Scattering from Free Atoms [nln93]

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

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

Contact interaction between gas atom at position $\mathbf{R}(t)$ and scattering radiation (see [nln89]) defines dynamical variable relevant for scattering process:

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

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

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

Formal solution:

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

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

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

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

Note symmetry property from [nln39]: $\tilde{S}_{AA}(\mathbf{q},-t) = \tilde{S}_{AA}(\mathbf{q},t-\imath\beta)$.

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

Dynamic structure factor via Fourier transform:

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

- Scattering is isotropic, only dependent on magnitude of **q**.
- Maximum intensity occurs when energy transfer ω and momentum transfer **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 [nln39]:

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

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

$$S_{AA}(\mathbf{q},\omega) \stackrel{M\to\infty}{\longrightarrow} 2\pi\delta(\omega).$$