

Scattering from Free Atoms [nl93]

Consider a dilute gas of atoms with mass M . Interaction between gas atoms limited to (rare) collisions.

Hamiltonian: $\mathcal{H} = \frac{p^2}{2M}$ (dominated by kinetic energy).

Contact interaction between gas atom at position $\mathbf{R}(t)$ and scattering radiation (see [nl93]) defines dynamical variable relevant for scattering process:

$$A(\mathbf{q}, t) = \int d^3r e^{i\mathbf{q}\cdot\mathbf{r}} \delta(\mathbf{r} - \mathbf{R}(t)) = e^{i\mathbf{q}\cdot\mathbf{R}(t)}. \quad (1)$$

Equation of motion (setting $\hbar \equiv 1$):¹

$$i \frac{\partial A}{\partial t} = [A, \mathcal{H}] = \frac{1}{2M} [e^{i\mathbf{q}\cdot\mathbf{R}}, p^2] = -A \frac{1}{2M} (2\mathbf{q} \cdot \mathbf{p} + q^2). \quad (2)$$

Formal solution:

$$A(\mathbf{q}, t) = e^{i\mathbf{q}\cdot\mathbf{R}(0)} \exp\left(\frac{it(2\mathbf{q} \cdot \mathbf{p} + q^2)}{2M}\right). \quad (3)$$

Correlation function: $\tilde{S}_{AA}(\mathbf{q}, t) \doteq \langle A^\dagger(\mathbf{q}, t) A(\mathbf{q}, 0) \rangle$.

$$\begin{aligned} \Rightarrow \tilde{S}_{AA}(\mathbf{q}, t) &\doteq e^{-itq^2/2M} \langle \exp(-it\mathbf{q} \cdot \mathbf{p}/M) \rangle \\ &= e^{-itq^2/2M} \frac{1}{Z} \int d^3p e^{-\beta p^2/2M} e^{-it\mathbf{q}\cdot\mathbf{p}/M} \\ &= e^{-itq^2/2M} \frac{1}{Z} \int d^3p \underbrace{\exp\left(\frac{(\sqrt{\beta}\mathbf{p} + it\mathbf{q}/\sqrt{\beta})^2}{2M}\right)}_Z e^{-q^2 t^2/2M\beta} \\ &= \exp\left(-\frac{q^2(t^2/\beta + it)}{2M}\right). \end{aligned} \quad (4)$$

Third line: Gaussian integral is unaffected by a constant shift in \mathbf{p} .

Note symmetry property from [nl93]: $\tilde{S}_{AA}(\mathbf{q}, -t) = \tilde{S}_{AA}(\mathbf{q}, t - i\beta)$.

¹Use $[\mathbf{R}, \mathbf{p}] = i$, $[A, \mathbf{p}] = -\mathbf{q}A$, $[A, p^2] = [A, \mathbf{p}] \cdot \mathbf{p} + \mathbf{p} \cdot [A, \mathbf{p}] = -A\mathbf{q} \cdot \mathbf{p} - \mathbf{p} \cdot \mathbf{q}A$, $A\mathbf{q} \cdot \mathbf{p} - \mathbf{p} \cdot \mathbf{q}A = -Aq^2$, $\Rightarrow [A, p^2] = -A(2\mathbf{q} \cdot \mathbf{p} + q^2)$.

Dynamic structure factor via Fourier transform:

$$\begin{aligned}
 S_{AA}(\mathbf{q}, \omega) &\doteq \int_{-\infty}^{+\infty} dt e^{i\omega t} \tilde{S}_{AA}(\mathbf{q}, t) \\
 &= \sqrt{\frac{2\pi M\beta}{q^2}} \exp\left(-\frac{M\beta}{2q^2} [\omega - q^2/2M]^2\right). \quad (5)
 \end{aligned}$$

- Scattering is isotropic, only dependent on magnitude of \mathbf{q} .
- Maximum intensity occurs when energy transfer ω and momentum transfer \mathbf{q} reflect energy momentum relation, $\omega = q^2/2M$, of free, non-relativistic gas particle.
- Lineshape broadens with increasing temperature and/or decreasing mass of gas atoms.
- Note detailed-balance condition from [nl39]:

$$S_{AA}(\mathbf{q}, -\omega) = e^{-\beta\omega} S_{AA}(\mathbf{q}, \omega).$$

- In the limit $M \rightarrow \infty$ at fixed temperature, the atoms slow down and come to rest. The scattering becomes elastic in nature, still isotropic and with zero energy transfer:

$$S_{AA}(\mathbf{q}, \omega) \xrightarrow{M \rightarrow \infty} 2\pi\delta(\omega).$$

