Neutron Scattering

Cross Section

in 7 easy steps

1. Scattering Probability (TDPT)
2. Adiabatic Switching of Potential
3. Scattering matrix (integral over time)
4. Transition matrix (correlation of events)
5. Density of states
6. Incoming flux
7. Thermal average

1. Scattering Probability

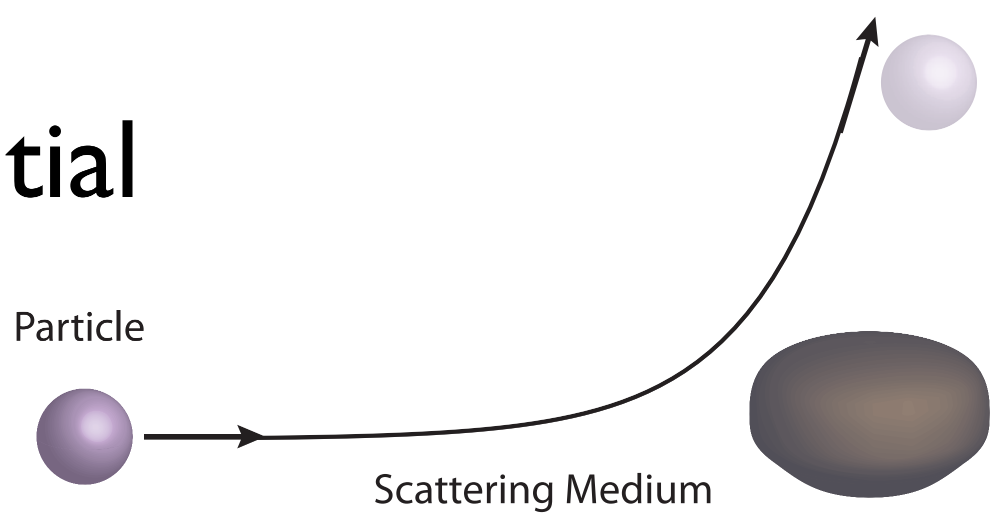
- Probability of final scattered state, when evolving under scattering interaction

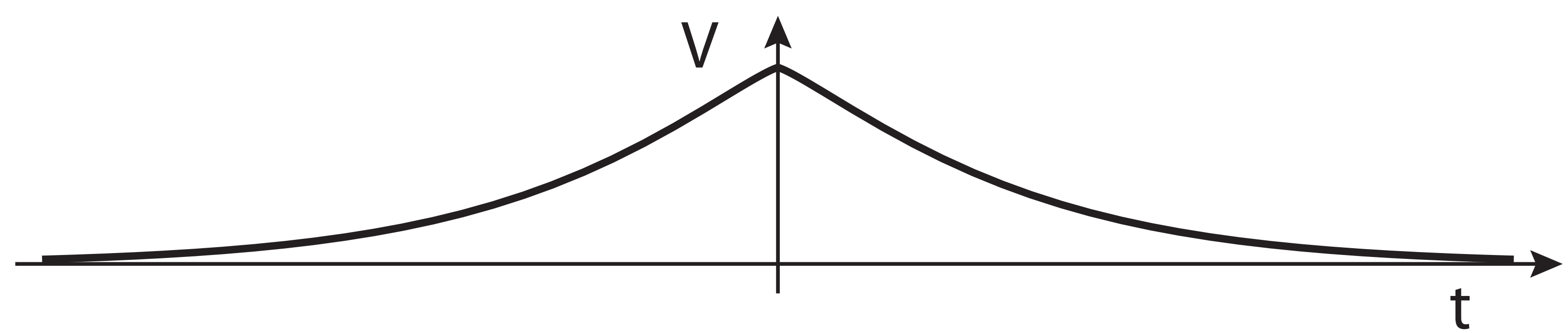
$$P_{scatt} = |\langle f| U_I(t) |i\rangle|^2$$

- Time-dependent perturbation theory (Dyson expansion)

2. Adiabatic Switching

- Slow switching of potential
  → time ∈ [-∞,∞]





- V is approximately constant

3. Scattering Matrix

- Propagator for time t=-∞ → t= ∞ is called the scattering matrix

$$|\langle f| U_I(t_i = -\infty, t_f = \infty) |i\rangle|^2 = |\langle f| S |i\rangle|^2$$

- S is expanded in series:

$$\langle f| S^{(1)} |i\rangle = -iV_{fi} \int_{-\infty}^{\infty} e^{i\omega_{fi} t} dt = -2\pi i \delta(\omega_f - \omega_i) V_{fi}$$

$$\langle f| S^{(2)} |i\rangle = -\langle f| \left(\sum_m V |m\rangle \langle m| V \right) |i\rangle \int_{-\infty}^{\infty} dt_1 e^{i\omega_{fm} t_1} \int_{-\infty}^{t_1} dt_2 e^{i\omega_{mi} t_2}$$

3. Scattering Matrix

- Be careful with integration (ε ...)

- First and second order simplify to

$$\langle f|\, S^{(1)}\, |i\rangle = -2\pi i\delta(\omega_f - \omega_i)\, \langle f|\, V\, |i\rangle$$

$$\langle f|\, S^{(2)}\, |i\rangle = -2\pi i\delta(\omega_f - \omega_i) \sum_m \frac{\langle f|\, V\, |m\rangle\, \langle m|\, V\, |i\rangle}{\omega_i - \omega_m}$$

4. Transition Matrix

- The scattering matrix is given by the transition matrix

$$\langle f| S |i\rangle = -2\pi i \delta(\omega_f - \omega_i) \ \langle f| T |i\rangle$$

- which has the following expansion

$$\langle f| T |i\rangle = \langle f| V |i\rangle + \sum_m \frac{\langle f| V |m\rangle \langle m| V |i\rangle}{\omega_i - \omega_m} + \sum_{m,n} \frac{V_{fm} V_{mn} V_{ni}}{(\omega_i - \omega_m)(\omega_i - \omega_n)} + \dots$$

4. Transition Matrix

- Scattering probability

$$P_s = 4\pi^2 |\langle f| T |i\rangle|^2 \delta^2(\omega_f - \omega_i) = 2\pi t |\langle f| T |i\rangle|^2 \delta(\omega_f - \omega_i)$$

(not well defined because of $t \to \infty$)

- Scattering rate

$$W_S = 2\pi |\langle f| T |i\rangle|^2 \delta(\omega_f - \omega_i)$$

4. Transition Matrix

- Target is left in one (of many possible) state.
- Radiation is left in a continuum state
- Separate the two subsystems
(no entanglement prior and after the scattering event)
and rewrite the transition matrix

4. Transition Matrix

- Target: $|m_k\rangle\,, \epsilon_k$
- Radiation: $|k\rangle\,, \omega_k$
- Scattering rate $W_{fi} = 2\pi |\langle f|\, T\, |i\rangle\,|^2 \delta(E_f - E_i)$

go back to definition, using explicit states

$$W_{fi} = |\,\langle m_f, k_f|\, T\, |m_i, k_i\rangle\,|^2 \int_{-\infty}^{\infty} e^{i(\omega_f + \epsilon_f - \omega_i - \epsilon_i)t}$$

4. Transition Matrix

- Work in Schrodinger pict. for radiation and Interaction pict. for target:

$$\langle m_f, k_f | T_{I_t I_r} | m_i, k_i \rangle = \langle m_f, k_f | T_{S_t S_r} | m_i, k_i \rangle \, e^{i(\omega_f - \omega_i)t} e^{i(\epsilon_f - \epsilon_i)t}$$

$$= \langle m_f, k_f | T_{I_t S_r}(t) | m_i, k_i \rangle \, e^{i(\omega_f - \omega_i)t} = \langle m_f | T_{k_f, k_i}(t) | m_i \rangle \, e^{i(\omega_f - \omega_i)t}$$

- Scattering rate is then a correlation

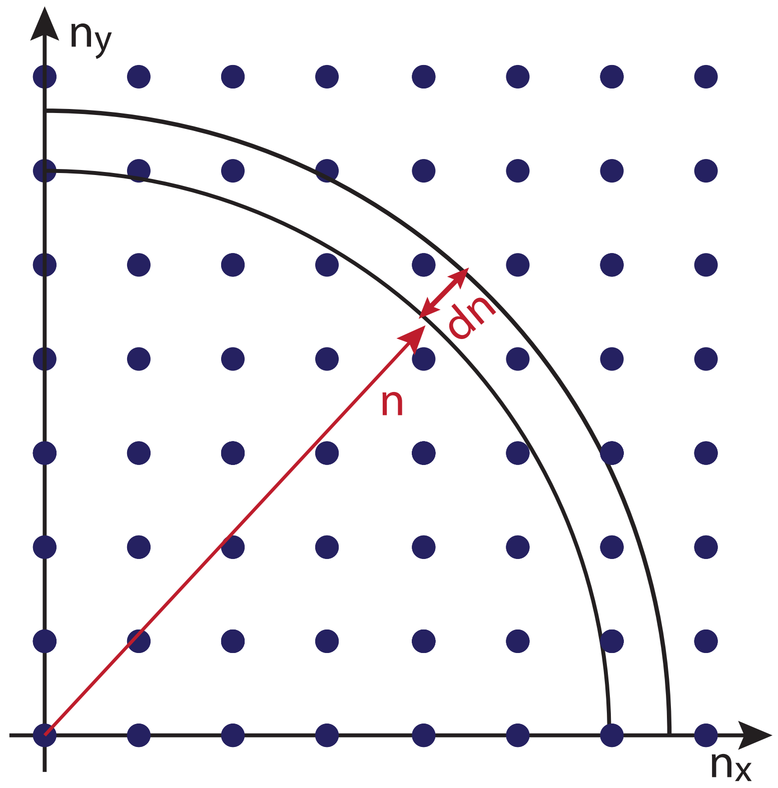
$$W_{fi} = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} e^{i(\omega_f - \omega_i)t} \langle m_i | T^{\dagger}_{k_f, k_i}(0) | m_f \rangle \langle m_f | T_{k_f, k_i}(t) | m_i \rangle$$

NOTE: Time evolution of target only

(e.g. lattice nuclei vibration)

5. Density of states

- # of states $\sum_k n(E_k) \approx \int d^3n(E)$
- Plane wave in a cubic cavity



$$k_x = \frac{2\pi}{L} n_x \to d^3n = \left(\frac{L}{2\pi}\right)^3 d^3k$$

$$\rho(E) dE d\Omega = \rho(k) d^3k = \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega$$

5. Density of states

- Photons, $k = E/\hbar c \to \dfrac{d\,k}{d\,E} = 1/\hbar c$

$$\rho(E) = 2\left(\frac{L}{2\pi}\right)^3 \frac{E^2}{\hbar^3 c^3} = 2\left(\frac{L}{2\pi}\right)^3 \frac{\omega_k^2}{\hbar c^3}$$

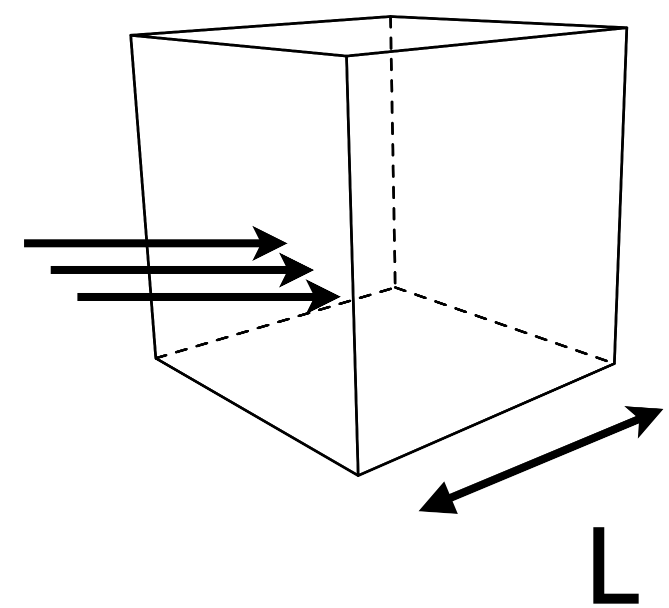
- Massive particles, $E = \dfrac{\hbar^2 k^2}{2m}$

$$\rho(E) = \left(\frac{L}{2\pi}\right)^3 \frac{k}{\hbar^2} = \left(\frac{L}{2\pi}\right)^3 \frac{\sqrt{2mE}}{\hbar^3}$$

6. Incoming Flux

- # scatterer per unit area and time

$$\Phi = \frac{\#}{A\,t} = \frac{v}{L^3}, \text{ since } t = L/v, \; A = L^2$$



- Photons, $\Phi = c/L^3$

- Massive particles, $\Phi = \dfrac{\hbar k}{m L^3}$

7. Thermal Average

- Average over initial state of target

$$W_S(i \to \Omega + d\Omega, E + dE) = \rho(E) \sum_i P_i \sum_f W_{fi}$$

- Scattering Cross Section

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{\hbar^2} \sum_f \int_{-\infty}^{\infty} dt e^{i\omega_{fi}t} \left\langle T_{if}^{\dagger}(0) T_{fi}(t) \right\rangle_{th} \frac{\rho(E)}{\Phi}$$

Neutrons

- Using Φ_{inc} and $\rho(E)$ for massive particles, the scattering cross section is:

$$\frac{d^2\sigma}{d\,\Omega d\omega} = \frac{1}{2\pi}\left(\frac{mL^3}{2\pi\hbar^2}\right)^2 \frac{k_f}{k_i}\int_{-\infty}^{\infty} e^{i\omega_{fi}t}\left\langle T_{if}^{\dagger}(0)T_{fi}(t)\right\rangle$$

Neutrons

- Evaluate T for neutrons, with states

$$|k_{i,f}\rangle \to \psi_k(r) = e^{ik\cdot r}/L^{3/2}$$

- we obtain $T_{k_f k_i}(t, Q)$ with $Q = k_f - k_i$

$$\langle k_f|\, T(t,r)\, |k_i\rangle = \int_{L^3} d^3r \quad {}^{*}_{k_f}(r) T(r,t) \quad {}_{k_i}(r)$$

$$= \frac{1}{L^3} \int_{L^3} d^3r\, e^{iQ\cdot r} T(r,t)$$

Neutron Transition Matrix

- We still need to take the expectation value with respect to the target states,

$$T_{fi} = \frac{1}{L^3} \int_{L^3} d^3r \, e^{iQ\cdot r} \, \langle m_f | \, T(r,t) \, | m_i \rangle$$

Fermi Potential

- T is an expansion of the interaction potential, here the nuclear potential

    - analyze at least first order...

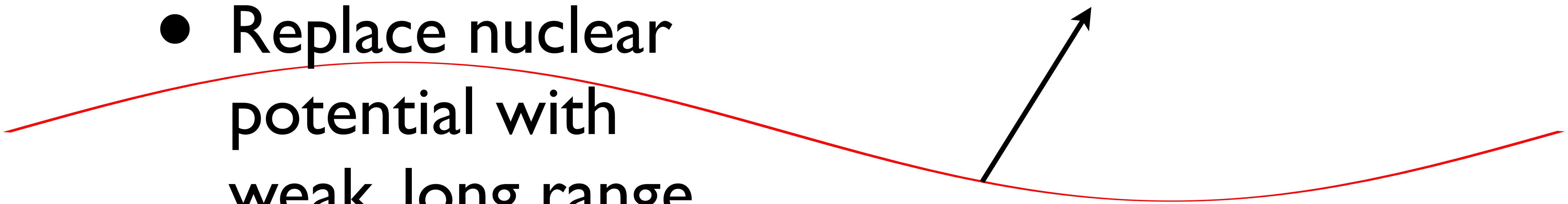
Fermi Potential

- Nuclear potential is very strong (V_0~30MeV)
- And short range (r_0 ~ 2fm)
  - Not good for perturbation theory!
- Fermi approximation
  - What is important is the product

$$a \propto V_0 r_0^3$$

(a = scattering length) if $kr_0 \ll 1$

Fermi Potential



- Replace nuclear potential with weak, long range pseudo-potential
- Still, short range compared to wavelength
    - Delta-function potential!

$$V(r) = \frac{2\pi\hbar^2}{\mu} a\delta(r)$$

Scattering Length

- Free scattering length a,

$$V(r) = \frac{2\pi\hbar^2}{\mu} a\delta(r) \rightarrow \frac{2\pi\hbar^2}{m_n} b\delta(r)$$

- bound scattering length b (include info about isotope and spin)

$$b = \frac{m_n}{\mu} a \approx \frac{A+1}{A} a$$

(reduced mass: $\mu = \frac{M m_n}{M + m_n}$)

Transition Matrix

- To first order, the transition matrix is just the potential

$$T_{fi} = \frac{1}{L^3} \int_{L^3} d^3r \, e^{iQ\cdot r} \, \langle m_f | \, V(r,t) \, | m_i \rangle$$

- Using the nuclear potential for a nucleus at a position R, we have

$$T_{fi} = \frac{1}{L^3} \int_{L^3} d^3r \, e^{iQ\cdot r} \frac{2\pi\hbar^2}{m_n} b(R)\delta(R)T(r,t) = \frac{2\pi\hbar^2}{m_n} b(R) e^{iQ\cdot R(t)}$$

Transition Matrix

- To first order, for many scatter at position r_i

$$T_{fi}(t) = \frac{2\pi\hbar^2}{m_n} \sum_i b_i e^{iQ\cdot r_i(t)}$$

- The scattering cross section becomes

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{2\pi}\frac{k_f}{k_i}\int_{-\infty}^{\infty} e^{i\omega_{fi}t} \sum_{\ell,j} b_\ell b_j \left\langle e^{-iQ\cdot r_\ell(0)} e^{iQ\cdot r_j(t)} \right\rangle_{th}$$

Scattering Lengths

- The bound scattering length depends on isotope and spin
- We need to take the average $b_\ell b_j \rightarrow \overline{b_\ell b_j}$
  - $j = \ell, \quad \overline{b_\ell b_j} = \overline{b^2}$
  - $j \neq \ell, \quad \overline{b_\ell b_j} = \bar{b}^2$
- Finally, $\overline{b_\ell b_j} = \overline{b^2}\delta_{j,\ell} + \bar{b}^2(1 - \delta_{j,\ell})$
- Coherent/Incoherent scattering length:

$$\overline{b_\ell b_j} = (\overline{b^2} - \bar{b}^2)\delta_{j,\ell} + \bar{b}^2 = b_i^2 + b_c^2$$

Scattering lengths

- **Coherent** scattering length

$$b_c = \bar{b}$$

  - Correlations in scattering events from the ***same*** target
(scale-length over which the incoming radiation is ***coherent*** in a QM sense)
  - Simple average over isotopes and spins

Scattering Lengths

- **Incoherent** scattering length

$$b_i^2 = (\overline{b^2} - \overline{b}^2)\delta_{j,\ell}$$

  - Correlation of scattering events between ***different*** targets
  - Variance of the scattering length over spin states and isotopes

Cross-section

- Averaging over the scattering lenght

$$\frac{d^2\sigma}{d\,\Omega d\omega} = \frac{1}{2\pi}\frac{k_f}{k_i}\int_{-\infty}^{\infty} e^{i\omega_{fi}t}\sum_{\ell,j}\overline{b_\ell b_j}\left\langle e^{-iQ\cdot r_\ell(0)}e^{iQ\cdot r_j(t)}\right\rangle_{th}$$

we obtain

$$S_S(Q,\omega)$$

$$\frac{d^2\sigma}{d\,\Omega d\omega} = \frac{1}{2\pi}\frac{k_f}{k_i}\int_{-\infty}^{\infty} e^{i\omega_{fi}t}\sum_{\ell,j}(b_i^2 + b_c^2)\left\langle e^{-iQ\cdot r_\ell(0)}e^{iQ\cdot r_j(t)}\right\rangle_{th}$$

$$S(Q,\omega)$$

Cross-section

- Using the dynamic structure factors, we can write the cross section as

$$\frac{d^2\sigma}{d\Omega d\omega} = N\frac{k_f}{k_i}\left[b_i^2 S_s(Q,\omega) + b_c^2 S(Q,\omega)\right]$$

- These functions encapsulate the target characteristics, or more precisely, the target response to a radiation of energy ω and wavevector $\vec{Q}$

Structure Factors

- Self dynamic structure factor (incoherent)

$$S_S(Q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega_{fi}t} \left\langle \frac{1}{N}\sum_{\ell} e^{-iQ\cdot r_\ell(0)} e^{iQ\cdot r_\ell(t)} \right\rangle$$

- Full dynamic structure factor (coherent)

$$S(Q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega_{fi}t} \left\langle \frac{1}{N}\sum_{\ell,j} e^{-iQ\cdot r_\ell(0)} e^{iQ\cdot r_j(t)} \right\rangle$$

Intermediate Scattering Functions

- Self dynamic structure factor

$$S_S(Q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega_{fi}t} F_s(Q,t)$$

$$F_s(Q,t) = \left\langle \frac{1}{N}\sum_{\ell} e^{-iQ\cdot r_\ell(0)} e^{iQ\cdot r_\ell(t)} \right\rangle$$

- Full dynamic structure factor

$$S(Q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega_{fi}t} F(Q,t)$$

$$F(Q,t) = \left\langle \frac{1}{N}\sum_{\ell,j} e^{-iQ\cdot r_j(0)} e^{iQ\cdot r_\ell(t)} \right\rangle$$

- These functions are the Fourier transform (wrt time) of the structure factors
- They contain information about the target and its time correlation.

  - Examples:
    - Lattice vibrations (phonons)
    - Liquid/Gas diffusion

Crystal Lattice

- Position in $F(Q,t) \sim \left\langle \sum_{\ell,j} e^{-iQ\cdot x_j(0)} e^{iQ\cdot x_\ell(t)} \right\rangle$ is the nuclear lattice position
- Model as 1D quantum harmonic oscillator
  - position: $x = \sqrt{\frac{\hbar}{2M\omega_0}}(a + a^\dagger)$
  - Hamiltonian (phonons)

$$\mathcal{H} = \frac{p^2}{2M} + \frac{M\omega_0^2}{2}x^2 = \hbar\omega_0(a^\dagger a + \tfrac{1}{2})$$

Crystal Lattice

- Assumption: 1D, 1 isotope, 1 spin state
  → Self-intermediate structure function:

$$F_S(Q,t) = \left\langle e^{-iQ\cdot x(0)} e^{iQ\cdot x(t)} \right\rangle$$

- Note: $[x(0), x(t)] \neq 0$ (but it's a number)

- Use BCH formula: $e^A e^B = e^{A+B} e^{[A,B]} \ldots$

$$F_S(Q,T) = \left\langle e^{-iQ\cdot[x(0)-x(t)]} e^{+\frac{1}{2}[Q\cdot x(0), Q\cdot x(t)]} \right\rangle$$

- Simplify using (Bloch) formula:

$$\left\langle e^{\alpha a+\beta a^\dagger} \right\rangle = e^{\left\langle (\alpha a+\beta a^\dagger)^2 \right\rangle}$$

- we get $F_S(Q,t) = e^{-Q^2\left\langle \Delta x^2 \right\rangle/2} e^{+\frac{1}{2}[Q\cdot x(0), Q\cdot x(t)]}$
- with

$$\left\langle \Delta x^2 \right\rangle = 2\left\langle x^2 \right\rangle + 2\left\langle x(0)x(t) \right\rangle - \left\langle [x(0), x(t)] \right\rangle$$

$$F_S(Q,t) = e^{-Q^2\langle x^2 \rangle} e^{-Q^2\langle x(0)x(t) \rangle}$$

- The crystal is usually in a thermal state.
  - Calculate F(Q,t) for a number state and then take a thermal average over Boltzman distribution

$$\langle n| x^2 |n\rangle = \frac{\hbar}{2M\omega_0}(2n+1)$$

$$\langle n| x(0)x(t) |n\rangle = \frac{\hbar}{2M\omega_0}[2n\cos(\omega_0 t) + e^{i\omega_0 t}]$$

  - Replace $n \to \langle n\rangle$

Phonon Expansion

- Low temperature $\langle n \rangle \approx 0$

$$\left\langle x^2 \right\rangle = \frac{\hbar}{2M\omega_0} \qquad \langle x(0)x(t)\rangle = \frac{\hbar}{2M\omega_0} e^{i\omega_0 t}$$

- Expand in series of $\frac{\hbar^2 Q^2}{2M}/(\hbar\omega_0) = E_{kin}/E_{bind}$ and calculate the dynamic structure factor

$$S_S(Q,\omega) = \mathcal{F}(F(Q,t)$$

$$S_S(Q,\omega) \approx e^{-Q^2 \frac{\hbar Q^2}{2M\omega_0}} \left[\delta(\omega) + \frac{\hbar Q^2}{2M\omega_0}\delta(\omega - \omega_0) + \frac{1}{2}\left(\frac{\hbar Q^2}{2M\omega_0}\right)^2 \delta(\omega - 2\omega_0) + \dots\right]$$

Phonon Expansion

- Neutron/q.h.o. energy exchange

Zero-phonon = no excitation (elastic scattering)

one-phonon = 1 quantum of Energy

$$S_S(Q,\omega) \approx e^{-Q^2 \frac{\hbar Q^2}{2M\omega_0}} \left[\delta(\omega) + \frac{\hbar Q^2}{2M\omega_0}\delta(\omega - \omega_0) + \frac{1}{2}\left(\frac{\hbar Q^2}{2M\omega_0}\right)^2 \delta(\omega - 2\omega_0) + \dots\right]$$

two-phonons = 2 quantum of Energy

n-phonons

High Temperature

- We find a "classical" result, where

$$F_S^{cl} = \mathcal{F}[G_s^{cl}(x,t)]$$

and the space-time self correlation (classical) function $G_s^{cl}(x,t)dx$ is the probability of finding the h.o. at x, at time t, if it was at the origin at time t=0.

$$F_z^{cl}(Q,T) = e^{-(k_b T Q^2/M\omega_0^2)[1-\cos(\omega_0 t)]}$$

22.51 Quantum Theory of Radiation Interactions
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