22.51 Problem Set 9 (due Fri, Dec. 7)

1 Born's Approximation

Question: Instead of using the heavier machinery of time-dependent perturbation theory, the differential scattering cross-section $d\sigma/d\Omega$ between neutron and a *static* potential field $V(\mathbf{x})$ can be derived by solving merely the steady-state Schrodinger's equation.

(**a**). Suppose $\psi(\mathbf{x})$ is a solution to the one-body problem,

$$\left(-\frac{\hbar^2\nabla^2}{2\mu}+V(\mathbf{x})\right)\psi(\mathbf{x}) \quad = \quad \frac{\hbar^2k^2}{2\mu}\psi(\mathbf{x}), \tag{1}$$

and it has the following asymptotic behavior at large $|\mathbf{x}|$,

$$\psi(\mathbf{x}) \quad = \quad e^{i\mathbf{k}\cdot\mathbf{x}}+f(\theta)\frac{e^{i|\mathbf{k}||\mathbf{x}|}}{|\mathbf{x}|}+\mathcal{O}(|\mathbf{x}|^{-2}), \tag{2}$$

where θ is the angle between $\mathbf{x}$ and the incident wave-vector $\mathbf{k}$. Show that,

$$\frac{d\sigma}{d\Omega} \quad = \quad |f(\theta)|^2.$$

(**b**). We may rewite (1) as,

$$\left(\nabla^2+k^2\right)\psi(\mathbf{x}) \quad = \quad \frac{2\mu V(\mathbf{x})}{\hbar^2}\psi(\mathbf{x}). \tag{3}$$

What are the general solutions $\{\psi_0(\mathbf{x})\}$ to,

$$\left(\nabla^2+k^2\right)\psi_0(\mathbf{x}) \quad = \quad 0, \qquad \mathbf{x}\in\mathbf{R}^3,$$

and what is the Green's function solution $g(\mathbf{x})$ to,

$$\left(\nabla^2+k^2\right)g(\mathbf{x}) \quad = \quad \delta(\mathbf{x}).$$

(**c**). Given the scattering problem context, pick the general solution $\psi_0(\mathbf{x})$, and write down a formal "solution" to (3).

(**d**). Following the same procedure as in time-dependent perturbation theory, write down a series expansion for the exact solution.

(**e**). Take the leading term and take the large $|\mathbf{x}|$ limit, derive $f(\theta)$ in terms of $V(\mathbf{x})$.

(**f**). Suppose,

$$V(\mathbf{x}) = -\frac{2\pi\hbar^2}{\mu} a\delta(\mathbf{x}),$$

what is the total scattering cross-section and how should one then interpret a?

(**g**). Show by rigorous quantum mechanics the relationship between a and b, the free and bound scattering lengths.

Answer:

(**a**). See Fig. 1. The incident beam $e^{i\mathbf{k}\cdot\mathbf{x}}$ does have finite width, which is enough to cover the sample, but will not be received by the detector.

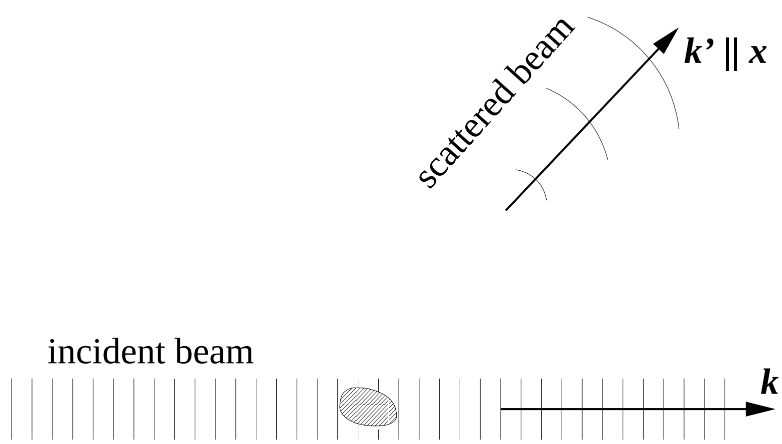

Figure 1: The incident beam $e^{i\mathbf{k}\cdot\mathbf{x}}$ does have finite width.

The particle flux formula is,

$$\mathbf{j} = -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right), \tag{4}$$

since,

$$\begin{aligned} -\nabla\cdot\mathbf{j} &= \frac{i\hbar}{2m}\nabla\cdot\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \\ &= \frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) \\ &= \psi^*\left(\dot{\psi} - \frac{V\psi}{i\hbar}\right) + \psi\left(\dot{\psi^*} + \frac{V\psi^*}{i\hbar}\right) \\ &= \psi^*\dot{\psi} + \psi\dot{\psi^*} \end{aligned}$$

$$= \quad \dot{\rho}. \tag{5}$$

One could work out the scattered flux exactly, but that is not necessary because at large $|\mathbf{x}|$, $f(\theta)e^{i|k||\mathbf{x}|}/|\mathbf{x}|$ behaves locally very much like a planewave $e^{i\mathbf{k}'\cdot\mathbf{x}}$, with,

$$\mathbf{k}' \equiv \frac{|\mathbf{k}|\mathbf{x}}{|\mathbf{x}|},$$

and amplitude $f(\theta)/|\mathbf{x}|$. The reason is because since,

$$\nabla = \mathbf{e}_r\partial_r + \frac{\mathbf{e}_\theta}{r}\partial_\theta + \frac{\mathbf{e}_\phi}{r\sin\theta}\partial_\phi,$$

the only $\mathcal{O}(r^{-1})$ term in (4) is from the radial derivative $\mathbf{e}_r\partial_r$. Thus, the scattered flux must be,

$$\frac{\Phi_{\text{scattered}}}{\Phi_{\text{incident}}} = \left|\frac{f(\theta)}{r}\right|^2,$$

compared to the incident flux because both are like planewaves. Therefore the number of outgoing quanta per unit time in solid angle $d\Omega$ is simply,

$$\frac{dN}{dt} = \Phi_{\text{scattered}}dS = \Phi_{\text{scattered}} \cdot r^2 d\Omega = \Phi_{\text{incident}}|f(\theta)|^2 d\Omega,$$

therefore,

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Phi_{\text{incident}}}\frac{dN}{d\Omega dt} = |f(\theta)|^2.$$

(**b**). The general solutions are planewaves $e^{i\mathbf{k}\cdot\mathbf{x}}$, $\forall\mathbf{k} \in \{|\mathbf{k}| = k\}$.

The Green's functions $g(\mathbf{x})$ are,

$$g(\mathbf{x}) = -\frac{e^{\pm ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}.$$

However, the $e^{-ik|\mathbf{x}|}/|\mathbf{x}|$ branch is not physically possible (mathematically speaking, it does not satisfy the boundary condition) because it represents spherically incoming wave. One can check that,

$$\begin{aligned}
\left(\nabla^2 + k^2\right)\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|} &= \left(r^{-2}\partial_r r^2\partial_r + k^2\right)\frac{e^{ikr}}{r} \\
&= r^{-2}\partial_r r^2\left(ik\frac{e^{ikr}}{r} - \frac{e^{ikr}}{r^2}\right) + k^2\frac{e^{ikr}}{r} \\
&= r^{-2}\partial_r\left(ikre^{ikr} - e^{ikr}\right) + k^2\frac{e^{ikr}}{r}
\end{aligned}$$

$$
\begin{aligned}
&= r^{-2}\left(ike^{ikr} - k^2 r e^{ikr} - ike^{ikr}\right) + k^2\frac{e^{ikr}}{r} \\
&= 0, \qquad r > 0. \qquad (6)
\end{aligned}
$$

When $r \to 0$, $-\frac{e^{ikr}}{4\pi r} \sim -\frac{1}{4\pi r}$, which was previously shown to be the Green's function to $\nabla^2 g(\mathbf{x}) = \delta(\mathbf{x})$ and has the same singular properties.

(**c**). Let us pick a particular planewave,

$$
\psi_0(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}},
$$

which is interpreted as the incident beam and a solution to (3) when $V(\mathbf{x}) = 0$. Using the Green's function, the formal solution to (3) when $V(\mathbf{x}) \neq 0$ can be simply written as,

$$
\begin{aligned}
\psi(\mathbf{x}) &= e^{i\mathbf{k}\cdot\mathbf{x}} - \int d\mathbf{x}' \frac{2\mu V(\mathbf{x}')\psi(\mathbf{x}')}{\hbar^2} \cdot \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \\
&= e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}' \tilde{V}(\mathbf{x}') \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\psi(\mathbf{x}'), \qquad (7)
\end{aligned}
$$

where,

$$
\tilde{V}(\mathbf{x}) \equiv -\frac{\mu}{2\pi\hbar^2} V(\mathbf{x}),
$$

is the reduced potential that has unit of length.

(**d**). The (7) solution for $\psi(\mathbf{x})$ is not directly usable because $\psi(\mathbf{x})$ itself is invoked in the expression. But under the conditions that $\tilde{V}(\mathbf{x})$ can be considered as small, one can use the trick of iterative replacement,

$$
\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}' \tilde{V}(\mathbf{x}') \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} e^{i\mathbf{k}\cdot\mathbf{x}'} + \int d\mathbf{x}' \tilde{V}(\mathbf{x}') \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \int d\mathbf{x}'' \tilde{V}(\mathbf{x}'') \frac{e^{ik|\mathbf{x}'-\mathbf{x}''|}}{|\mathbf{x}'-\mathbf{x}''|} e^{i\mathbf{k}\cdot\mathbf{x}''} + \ldots,
$$

which is in effect an expansion in orders of $\tilde{V}(\mathbf{x})$.

(**e**). The leading order term is,

$$
\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}' \tilde{V}(\mathbf{x}') \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} e^{i\mathbf{k}\cdot\mathbf{x}'}.
$$

In the limit of large $|\mathbf{x}|$: $|\mathbf{x}| \gg |\mathbf{x}'|$,

$$
|\mathbf{x}-\mathbf{x}'| = |\mathbf{x}| - \frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|} + \mathcal{O}\left(\frac{|\mathbf{x}'|^2}{|\mathbf{x}|}\right),
$$

Let us define,

$$\mathbf{k}' \equiv k\frac{\mathbf{x}}{|\mathbf{x}|},$$

then,

$$e^{ik|\mathbf{x}-\mathbf{x}'|} \approx e^{ik|\mathbf{x}|}e^{-i\mathbf{k}'\cdot\mathbf{x}'}.$$

Also,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{|\mathbf{x}|} + \mathcal{O}\left(\frac{|\mathbf{x}'|}{|\mathbf{x}|^2}\right).$$

Therefore,

$$\psi(\mathbf{x}) \approx e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}'\tilde{V}(\mathbf{x}')\frac{e^{ik|\mathbf{x}|}e^{-i\mathbf{k}'\cdot\mathbf{x}'}}{|\mathbf{x}|}e^{i\mathbf{k}\cdot\mathbf{x}'} = e^{i\mathbf{k}\cdot\mathbf{x}} + f(\theta)\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|},$$

with,

$$f(\theta) = \int d\mathbf{x}'\tilde{V}(\mathbf{x}')e^{i\mathbf{Q}\cdot\mathbf{x}'}, \qquad \mathbf{Q} \equiv \mathbf{k} - \mathbf{k}'.$$

In other words, $f(\theta)$ is simply the spatial Fourier transform of $\tilde{V}(\mathbf{x})$ in wavevector $\mathbf{Q}$ which spans angle θ.

(**f**). Clearly $\tilde{V}(\mathbf{x}) = a\delta(\mathbf{x})$ and $f(\theta) = a$. Therefore the total scattering cross-section is $4\pi a^2$. In a one-body problem where,

$$\tilde{V}(\mathbf{x}) = \begin{cases} \infty, & |\mathbf{x}| < a \\ 0, & |\mathbf{x}| \geq a \end{cases},$$

the quantum mechanical total scattering cross section turns out to be $4\pi a^2$ in the long-wavelength limit (as compared to πa^2 total scattering cross section in classical mechanics). Therefore, a can be interpreted as the interaction cutoff distance between hard spheres.

(**g**). A two-body quantum mechanics problem,

$$\left(-\frac{\hbar^2\nabla_1^2}{2m_1} - \frac{\hbar^2\nabla_2^2}{2m_2} + V(\mathbf{x}_1 - \mathbf{x}_2)\right)\Psi(\mathbf{x}_1,\mathbf{x}_2) = \tilde{E}\Psi(\mathbf{x}_1,\mathbf{x}_2),$$

can be transformed to,

$$\left(-\frac{\hbar^2\nabla_\mathbf{x}^2}{2\mu} - \frac{\hbar^2\nabla_\mathbf{X}^2}{2M} + V(\mathbf{x})\right)\Psi(\mathbf{x},\mathbf{X}) = \tilde{E}\Psi(\mathbf{x},\mathbf{X}),$$

where,

$$\mathbf{x} \equiv \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{X} \equiv \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}, \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}, \quad M \equiv m_1 + m_2,$$

so,

$$\Psi(\mathbf{x}, \mathbf{X}) = \psi(\mathbf{x}) e^{i\mathbf{K}\cdot\mathbf{X}}, \quad \tilde{E} = E + \frac{\hbar^2 K^2}{2M},$$

with,

$$\left(-\frac{\hbar^2 \nabla_{\mathbf{x}}^2}{2\mu} + V(\mathbf{x})\right)\psi(\mathbf{x}) = E\psi(\mathbf{x}).$$

The scattering cross-section is clearly 0 when $V = 0$. Since,

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{x}) = \frac{2\mu V(\mathbf{x})}{\hbar^2}\psi(\mathbf{x}),$$

the leading order perturbation to $\psi(\mathbf{x})$ is also proportional to μ. Therefore,

$$\sigma_{\text{bound}} = \left(1 + \frac{m_{\text{N}}}{m_{\text{A}}}\right)^2 \sigma_{\text{free}},$$

in the long wavelength limit and when the Born approximation is valid.

2 Contrast Variation

Question: A certain element E has two isotopes, E^{41} and E^{44}. E^{41} has spin $2\hbar$, E^{44} has spin $3\hbar$. The scattering lengths are,

$$b^+_{\text{E}^{41}} = 1 \times 10^{-12}\text{cm}, \quad b^-_{\text{E}^{41}} = 3 \times 10^{-12}\text{cm}, \quad b^+_{\text{E}^{44}} = -2 \times 10^{-12}\text{cm}, \quad b^-_{\text{E}^{44}} = -4 \times 10^{-12}\text{cm},$$

where $+$ and $-$ means spin aligned and anti-aligned between incoming neutron and the nucleus, respectively.

(**a**). What are the coherent and incoherent scattering lengths for E^{41} and E^{44}, suppose each isotope appears in pure form, respectively?

(**b**). Suppose the natural abundance of E^{41} is 80% and that of E^{44} is 20%, calculate the coherent and incoherent scattering lengths of pure natural E.

(**c**). Calculate the desired abundance of E^{41} in order to have only incoherent scattering.

(**d**). There is simple mixing rule for b_{coh}. Is there for b_{inc}? for b^2_{inc}? (e.g., if there is 80% E^{41}

and 20% E^{44}, is $b_{\text{inc}}^2(\text{E}) = 0.8 b_{\text{inc}}^2(\text{pure E}^{41}) + 0.2 b_{\text{inc}}^2(\text{pure E}^{44})$?)

Answer:

(**a**). For pure E^{41},

$$b_{\text{coh}} = \frac{2\times 2+2}{4\times 2+2}\times 1 + \frac{2\times 2}{4\times 2+2}\times 3 = 1.8\sqrt{\text{barn}},$$

$$\overline{b^2} = \frac{2\times 2+2}{4\times 2+2}\times 1 + \frac{2\times 2}{4\times 2+2}\times 9 = 4.2 \text{ barn},$$

so,

$$b_{\text{inc}} = \sqrt{\overline{b^2} - b_{\text{coh}}^2} = 0.9798\sqrt{\text{barn}}.$$

For pure E^{44},

$$b_{\text{coh}} = \frac{2\times 3+2}{4\times 3+2}\times (-2) + \frac{2\times 3}{4\times 3+2}\times (-4) = -2.8571\sqrt{\text{barn}},$$

$$\overline{b^2} = \frac{2\times 3+2}{4\times 3+2}\times 4 + \frac{2\times 3}{4\times 3+2}\times 16 = 9.1429 \text{ barn},$$

so,

$$b_{\text{inc}} = \sqrt{\overline{b^2} - b_{\text{coh}}^2} = 0.9899\sqrt{\text{barn}}.$$

(**b**).

$$b_{\text{coh}} = 0.8\times 1.8 + 0.2\times(-2.8571) = 0.8686\sqrt{\text{barn}}.$$

$$\overline{b^2} = 0.8\times 4.2 + 0.2\times 9.1429 = 5.1886 \text{ barn},$$

so,

$$b_{\text{inc}} = \sqrt{\overline{b^2} - b_{\text{coh}}^2} = 2.1057\sqrt{\text{barn}}.$$

(**c**). Let the abundance of E^{41} be x, then,

$$b_{\text{coh}} = x\times 1.8 + (1-x)\times(-2.8571) = 0,$$

demands that $x = 0.6135$.

(**d**). There is no simple mixing rule for either b_{inc} or b_{inc}^2. We can have isotopes of the same b_{inc}, but if their b_{coh}'s are different, their mixed b_{inc} is going to be enhanced.

3 Dynamic Structure Factor

Question:

(**a**). Calculate the thermally averaged self intermediate scattering function,

$$F_s(\mathbf{Q}, t) \equiv \left\langle e^{-i\mathbf{Q}\cdot\hat{\mathbf{x}}(0)} e^{i\mathbf{Q}\cdot\hat{\mathbf{x}}(t)} \right\rangle,$$

and the self dynamic structure factor $S_s(\mathbf{Q}, \omega)$ for ideal gas at temperature T.

(**b**). Do the same for a single harmonic oscillator of frequency Ω at temperature T.

Hint: Use the Baker-Hausdorff theorem.

Answer:

Let me do (**b**) first, and then by taking the $\Omega \to 0$ limit, we can obtain the ideal gas behavior.

(**b**). For 1D simple harmonic oscillator, we know that,

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m_A\Omega}} \left(\hat{a}(t) + \hat{a}^\dagger(t)\right), \quad \hat{a}(t) = \hat{a}e^{-i\Omega t}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger e^{i\Omega t},$$

in the Heisenberg picture. Therefore,

$$[\hat{x}(0), \hat{x}(t)] = \frac{\hbar}{2m_A\Omega}\left[\hat{a} + \hat{a}^\dagger, \hat{a}e^{-i\Omega t} + \hat{a}^\dagger e^{i\Omega t}\right] = \frac{\hbar}{2m_A\Omega} 2i\sin\Omega t = \frac{i\hbar}{m_A\Omega}\sin\Omega t.$$

Since it is just a constant which commutes with *any* operator, we can use the Baker-Hausdorff theorem,

$$\begin{aligned} e^{-iQ\hat{x}(0)}e^{iQ\hat{x}(t)} &= \exp\left(iQ\sqrt{\frac{\hbar}{2m_A\Omega}}\left[(e^{-i\Omega t}-1)\hat{a} + (e^{i\Omega t}-1)\hat{a}^\dagger\right] + \frac{iQ^2\hbar}{2m_A\Omega}\sin\Omega t\right) \\ &= \exp\left(\frac{iQ^2\hbar}{2m_A\Omega}\sin\Omega t\right)\hat{D}(\alpha(t)), \end{aligned} \tag{8}$$

where $\hat{D}(\alpha(t))$ is the displacement operator, with,

$$\alpha(t) \equiv iQ\sqrt{\frac{\hbar}{2m_A\Omega}}(e^{i\Omega t} - 1).$$

We would like to calculate the thermal average $\langle \hat{D}(\alpha)\rangle$ using complete but non-orthogonal coherent states basis. The following identities will be used.

$$
\begin{aligned}
\hat{D}(\alpha)\hat{D}(\beta) &= e^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\hat{D}(\alpha+\beta). \\
\langle\alpha|\beta\rangle &= e^{\alpha^*\beta-\frac{1}{2}(|\alpha|^2+|\beta|^2)}. \\
\int\frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| &= \mathbf{I}. \\
\langle n|\beta\rangle &= e^{-\frac{1}{2}|\beta|^2}\frac{\beta^n}{\sqrt{n!}}.
\end{aligned}
$$

Now consider,

$$
\begin{aligned}
\langle n|\hat{D}(\alpha)|n\rangle &= \int\frac{d^2\gamma}{\pi}\int\frac{d^2\beta}{\pi}\langle n|\gamma\rangle\langle\gamma|\hat{D}(\alpha)|\beta\rangle\langle\beta|n\rangle \\
&= \int\frac{d^2\gamma}{\pi}\int\frac{d^2\beta}{\pi}e^{-\frac{1}{2}|\gamma|^2}\frac{\gamma^n}{\sqrt{n!}}\langle\gamma|\hat{D}(\alpha)|\beta\rangle e^{-\frac{1}{2}|\beta|^2}\frac{\beta^{*n}}{\sqrt{n!}} \\
&= \int\frac{d^2\gamma}{\pi}\int\frac{d^2\beta}{\pi}e^{-\frac{1}{2}(|\gamma|^2+|\beta|^2)}\frac{(\beta^*\gamma)^n}{n!}\langle\gamma|\hat{D}(\alpha)\hat{D}(\beta)|0\rangle \\
&= \int\frac{d^2\gamma}{\pi}\int\frac{d^2\beta}{\pi}e^{-\frac{1}{2}(|\gamma|^2+|\beta|^2)}\frac{(\beta^*\gamma)^n}{n!}e^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\langle\gamma|\alpha+\beta\rangle \\
&= \int\frac{d^2\gamma}{\pi}\int\frac{d^2\beta}{\pi}e^{-\frac{1}{2}(|\gamma|^2+|\beta|^2)}\frac{(\beta^*\gamma)^n}{n!}e^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}e^{\gamma^*(\alpha+\beta)-\frac{1}{2}(|\gamma|^2+|\alpha+\beta|^2)}. \quad (9)
\end{aligned}
$$

Since,

$$
\sum_{n=0}^{\infty}e^{-\frac{n\hbar\Omega}{k_{\mathrm{B}}T}} = \frac{1}{1-e^{-\frac{\hbar\Omega}{k_{\mathrm{B}}T}}} = \frac{1}{1-d},\quad \sum_{n=0}^{\infty}e^{-\frac{n\hbar\Omega}{k_{\mathrm{B}}T}}\frac{(\beta^*\gamma)^n}{n!} = \exp\left(e^{-\frac{\hbar\Omega}{k_{\mathrm{B}}T}}\beta^*\gamma\right) = e^{d\beta^*\gamma},\quad d\equiv e^{-\frac{\hbar\Omega}{k_{\mathrm{B}}T}}.
$$

we have,

$$
\begin{aligned}
\langle\hat{D}(\alpha)\rangle = &\quad (1-d)\int\frac{d^2\gamma d^2\beta}{\pi^2}e^{-\frac{1}{2}(|\gamma|^2+|\beta|^2)}e^{d\beta^*\gamma}e^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)+\gamma^*\alpha+\gamma^*\beta-\frac{1}{2}(|\gamma|^2+|\alpha|^2+|\beta|^2+\alpha^*\beta+\alpha\beta^*)} \\
= &\quad (1-d)e^{-\frac{1}{2}|\alpha|^2}\int\frac{d^2\gamma d^2\beta}{\pi^2}e^{-|\gamma|^2-|\beta|^2+d\beta^*\gamma+\gamma^*\beta+\gamma^*\alpha-\alpha^*\beta}. \quad (10)
\end{aligned}
$$

The above is just a Gaussian integral in 4D. Let,

$$
\alpha \equiv \alpha_x+i\alpha_y,\quad \beta \equiv \beta_x+i\beta_y,\quad \gamma \equiv \gamma_x+i\gamma_y,
$$

we have,

$$
\beta^*\gamma = (\beta_x-i\beta_y)(\gamma_x+i\gamma_y) = \beta_x\gamma_x+\beta_y\gamma_y+i(\beta_x\gamma_y-\beta_y\gamma_x),
$$

$$\gamma^*\beta \;=\; \gamma_x\beta_x + \gamma_y\beta_y + i(\gamma_x\beta_y - \gamma_y\beta_x).$$

Thus, inside the exponential, the function is,

$$-\begin{pmatrix} \beta_x & \beta_y & \gamma_x & \gamma_y \end{pmatrix} \begin{pmatrix} 1 & 0 & -\frac{1+d}{2} & -\frac{1-d}{2i} \\ 0 & 1 & \frac{1-d}{2i} & -\frac{1+d}{2} \\ -\frac{1+d}{2} & \frac{1-d}{2i} & 1 & 0 \\ -\frac{1-d}{2i} & -\frac{1+d}{2} & 0 & 1 \end{pmatrix} \begin{pmatrix} \beta_x \\ \beta_y \\ \gamma_x \\ \gamma_y \end{pmatrix} \quad + \quad \begin{pmatrix} -\alpha^* & -i\alpha^* & \alpha & -i\alpha \end{pmatrix} \begin{pmatrix} \beta_x \\ \beta_y \\ \gamma_x \\ \gamma_y \end{pmatrix} \quad , \tag{11}$$

and since,

$$\int d^D\mathbf{x} \exp\left(-\mathbf{x}^T\mathbf{A}\mathbf{x} + \mathbf{b}\mathbf{x}\right) \;=\; \frac{(\pi)^{D/2}}{\sqrt{\det|\mathbf{A}|}} \exp\left(-\frac{1}{4}\mathbf{b}^T\mathbf{A}^{-1}\mathbf{b}\right),$$

the integral is straightforward, but cumbersome. Therefore using Maple we get,

$$\langle\hat{D}(\alpha)\rangle \;=\; (1-d)e^{-\frac{1}{2}|\alpha|^2}\frac{1}{\pi^2}\cdot\frac{e^{-\frac{d|\alpha|^2}{1-d}}\pi^2}{1-d} \;=\; e^{-\frac{1}{2}|\alpha|^2}e^{-\frac{d|\alpha|^2}{1-d}} \;=\; e^{-\frac{|\alpha|^2(1+d)}{2(1-d)}}. \tag{12}$$

```
> restart: int(int(int(
  exp(-GX^2-GY^2-BX^2-BY^2+d*(BX-I*BY)*(GX+I*GY)+(GX-I*GY)*(BX+I*BY)
  +(GX-I*GY)*a-conjugate(a)*(BX+I*BY)),GX=-infinity..infinity),GY=-i
  nfinity..infinity),BY=-infinity..infinity);
```

$$\begin{cases} \dfrac{\mathbf{e}^{\left(1/4\,\frac{4\,d^2\,BX\,a-4\,d\,BX\,a-4\,\bar{a}\,BX\,d+4\,\bar{a}\,BX+4\,d^2\,BX^2-8\,d\,BX^2+4\,BX^2+d^2\,a^2+2\,d\,a\,\bar{a}+\bar{a}^2}{d-1}\right)}\,\pi^{(3/2)}}{\sqrt{-d+1}}, & -\mathrm{csgn}(d-1)=1 \\ \infty, & \mathit{otherwise} \end{cases}$$

```
> int(exp(1/4*(4*d^2*BX*a-4*d*BX*a-4*conjugate(a)*BX*d+4*conjugate(a
  )*BX+4*d^2*BX^2-8*d*BX^2+4*BX^2+d^2*a^2+2*d*a*conjugate(a)+conjuga
  te(a)^2)/(d-1))*Pi^(3/2)/(-d+1)^(1/2), BX=-infinity..infinity);
```

$$\begin{cases} \dfrac{\mathbf{e}^{\left(\frac{d\,a\,\bar{a}}{d-1}\right)}\,\pi^2}{-d+1} & \mathrm{csgn}\left(-\dfrac{d^2}{d-1}+\dfrac{2\,d}{d-1}-\dfrac{1}{d-1}\right)=1 \\ \infty & \mathit{otherwise} \end{cases}$$

Thus,

$$
\begin{aligned}
& \langle e^{-iQ\hat{x}(0)} e^{iQ\hat{x}(t)} \rangle \\
= \quad & \exp\left(\frac{iQ^2\hbar}{2m_A\Omega} \sin\Omega t - \frac{|\alpha(t)|^2(1+d)}{2(1-d)} \right) \\
= \quad & \exp\left(\frac{iQ^2\hbar}{2m_A\Omega} \sin\Omega t - \frac{Q^2\hbar}{2m_A\Omega}(e^{i\Omega t}-1)(e^{-i\Omega t}-1)\frac{(1+d)}{2(1-d)} \right) \\
= \quad & \exp\left(\frac{Q^2\hbar}{4m_A\Omega} \left(e^{i\Omega t} - e^{-i\Omega t} - (2 - e^{i\Omega t} - e^{-i\Omega t})\frac{1+d}{1-d} \right) \right) \\
= \quad & \exp\left(\frac{Q^2\hbar}{4m_A\Omega} \frac{(1-d)e^{i\Omega t} - (1-d)e^{-i\Omega t} - 2(1+d) + (1+d)e^{i\Omega t} + (1+d)e^{-i\Omega t}}{1-d} \right) \\
= \quad & \exp\left(\frac{Q^2\hbar}{4m_A\Omega} \frac{2e^{i\Omega t} + 2de^{-i\Omega t} - 2(1+d)}{1-d} \right) \\
= \quad & \exp\left(\frac{Q^2\hbar}{2m_A\Omega} \frac{(e^{i\Omega t}-1) + d(e^{-i\Omega t}-1)}{1-d} \right). \qquad (13)
\end{aligned}
$$

At low T, $d \sim 0$, so,

$$\langle e^{-iQ\hat{x}(0)} e^{iQ\hat{x}(t)} \rangle = \exp\left(\frac{Q^2\hbar}{2m_A\Omega}(e^{i\Omega t}-1) \right) = \exp\left(-\frac{Q^2\hbar}{2m_A\Omega} \right) \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{Q^2\hbar}{2m_A\Omega} \right)^n e^{in\Omega t},$$

and,

$$S_s(Q,\omega) = \exp\left(-\frac{Q^2\hbar}{2m_A\Omega} \right) \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{Q^2\hbar}{2m_A\Omega} \right)^n \delta(\omega - n\Omega),$$

so the neutron is only able to deposit energy in quantas of $\hbar\Omega$.

At high T, $d \sim 1 - \frac{\hbar\Omega}{k_{\mathrm{B}}T}$, so,

$$\frac{(e^{i\Omega t}-1) + d(e^{-i\Omega t}-1)}{1-d} \approx \frac{k_{\mathrm{B}}T}{\hbar\Omega} \left(e^{i\Omega t} + de^{-i\Omega t} - 1 - d \right),$$

and we will find that the neutron is able to both extract and deposit energy, with the probability of the latter a little bit greater.

In 3D, we would have,

$$\langle e^{-i\mathbf{Q}\cdot\hat{x}(0)} e^{i\mathbf{Q}\cdot\hat{x}(t)} \rangle = \prod_{i=1}^{3} \exp\left(\frac{Q_i^2\hbar}{2m_A\Omega_i} \frac{(e^{i\Omega_i t}-1) + d_i(e^{-i\Omega_i t}-1)}{1-d_i} \right),$$

where Ω_x, Ω_y, Ω_z are the oscillator frequencies in three directions.

(**a**). Let us take the $\Omega \to 0$ limit. Since,

$$
\begin{aligned}
\frac{(e^{i\Omega t}-1)+d(e^{-i\Omega t}-1)}{\Omega(1-d)} &\approx \frac{k_{\rm B}T}{\hbar\Omega^2}\left(i\Omega t-\frac{\Omega^2t^2}{2}+d(-i\Omega t)-d\frac{\Omega^2t^2}{2}\right)\\
&= \frac{k_{\rm B}T}{\hbar\Omega^2}\left(\frac{\hbar\Omega}{k_{\rm B}T}i\Omega t-\Omega^2t^2\right)\\
&= it-\frac{k_{\rm B}Tt^2}{\hbar}, \qquad (14)
\end{aligned}
$$

we have,

$$
\langle e^{-i\mathbf{Q}\cdot\hat{x}(0)}e^{i\mathbf{Q}\cdot\hat{x}(t)}\rangle = \exp\left(-\frac{|\mathbf{Q}|^2\hbar}{2m_A}\left(\frac{k_{\rm B}Tt^2}{\hbar}-it\right)\right).
$$

```
> restart: simplify(int(
  exp(-Q^2*hbar/2/m*(k*T*t^2/hbar-I*t)-I*omega*t)/2/Pi,
  t=-infinity..infinity));
```

$$
\begin{cases} \dfrac{1}{2}\dfrac{e^{\left(-1/8\frac{(-Q^2\,hbar+2\,\omega\,m)^2}{m\,Q^2\,k\,T}\right)}\sqrt{2}}{\sqrt{\pi}\sqrt{\dfrac{Q^2\,k\,T}{m}}} & \mathrm{csgn}(Q^2\,\overline{m}\,k\,T)=1 \\ \infty & \textit{otherwise} \end{cases}
$$

Thus, the dynamic structure factor of ideal gas is,

$$
S(\mathbf{Q},\omega) = S_s(\mathbf{Q},\omega) = \frac{1}{\sqrt{2\pi|\mathbf{Q}|^2k_{\rm B}T/m_A}}\exp\left(-\frac{(|\mathbf{Q}|^2\hbar-2m_A\omega)^2}{8m_A|\mathbf{Q}|^2k_{\rm B}T}\right),
$$

with the loss peaking at,

$$
\omega_0 = \frac{\hbar|\mathbf{Q}|^2}{2m_A}.
$$

When $T=0$, it is a free standing particle, and,

$$
S(\mathbf{Q},\omega) = \delta\left(\omega-\frac{\hbar|\mathbf{Q}|^2}{2m_A}\right).
$$

So,

$$
\frac{d^2\sigma}{d\Omega d\omega} = b^2\left(\frac{k'}{k}\right)S(\mathbf{Q},\omega) = b^2\left(\frac{k'}{k}\right)\delta\left(\omega-\frac{\hbar|\mathbf{Q}|^2}{2m_A}\right),
$$

or,

$$\frac{d^2\sigma}{d\Omega dE'} = b^2\left(\frac{k'}{k}\right)\delta\left(E-E'-\frac{\hbar^2|\mathbf{Q}|^2}{2m_A}\right).$$

At this moment it is important to remember what the dependent variables are. Recall that in the derivation, we are lastly down to counting $d^3\mathbf{k}'^3$ of the outgoing radiation, and it is converted to spherical shell differential $dE'd\Omega$. Therefore, the dependent variables are direction Ω ($\cos\theta$) and E' which are just indices for counting $\mathbf{k}'$. A common mistake is to think that $\mathbf{Q}$ and ω are somehow the dependent variables since $S(\mathbf{Q},\omega)$ is *expressed* in them. It is not so. For example, the partial integration in ω of $\delta\left(\omega-\frac{\hbar|\mathbf{Q}|^2}{2m_A}\right)$ gives 1 if $\mathbf{Q}$ and ω are considered independent, but that is the wrong answer. The correct answer, when considering the dependence of $|\mathbf{Q}|^2$ on ω for fixed $\cos\theta$, would give a factor different from 1.

$$\frac{\hbar^2|\mathbf{Q}|^2}{2m_A} = \frac{\hbar^2|\mathbf{k}-\mathbf{k}'|^2}{2m_A} = \frac{\hbar^2|\mathbf{k}|^2}{2m_A}+\frac{\hbar^2|\mathbf{k}'|^2}{2m_A}-\frac{\hbar^2\mathbf{k}\cdot\mathbf{k}'}{m_A} = \frac{\hbar^2k^2}{2m_A}+\frac{\hbar^2k'^2}{2m_A}-\frac{\hbar^2kk'\cos\theta}{m_A},$$

so,

$$d\left(\frac{\hbar^2|\mathbf{Q}|^2}{2m_A}\right) = \left(\frac{\hbar^2k'}{m_A}-\frac{\hbar^2k\cos\theta}{m_A}\right)dk',$$

and therefore,

$$\int dE'\delta\left(E-E'-\frac{\hbar^2|\mathbf{Q}|^2}{2m_A}\right)...$$

integration would give an extra factor,

$$\frac{\frac{\hbar^2k'}{m_N}dk'}{\frac{\hbar^2k'}{m_N}dk'+\left(\frac{\hbar^2k'}{m_A}-\frac{\hbar^2k\cos\theta}{m_A}\right)dk'} = \frac{\frac{m_A}{m_N}\frac{k'}{k}}{\frac{(m_A+m_N)k'}{m_Nk}-\cos\theta}.$$

To get k'/k, we use,

$$E'=\frac{\hbar^2|\mathbf{k}'|^2}{2m_N}=\frac{\hbar^2|\mathbf{k}|^2}{2m_N}-\frac{\hbar^2|\mathbf{Q}|^2}{2m_A}=\frac{\hbar^2|\mathbf{k}|^2}{2m_N}-\frac{\hbar^2|\mathbf{k}-\mathbf{k}'|^2}{2m_A}=\frac{\hbar^2|\mathbf{k}|^2}{2m_N}-\frac{\hbar^2|\mathbf{k}|^2}{2m_A}-\frac{\hbar^2|\mathbf{k}'|^2}{2m_A}+\frac{\hbar^2\mathbf{k}\cdot\mathbf{k}'}{m_A},$$

or,

$$m_A|\mathbf{k}'|^2 = m_A|\mathbf{k}|^2-m_N|\mathbf{k}|^2-m_N|\mathbf{k}'|^2+2m_N|\mathbf{k}||\mathbf{k}'|\cos\theta,$$

and so,

$$(m_N+m_A)k'^2-2m_N\cos\theta k'k+(m_N-m_A)k^2=0,$$

thus,

$$\frac{k'}{k} = \frac{2m_N\cos\theta\pm\sqrt{4m_N^2\cos^2\theta-4(m_N+m_A)(m_N-m_A)}}{2(m_N+m_A)}.$$

We take the + branch because k'/k should be positive, so,

$$\frac{k'}{k} = \frac{m_N \cos\theta + \sqrt{m_N^2 \cos^2\theta + m_A^2 - m_N^2}}{m_N + m_A}.$$

Therefore,

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= b^2 \left(\frac{k'}{k}\right) \frac{\frac{m_A}{m_N}\frac{k'}{k}}{\frac{(m_A+m_N)k'}{m_N k} - \cos\theta} = b^2 \frac{\frac{m_A}{m_N}\left(\frac{k'}{k}\right)^2}{\frac{(m_A+m_N)k'}{m_N k} - \cos\theta} \\ &= \frac{m_A b^2}{\sqrt{m_N^2\cos^2\theta + m_A^2 - m_N^2}} \left(\frac{m_N\cos\theta + \sqrt{m_N^2\cos^2\theta + m_A^2 - m_N^2}}{m_N + m_A}\right)^2. \end{aligned} \tag{15}$$

```
> restart: m:=2: M:=5: evalf( int ( 2*Pi*((m*x + sqrt(m^2*x^2 + M^2
  - m^2)) / (m + M))^2 * M / sqrt(m^2*x^2 + M^2 - m^2), x = -1..1) -
  4*Pi*(M/(m+M))^2);
                                  0.
> m:=1: M:=10.7: evalf( int ( 2*Pi*((m*x + sqrt(m^2*x^2 + M^2 -
  m^2)) / (m + M))^2 * M / sqrt(m^2*x^2 + M^2 - m^2), x = -1..1) -
  4*Pi*(M/(m+M))^2);
                                  0.
> m:=3.9: M:=17.7: evalf( int ( 2*Pi*((m*x + sqrt(m^2*x^2 + M^2 -
  m^2)) / (m + M))^2 * M / sqrt(m^2*x^2 + M^2 - m^2), x = -1..1) -
  4*Pi*(M/(m+M))^2);
                                  0.
```

It has been verified numerically to give the following total cross-section,

$$\begin{aligned}\sigma &= 2\pi \int_{-1}^{1} dx \frac{m_A b^2}{\sqrt{m_N^2 x^2 + m_A^2 - m_N^2}} \left(\frac{m_N x + \sqrt{m_N^2 x^2 + m_A^2 - m_N^2}}{m_N + m_A}\right)^2 \\ &= 4\pi b^2 \left(\frac{m_A}{m_N + m_A}\right)^2 \\ &= 4\pi a^2, \end{aligned} \tag{16}$$

in agreement with the simpler derivations using Born's approximation.