\frac{1}{N}\sum_{j,n}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_n(t))\right\rangle d\mathbf{r}'$$

$$G_s(\mathbf{r},t)=\frac{1}{N}\sum_{j}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_j(t))\right\rangle d\mathbf{r}'$$

Свойства G(**r**,t) и G_s(**r**,t)

$$\int G(\mathbf{r},t)d\mathbf{r} = N \qquad \int G_s(\mathbf{r},t)d\mathbf{r} = 1$$

$t = 0$ статические корреляторы

$$G(\mathbf{r},0) = \frac{1}{N}\sum_{j,n}\int\left\langle \delta(\mathbf{r}'-\mathbf{R}_j)\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_n)\right\rangle d\mathbf{r}'$$

$$= \frac{1}{N}\sum_{j,n}\left\langle \delta(\mathbf{R}_j+\mathbf{r}-\mathbf{R}_n)\right\rangle = \sum_{j}\left\langle \delta(\mathbf{r}-\mathbf{R}_0+\mathbf{R}_j)\right\rangle$$

$$G(\mathbf{r},0) = \delta(\mathbf{r}) + \sum_{j\neq 0}\left\langle \delta(\mathbf{r}-\mathbf{R}_0+\mathbf{R}_j)\right\rangle$$

$$G_s(\mathbf{r},0) = \delta(\mathbf{r})$$

Статическая парная функция распределения

Свойства G(**r**,t) и G_s(**r**,t). Классический предел.

$$G(\mathbf{r},t)=\frac{1}{N}\sum_{j,n}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_n(t))\right\rangle d\mathbf{r}'$$

$$=\frac{1}{N}\sum_{j,n}\left\langle\delta(\mathbf{r}+\mathbf{R}_j(0)-\mathbf{R}_n(t))\right\rangle=\sum_{n}\left\langle\delta(\mathbf{r}+\mathbf{R}_0(0)-\mathbf{R}_n(t))\right\rangle$$

$$G_s(\mathbf{r},t)=\frac{1}{N}\sum_{j}\int\left\langle\delta(\mathbf{r}'-\mathbf{R}_j(0))\delta(\mathbf{r}'+\mathbf{r}-\mathbf{R}_j(t))\right\rangle d\mathbf{r}'$$

$$=\left\langle\delta(\mathbf{r}+\mathbf{R}_0(0)-\mathbf{R}_0(t))\right\rangle$$

Аналитические свойства корреляционных функций

$$\left.\begin{aligned}
\rho(\mathbf{r},t) &= \sum_j \delta(\mathbf{r}-\mathbf{R}_j(t)) \\
\rho(\mathbf{r},t) &= \frac{1}{(2\pi)^3}\int \rho(\mathbf{Q},t)e^{i\mathbf{Qr}}d\mathbf{Q} \\
\rho(\mathbf{Q},t) &= \sum_j e^{-i\mathbf{QR}_j(t)}
\end{aligned}\right\}$$

$$\rho(\mathbf{r},t)^{+} = \rho(\mathbf{r},t)$$

$$\rho(\mathbf{Q},t)^{+} = \rho(-\mathbf{Q},t)$$

$$I(\mathbf{Q},t) = \frac{1}{N}\left\langle \rho(\mathbf{Q},0)\rho(-\mathbf{Q},t)\right\rangle$$

$$G(\mathbf{r},t) = \frac{1}{N}\int \left\langle \rho(\mathbf{r}',0)\rho(\mathbf{r}'+\mathbf{r},t)\right\rangle d\mathbf{r}'$$

Аналитические свойства корреляционных функций

1. $I(\mathbf{Q},t) = I(\mathbf{Q},-t)^*$ 2. $G(\mathbf{r},t) = G(-\mathbf{r},-t)^*$ 3. $S(\mathbf{Q},\omega) = S(\mathbf{Q},\omega)^*$

$$\rho(\mathbf{r},t)^+ = \rho(\mathbf{r},t)$$

$$\rho(\mathbf{Q},t)^+ = \rho(-\mathbf{Q},t)$$

1. $$I(\mathbf{Q},-t)^* = \frac{1}{N}\langle \rho(\mathbf{Q},0)\rho(-\mathbf{Q},-t)\rangle^*$$

$$= \frac{1}{N}\langle \rho(\mathbf{Q},-t)\rho(-\mathbf{Q},0)\rangle = \frac{1}{N}\langle \rho(\mathbf{Q},0)\rho(-\mathbf{Q},t)\rangle = I(\mathbf{Q},t)$$

2. $$G(-\mathbf{r},-t)^* = \frac{1}{N}\int \langle \rho(\mathbf{r}',0)\rho(\mathbf{r}'-\mathbf{r},-t)\rangle^* d\mathbf{r}'$$

$$= \frac{1}{N}\int \langle \rho(\mathbf{r}'-\mathbf{r},-t)\rho(\mathbf{r}',0)\rangle d\mathbf{r}' = \frac{1}{N}\int \langle \rho(\mathbf{r}'-\mathbf{r},0)\rho(\mathbf{r}',t)\rangle d\mathbf{r}'$$

$$= \frac{1}{N}\int \langle \rho(\mathbf{r}',0)\rho(\mathbf{r}'+\mathbf{r},t)\rangle d\mathbf{r}' = G(\mathbf{r},t)$$

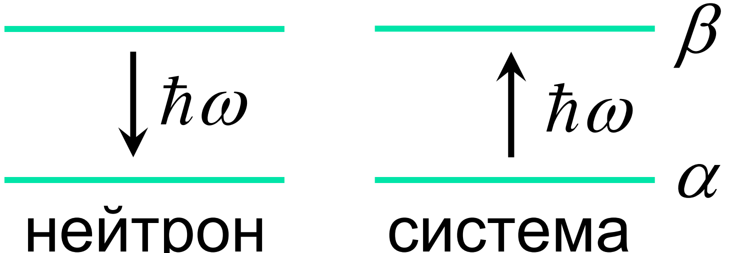
Принцип детального равновесия

$$\left(\frac{d^2\sigma}{dE_f\,d\Omega_f}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k_f}{k_i}\sum_{\alpha,\beta} P_\alpha \left|\sum_j \left\langle \beta \left| e^{i\mathbf{Q}\mathbf{R}_j} \right| \alpha \right\rangle\right|^2 \delta\left(E_\alpha - E_\beta + \hbar\omega\right)$$

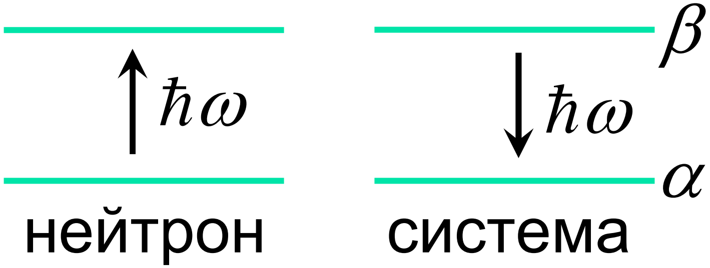
$$S(\mathbf{Q},\omega) = \frac{1}{NZ}\sum_{\alpha,\beta} e^{-E_\alpha/(k_b T)} \left|\sum_j \left\langle \beta \left| e^{i\mathbf{Q}\mathbf{R}_j} \right| \alpha \right\rangle\right|^2 \delta\left(E_\alpha - E_\beta + \hbar\omega\right)$$

$$S(\mathbf{Q},\omega) = e^{\frac{\hbar\omega}{k_B T}} S(-\mathbf{Q},-\omega)$$

$S(\mathbf{Q},\omega)$



$S(-\mathbf{Q},-\omega)$



$$S(\mathbf{Q},\omega)=\frac{1}{NZ}\sum_{\alpha,\beta}e^{-E_\alpha/(k_bT)}\left|\sum_j\left\langle\beta\left|e^{i\mathbf{QR}_j}\right|\alpha\right\rangle\right|^2\delta\left(E_\alpha-E_\beta+\hbar\omega\right)$$

$$S(-\mathbf{Q},-\omega)=\frac{1}{NZ}\sum_{\alpha,\beta}e^{-E_\alpha/(k_bT)}\left|\sum_j\left\langle\beta\left|e^{-i\mathbf{QR}_j}\right|\alpha\right\rangle\right|^2\delta\left(E_\alpha-E_\beta-\hbar\omega\right)$$

$$=\frac{1}{NZ}\sum_{\alpha,\beta}e^{-E_\beta/(k_bT)}\left|\sum_j\left\langle\alpha\left|e^{-i\mathbf{QR}_j}\right|\beta\right\rangle\right|^2\delta\left(E_\beta-E_\alpha-\hbar\omega\right)$$

$$=\frac{1}{NZ}\sum_{\alpha,\beta}e^{-E_\beta/(k_bT)}\left|\sum_j\left\langle\beta\left|e^{i\mathbf{QR}_j}\right|\alpha\right\rangle\right|^2\delta\left(E_\alpha-E_\beta+\hbar\omega\right)$$

$$=\frac{1}{NZ}e^{-(E_\beta-E_\alpha)/(k_bT)}\sum_{\alpha,\beta}e^{-E_\alpha/(k_bT)}\left|\sum_j\left\langle\beta\left|e^{i\mathbf{QR}_j}\right|\alpha\right\rangle\right|^2\delta\left(E_\alpha-E_\beta+\hbar\omega\right)$$

$$=e^{-\hbar\omega/(k_bT)}S(\mathbf{Q},\omega)$$

Связь сечения когерентного упругого рассеяния с I(**Q**,∞)

$$I(\mathbf{Q},t) = I(\mathbf{Q},\infty) + I'(\mathbf{Q},t)$$

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} I(\mathbf{Q},t)e^{-i\omega t}dt = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\left(I(\mathbf{Q},\infty) + I'(\mathbf{Q},t)\right)e^{-i\omega t}dt$$

$$= \frac{1}{\hbar}\delta(\omega)I(\mathbf{Q},\infty) + \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} I'(\mathbf{Q},t)e^{-i\omega t}dt$$

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\mathrm{coh,el}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{N}{\hbar}\delta(\omega)I(\mathbf{Q},\infty)$$

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\mathrm{coh,el}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}NI(\mathbf{Q},\infty)$$

$$I(\mathbf{Q},\infty)=\frac{1}{N}\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j(0)}e^{i\mathbf{QR}_n(\infty)}\right\rangle=\frac{1}{N}\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j(0)}\right\rangle\left\langle e^{i\mathbf{QR}_n(\infty)}\right\rangle$$

$$=\frac{1}{N}\sum_{j,n}\left\langle e^{-i\mathbf{QR}_j}\right\rangle\left\langle e^{i\mathbf{QR}_n}\right\rangle=e^{\left\langle U^2\right\rangle}\frac{1}{N}\sum_{j,n}e^{-i\mathbf{QR}_j^{(0)}}e^{i\mathbf{QR}_n^{(0)}}$$

$$=e^{-2W}\frac{(2\pi)^3}{\mathrm{V}_0}\sum_{\boldsymbol{\tau}}\delta(\mathbf{Q}-\boldsymbol{\tau})$$

$$\left\langle e^{-i\mathbf{QR}_j}\right\rangle=e^{-i\mathbf{QR}_j^{(0)}}\left\langle e^{-i\mathbf{Qu}_j}\right\rangle=e^{-i\mathbf{QR}_j^{(0)}}\left\langle e^{U}\right\rangle=e^{-i\mathbf{QR}_j^{(0)}}e^{\frac{1}{2}\left\langle U^2\right\rangle}$$

$$\mathbf{R}_j=\mathbf{R}_j^{(0)}+\mathbf{u}_j \qquad \left\langle e^{U+V}\right\rangle=e^{\frac{1}{2}\left\langle (U+V)^2\right\rangle} \qquad \sum_j e^{i\mathbf{QR}_j^{(0)}}=\frac{(2\pi)^3}{\mathrm{V}_0}\sum_{\boldsymbol{\tau}}\delta(\mathbf{Q}-\boldsymbol{\tau})$$

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\mathrm{coh,el}}=\frac{\sigma_{\mathrm{coh}}}{4\pi}NI(\mathbf{Q},\infty)=\frac{\sigma_{\mathrm{coh}}}{4\pi}Ne^{-2W}\frac{(2\pi)^3}{\mathrm{V}_0}\sum_{\boldsymbol{\tau}}\delta(\mathbf{Q}-\boldsymbol{\tau})$$

Связь сечения некогерентного упругого рассеяния с $I_s(\mathbf{Q},\infty)$

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{inc,el}} = \frac{\sigma_{\text{inc}}}{4\pi} N I_s(\mathbf{Q},\infty)$$

$$I_s(\mathbf{Q},\infty) = \frac{1}{N}\sum_j \left\langle e^{-i\mathbf{Q}\mathbf{R}_j(0)} e^{i\mathbf{Q}\mathbf{R}_j(\infty)} \right\rangle = \frac{1}{N}\sum_j \left\langle e^{-i\mathbf{Q}\mathbf{R}_j(0)} \right\rangle \left\langle e^{i\mathbf{Q}\mathbf{R}_j(\infty)} \right\rangle$$

$$= \frac{1}{N}\sum_j \left\langle e^{-i\mathbf{Q}\mathbf{R}_j} \right\rangle \left\langle e^{i\mathbf{Q}\mathbf{R}_j} \right\rangle = e^{\left\langle U^2 \right\rangle} \frac{1}{N}\sum_j e^{-i\mathbf{Q}\mathbf{R}_j^{(0)}} e^{i\mathbf{Q}\mathbf{R}_j^{(0)}} = e^{-2W}$$

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{inc,el}} = \frac{\sigma_{\text{inc}}}{4\pi} N e^{-2W}$$

Статическое приближение

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\text{coh}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\sum_{\alpha,\beta} P_\alpha \left|\sum_j \left\langle \beta \left| e^{i\mathbf{QR}_j} \right| \alpha \right\rangle\right|^2 \delta\left(E_\alpha - E_\beta + \hbar\omega\right)$$

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)^{\text{sa}}_{\text{coh}} = \frac{\sigma_{\text{coh}}}{4\pi}\sum_{\alpha,\beta} P_\alpha \sum_{j,n} \left\langle \alpha \left| e^{-i\mathbf{QR}_n} \right| \beta \right\rangle \left\langle \beta \left| e^{i\mathbf{QR}_j} \right| \alpha \right\rangle \delta\left(\hbar\omega\right)$$

$$= \frac{\sigma_{\text{coh}}}{4\pi}\sum_{\alpha} P_\alpha \sum_{j,n} \left\langle \alpha \left| e^{-i\mathbf{QR}_n} e^{i\mathbf{QR}_j} \right| \alpha \right\rangle \delta\left(\hbar\omega\right) = \frac{\sigma_{\text{coh}}}{4\pi}\sum_{j,n} \left\langle e^{i\mathbf{Q}\left(\mathbf{R}_j - \mathbf{R}_n\right)} \right\rangle \delta\left(\hbar\omega\right)$$

$$\left(\frac{d\sigma}{d\Omega_f}\right)^{\text{sa}}_{\text{coh}} = \frac{\sigma_{\text{coh}}}{4\pi} N I(\mathbf{Q}, 0) = \frac{\sigma_{\text{coh}}}{4\pi} N \int G(\mathbf{r}, 0) e^{i\mathbf{Qr}} d\mathbf{r}$$

Область применимости статического приближения

$$\frac{\hbar^2}{2m}(k_{\max}^2 - k^2) \sim \omega_m \qquad \frac{\hbar^2}{2m}(k^2 - k_{\min}^2) \sim \omega_m$$

$$\frac{\hbar^2}{m}k_f \Delta k_f \sim \omega_m \quad \Rightarrow \quad \frac{\Delta k_f}{k_f} \sim \frac{\omega_m}{E}$$

$$\Delta k_f \ll k_f \quad \Rightarrow \quad \boxed{E \gg \omega_m}$$

$$\omega_m \sim \frac{\hbar}{\tau} \qquad E = \frac{m\text{v}^2}{2} = \frac{\hbar k \text{v}}{2} \sim \frac{\hbar \text{v}}{\lambda}$$

$$\frac{\hbar}{\tau} \ll \frac{\hbar \text{v}}{\lambda} \quad \Rightarrow \quad \frac{1}{\tau} \ll \frac{\text{v}}{\lambda}$$

$$\frac{\lambda}{\text{v}} \sim \frac{a}{\text{v}} \sim t_n \quad \Rightarrow \quad \boxed{t_n \ll \tau}$$

$$\tau \sim 10^{-13} \div 10^{-12} \text{ сек}$$

$$t_n \sim 10^{-13} \text{ сек}$$

$$t_{X-rays} \sim 10^{-18} \text{ сек}$$