### 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 \(V(x)\) can be derived by solving merely the steady-state Schrodinger’s equation.

(a). Suppose \(\psi(x)\) is a solution to the one-body problem,

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

and it has the following asymptotic behavior at large \(|x|\),

\[
\psi(x) = e^{ik \cdot x} + f(\theta)\frac{e^{i|k||x|}}{|x|} + O(|x|^{-2}),
\]

where \(\theta\) is the angle between \(x\) and the incident wave-vector \(k\). Show that,

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

(b). We may rewrite (1) as,

\[
\left(\nabla^2 + k^2\right)\psi(x) = \frac{2\mu V(x)}{\hbar^2} \psi(x).
\]

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

\[
\left(\nabla^2 + k^2\right)\psi_0(x) = 0, \quad x \in \mathbb{R}^3,
\]

and what is the Green’s function solution \(g(x)\) to,

\[
\left(\nabla^2 + k^2\right) g(x) = \delta(x).
\]

(c). Given the scattering problem context, pick the general solution \(\psi_0(x)\), 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 $|x|$ limit, derive $f(\theta)$ in terms of $V(x)$.

(f). Suppose,

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

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 $e^{ik\cdot x}$ does have finite width, which is enough to cover the sample, but will not be received by the detector.

![Figure 1: The incident beam $e^{ik\cdot x}$ does have finite width.](image)

The particle flux formula is,

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

since,

$$-\nabla \cdot j = \frac{i\hbar}{2m} \nabla \cdot (\psi^*\nabla\psi - \psi\nabla\psi^*)$$

$$= \frac{i\hbar}{2m} (\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)$$

$$= \psi^*\left(\psi - \frac{V\psi}{i\hbar}\right) + \psi\left(\psi^* + \frac{V\psi^*}{i\hbar}\right)$$

$$= \psi^*\dot{\psi} + \psi\dot{\psi}^*$$
One could work out the scattered flux exactly, but that is not necessary because at large $|x|$, $f(\theta)e^{ ik| |x| }/|x|$ behaves locally very much like a planewave $e^{ ik\cdot x }$, with,

\[
 k' \equiv \frac{|k|x}{|x|},
\]

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

\[
 \nabla = e_r \partial_r + \frac{e_\theta}{r} \partial_\theta + \frac{e_\phi}{r \sin \theta} \partial_\phi,
\]

the only $O(r^{-1})$ term in (4) is from the radial derivative $e_r \partial_r$. 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 $e^{ ik\cdot x }$, $\forall k \in \{|k| = k\}$.

The Green’s functions $g(x)$ are,

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

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

\[
 (\nabla^2 + k^2) \frac{e^{ ik|x| }}{|x|} = \left( r^{-2} \partial_r r^2 \partial_r + k^2 \right) \frac{ e^{ ikr } }{ r } \\
 = r^{-2} \partial_r r^2 \left( ik \frac{ e^{ ikr } }{ r } - \frac{ e^{ ikr } }{ r^2 } \right) + k^2 \frac{ e^{ ikr } }{ r } \\
 = r^{-2} \partial_r \left( ik r e^{ ikr } - e^{ ikr } \right) + k^2 \frac{ e^{ ikr } }{ r }.
\]
\[ r^{-2} (ike^{ikr} - k^2 re^{ikr} - ike^{ikr}) + k^2 e^{ikr} r = 0, \quad r > 0. \tag{6} \]

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 \( \nabla^2 g(x) = \delta(x) \) and has the same singular properties.

(c). Let us pick a particular planewave,

\[ \psi_0(x) = e^{ikx}, \]

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

\[ \psi(x) = e^{ikx} - \int dx' \frac{2\mu V(x') \psi(x')}{h^2} \cdot \frac{e^{ik|x-x'|}}{4\pi|x-x'|} \]

\[ = e^{ikx} + \int dx' \tilde{V}(x') \frac{e^{ik|x-x'|}}{|x-x'|} \psi(x'), \tag{7} \]

where,

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

is the reduced potential that has unit of length.

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

\[ \psi(x) = e^{ikx} + \int dx' \tilde{V}(x') \frac{e^{ik|x-x'|}}{|x-x'|} e^{ikx'} + \int dx' \tilde{V}(x') \frac{e^{ik|x-x'|}}{|x-x'|} \int dx'' \tilde{V}(x'') \frac{e^{ik|x-x''|}}{|x'-x''|} e^{ikx''} + ..., \]

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

(e). The leading order term is,

\[ \psi(x) = e^{ikx} + \int dx' \tilde{V}(x') \frac{e^{ik|x-x'|}}{|x-x'|} e^{ikx'} \]

In the limit of large \( |x| \): \( |x| \gg |x'| \),

\[ |x - x'| = |x| - \frac{x \cdot x'}{|x|} + O \left( \frac{|x'|^2}{|x|} \right), \]
Let us define,
\[ k' \equiv k \frac{x}{|x|}, \]
then,
\[ e^{ik|x-x'|} \approx e^{ik|x|} e^{-ik' \cdot x'}. \]
Also,
\[ \frac{1}{|x-x'|} = \frac{1}{|x|} + O \left( \frac{|x'|}{|x|^2} \right). \]
Therefore,
\[ \psi(x) \approx e^{ik \cdot x} + \int dx' \tilde{V}(x') \frac{e^{ik|x|} e^{-ik' \cdot x'}}{|x|} e^{ik \cdot x'} = e^{ik \cdot x} + f(\theta) e^{ik|x|}, \]
with,
\[ f(\theta) = \int dx' \tilde{V}(x') e^{iQ \cdot x'}, \quad Q \equiv k - k'. \]
In other words, \( f(\theta) \) is simply the spatial Fourier transform of \( \tilde{V}(x) \) in wavevector \( Q \) which spans angle \( \theta \).

(f). Clearly \( \tilde{V}(x) = a\delta(x) \) and \( f(\theta) = a \). Therefore the total scattering cross-section is \( 4\pi a^2 \).

In a one-body problem where,
\[ \tilde{V}(x) = \begin{cases} \infty, & |x| < a \\ 0, & |x| \geq a \end{cases}, \]
the quantum mechanical total scattering cross section turns out to be \( 4\pi a^2 \) in the long-wavelength limit (as compared to \( \pi a^2 \) 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,
\[ \left( -\frac{\hbar^2 \nabla^2_1}{2m_1} - \frac{\hbar^2 \nabla^2_2}{2m_2} + V(x_1 - x_2) \right) \Psi(x_1, x_2) = \tilde{E} \Psi(x_1, x_2), \]
can be transformed to,
\[ \left( -\frac{\hbar^2 \nabla^2_x}{2\mu} - \frac{\hbar^2 \nabla^2_X}{2M} + V(x) \right) \Psi(x, X) = \tilde{E} \Psi(x, X), \]
where,
\[
x \equiv x_1 - x_2, \quad X \equiv \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}, \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}, \quad M \equiv m_1 + m_2,
\]
so,
\[
\Psi(x, X) = \psi(x)e^{iK \cdot X}, \quad \tilde{E} = E + \frac{\hbar^2 K^2}{2M},
\]
with,
\[
\left(-\frac{\hbar^2 \nabla_x^2}{2\mu} + V(x)\right)\psi(x) = E\psi(x).
\]
The scattering cross-section is clearly 0 when \(V = 0\). Since,
\[
\left(\nabla^2 + k^2\right)\psi(x) = \frac{2\mu V(x)}{\hbar^2}\psi(x),
\]
the leading order perturbation to \(\psi(x)\) is also proportional to \(\mu\). Therefore,
\[
\sigma_{\text{bound}} = \left(1 + \frac{m_N}{m_A}\right)^2 \sigma_{\text{free}},
\]
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,
\[
b_+^{E^{41}} = 1 \times 10^{-12} \text{ cm}, \quad b_-^{E^{41}} = 3 \times 10^{-12} \text{ cm}, \quad b_+^{E^{44}} = -2 \times 10^{-12} \text{ cm}, \quad b_-^{E^{44}} = -4 \times 10^{-12} \text{ cm},
\]
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 \(b_{\text{coh}}\). Is there for \(b_{\text{inc}}\)? for \(b_{\text{inc}}^2\)? (e.g., if there is 80\% \(E^{41}\)
and 20% E$^{44}$, is $b_{\text{inc}}^2(E) = 0.8b_{\text{inc}}^2(\text{pure E}^{41}) + 0.2b_{\text{inc}}^2(\text{pure E}^{44})$?

**Answer:**

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

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

\[
\sqrt{\bar{b}} = \frac{2 \times 2 + 2}{4 \times 2 + 2} \times 1 + \frac{2 \times 2}{4 \times 2 + 2} \times 9 = 4.2 \text{ barn},
\]

so,

\[
b_{\text{inc}} = \sqrt{\bar{b}}^2 - b_{\text{coh}}^2 = 0.9798 \sqrt{\text{barn}}.
\]

For pure E$^{44}$,

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

\[
\sqrt{\bar{b}} = \frac{2 \times 3 + 2}{4 \times 3 + 2} \times 4 + \frac{2 \times 3}{4 \times 3 + 2} \times 16 = 9.1429 \text{ barn},
\]

so,

\[
b_{\text{inc}} = \sqrt{\bar{b}}^2 - b_{\text{coh}}^2 = 0.9899 \sqrt{\text{barn}}.
\]

(b).

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

\[
\sqrt{\bar{b}} = 0.8 \times 4.2 + 0.2 \times 9.1429 = 5.1886 \text{ barn},
\]

so,

\[
b_{\text{inc}} = \sqrt{\bar{b}}^2 - b_{\text{coh}}^2 = 2.1057 \sqrt{\text{barn}}.
\]

(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 $b_{\text{inc}}$ or $b_{\text{inc}}^2$. We can have isotopes of the same $b_{\text{inc}}$, but if their $b_{\text{coh}}$’s are different, their mixed $b_{\text{inc}}$ is going to be enhanced.
3 Dynamic Structure Factor

Question:
(a). Calculate the thermally averaged self intermediate scattering function,
\[ F_s(Q, t) \equiv \langle e^{-iQ \cdot \hat{x}(0)} e^{iQ \cdot \hat{x}(t)} \rangle, \]
and the self dynamic structure factor \( S_s(Q, \omega) \) for ideal gas at temperature \( T \).
(b). Do the same for a single harmonic oscillator of frequency \( \Omega \) 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,
\[ e^{-iQ \hat{x}(0)} e^{iQ \hat{x}(t)} = \exp \left( iQ \sqrt{\frac{\hbar}{2m_A \Omega}} \left[ (e^{-i\Omega t} - 1)\hat{a} + (e^{i\Omega t} - 1)\hat{a}^\dagger \right] + \frac{iQ^2 \hbar}{2m_A \Omega} \sin \Omega t \right) \]
\[ = \exp \left( \frac{iQ^2 \hbar}{2m_A \Omega} \sin \Omega t \right) \hat{D}(\alpha(t)), \quad (8) \]

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.

$$\hat{D}(\alpha)\hat{D}(\beta) = e^{\frac{1}{2} (\alpha \beta^* - \alpha^* \beta)} \hat{D}(\alpha + \beta).$$

$$\langle \alpha | \beta \rangle = e^{\alpha \beta^* - \frac{1}{2} (|\alpha|^2 + |\beta|^2)}.$$

$$\int \frac{d^2 \alpha}{\pi} |\alpha\rangle \langle \alpha| = 1.$$

$$\langle n | \beta \rangle = e^{-\frac{1}{2} |\beta|^2} \frac{\beta^n}{\sqrt{n!}}.$$

Now consider,

$$\langle n | \hat{D}(\alpha) | n \rangle = \int \frac{d^2 \gamma}{\pi} \int \frac{d^2 \beta}{\pi} \langle n | \gamma \rangle \langle \gamma | \hat{D}(\alpha) | \beta \rangle \langle \beta | n \rangle$$

$$= \int \frac{d^2 \gamma}{\pi} \int \frac{d^2 \beta}{\pi} e^{-\frac{1}{2} |\gamma|^2} e^{\frac{n}{n!}} \langle \gamma | \hat{D}(\alpha) | \beta \rangle e^{-\frac{1}{2} |\beta|^2} \beta^n \frac{\beta^n}{\sqrt{n!}}$$

$$= \int \frac{d^2 \gamma}{\pi} \int \frac{d^2 \beta}{\pi} e^{-\frac{1}{2} (|\gamma|^2 + |\beta|^2)} \frac{(\beta^* \gamma)^n}{n!} \langle \gamma | \hat{D}(\alpha) | \beta \rangle |0\rangle$$

$$= \int \frac{d^2 \gamma}{\pi} \int \frac{d^2 \beta}{\pi} e^{-\frac{1}{2} (|\gamma|^2 + |\beta|^2)} \frac{(\beta^* \gamma)^n}{n!} e^{\frac{1}{2} (\alpha \beta^* - \alpha^* \beta)} |\gamma \rangle |\alpha + \beta\rangle$$

$$= \int \frac{d^2 \gamma}{\pi} \int \frac{d^2 \beta}{\pi} e^{-\frac{1}{2} (|\gamma|^2 + |\beta|^2)} \beta^n \frac{(\beta^* \gamma)^n}{n!} e^{\frac{1}{2} (\alpha \beta^* - \alpha^* \beta)} e^{\gamma^* (\alpha + \beta) - \frac{1}{2} (|\gamma|^2 + |\beta|^2)}.$$  (9)

Since,

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

we have,

$$\langle \hat{D}(\alpha) \rangle = (1 - d) \int \frac{d^2 \gamma \beta d^2 \beta}{\pi^2} e^{-\frac{1}{2} (|\gamma|^2 + |\beta|^2)} e^{d \beta^* \gamma} e^{\frac{1}{2} (\alpha \beta^* - \alpha^* \beta) + \gamma^* \gamma - \frac{1}{2} (|\gamma|^2 + |\beta|^2 + |\alpha|^2 + |\beta|^2 + \alpha \beta^* + \alpha^* \beta^*)}$$

$$= (1 - d) e^{-\frac{1}{2} |\alpha|^2} \int \frac{d^2 \gamma \beta d^2 \beta}{\pi^2} e^{-\frac{1}{2} |\gamma|^2 + |\beta|^2 + d \beta^* \gamma + \gamma^* \beta^* + \gamma^* \alpha - \alpha^* \beta}.$$  (10)

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,

\[-\left( \begin{array}{lll} \beta_x & \beta_y & \gamma_x \\ \gamma_y \end{array} \right) \left( \begin{array}{ccc} 1 & 0 & -\frac{1+d}{2i} \\ 0 & 1 & -\frac{1-d}{2i} \\ -\frac{1+d}{2i} & 1 & 0 \\ -\frac{1-d}{2i} & 0 & 1 \end{array} \right) \left( \begin{array}{c} \beta_x \\ \beta_y \\ \gamma_x \\ \gamma_y \end{array} \right) +
\left( \begin{array}{cc} -\alpha^* & -i\alpha^* \\ -i\alpha & \alpha \end{array} \right) \left( \begin{array}{c} \beta_x \\ \beta_y \\ \gamma_x \\ \gamma_y \end{array} \right) \right], \quad (11)\]

and since,

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

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

\[ \langle \hat{D}(\alpha) \rangle = (1 - d)e^{-\frac{1}{2}|\alpha|^2} \frac{e^{-\frac{1}{4}\text{det} |A|}}{1 - d} = e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{\text{det} |A|}{2(1-d)}}. \quad (12) \]
Thus,

\[
\langle e^{-i\mathbf{Q} \cdot \hat{x}(0)} e^{i\mathbf{Q} \cdot \hat{x}(t)} \rangle = \exp \left( \frac{iQ^2 \hbar}{2m_A \Omega} \sin \Omega t - \frac{|\alpha(t)|^2(1 + d)}{2(1 - d)} \right) \\
= \exp \left( \frac{iQ^2 \hbar}{2m_A \Omega} \sin \Omega t - \frac{Q^2 \hbar}{2m_A \Omega} (e^{i\Omega t} - 1)(e^{-i\Omega t} - 1) \frac{(1 + d)}{2(1 - d)} \right) \\
= \exp \left( \frac{Q^2 \hbar}{4m_A \Omega} \left( e^{i\Omega t} - e^{-i\Omega t} - (2 - e^{i\Omega t} - e^{-i\Omega t}) \frac{1 + d}{1 - d} \right) \right) \\
= \exp \left( \frac{Q^2 \hbar}{4m_A \Omega} \left( (1 - d)e^{i\Omega t} - (1 - d)e^{-i\Omega t} - 2(1 + d) + (1 + d)e^{i\Omega t} + (1 + d)e^{-i\Omega t} \right) \right) \\
= \exp \left( \frac{Q^2 \hbar}{2m_A \Omega} \frac{(e^{i\Omega t} - 1) + d(e^{-i\Omega t} - 1)}{1 - d} \right). \tag{13}
\]

At low \( T \), \( d \sim 0 \), so,

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

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 quanta of \( \hbar \Omega \).

At high \( T \), \( d \sim 1 - \frac{m_A \Omega}{\hbar k_B T} \), so,

\[
\frac{(e^{i\Omega t} - 1) + d(e^{-i\Omega t} - 1)}{1 - d} \approx \frac{k_B T}{\hbar \Omega} \left( e^{i\Omega t} + d e^{-i\Omega t} - 1 - d \right),
\]

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 \( \Omega_x, \Omega_y, \Omega_z \) are the oscillator frequencies in three directions.
(a). Let us take the $\Omega \to 0$ limit. Since,

$$
\frac{(e^{i\Omega t} - 1) + d(e^{-i\Omega t} - 1)}{\Omega(1 - d)} \approx \frac{k_B T}{h\Omega^2} \left( i\Omega t - \frac{\Omega^2 t^2}{2} + d(-i\Omega t) - \frac{\Omega^2 t^2}{2} \right)
$$

$$
= \frac{k_B T}{h\Omega^2} \left( \frac{h\Omega}{k_B T} i\Omega t - \Omega^2 t^2 \right)
$$

$$
= it - \frac{k_B T t^2}{\hbar},
$$

we have,

$$
\langle e^{-iQ\hat{\mathbf{x}}(0)} e^{iQ\hat{\mathbf{x}}(t)} \rangle = \exp \left( -\frac{|Q|^2 \hbar}{2m_A} \left( \frac{k_B T t^2}{\hbar} - it \right) \right).
$$

Thus, the dynamic structure factor of ideal gas is,

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

with the loss peaking at,

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

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

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

So,

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

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

\[
d \left( \frac{\hbar^2|Q|^2}{2m_A} \right) = \left( \frac{\hbar^2 k'}{m_A} - \frac{\hbar^2 k \cos \theta}{m_A} \right) dk',
\]
and therefore,

\[
\int dE' \delta \left( E - E' - \frac{\hbar^2|Q|^2}{2m_A} \right) ...
\]
integration would give an extra factor,

\[
\frac{\hbar^2 k' dk'}{m_N} + \left( \frac{\hbar^2 k'}{m_A} - \frac{\hbar^2 k \cos \theta}{m_A} \right) dk' = \frac{m_A k'}{(n_A + m_N k') - \cos \theta}.
\]
To get \( k'/k \), we use,

\[
E' = \frac{\hbar^2|k'|^2}{2m_N} = \frac{\hbar^2|k|^2}{2m_N} - \frac{\hbar^2|Q|^2}{2m_A} = \frac{\hbar^2|k|^2}{2m_N} - \frac{\hbar^2|k - k'|^2}{2m_A} = \frac{\hbar^2|k|^2}{2m_N} - \frac{\hbar^2|k|^2}{2m_A} - \frac{\hbar^2|k'|^2}{2m_A} + \frac{\hbar^2 k \cdot k'}{m_A},
\]
or,

\[
m_A|k'|^2 = m_A|k|^2 - m_N|k|^2 - m_N|k'|^2 + 2m_N|k||k'| \cos \theta,
\]
and so,

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

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

\[
\frac{d\sigma}{d\Omega} = b^2 \left( \frac{k'}{k} \right) \frac{m_A k'}{m_N k} \left( \frac{m_{A} k'}{m_N k} - \cos \theta \right) = b^2 \left( \frac{m_{A} k'}{m_N k} \right)^2 \left( \frac{m_{N} \cos \theta + \sqrt{m_N^2 \cos^2 \theta + m_A^2 - m_N^2}}{m_N + m_A} \right)^2.
\]

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

\[
\sigma = 2\pi \int_{-1}^{1} dx \frac{m_A b^2}{\sqrt{m_N^2 x^2 + m_A^2 - m_N^2}} \left( \frac{m_N x + \sqrt{m_N^2 x^2 + m_A^2 - m_N^2}}{m_N + m_A} \right)^2 = 4\pi b^2 \left( \frac{m_A}{m_N + m_A} \right)^2 = 4\pi a^2,
\]

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