Zhi Chen HW#13

44) <u>The radial distribution function $g(r)$:</u>

a) Calculate $\rho\lambda_{th}^3$, determine whether it is appropriate to use classical approach.

$$\rho\lambda_{th}^3 = \rho\left(\frac{h^2}{2\pi m k_B T}\right)^{3/2}$$

$$\overset{!}{=}\left(0.02125 \times \left(10^{10}\ m^{-1}\right)^3\right)\frac{\left(6.626\times10^{-34}\ J\cdot s\right)^3}{\left(2\pi\left(6.6335\times10^{-26}\ kg\right)\left(1.380649\times10^{-23}\times 84\right)J\right)^{3/2}}$$

$$\boxed{\rho\lambda_{th}^3 \overset{!}{=} 0.00057}$$

We see since $\rho\lambda_{th}^3 \ll 1$, it is suitable to use classical approach.

b) Show that minimum of Lennard-Jones potential occurs at $r_0 = 2^{1/6}\sigma$ and $u(r_0) = -\varepsilon$.

$$\frac{\partial}{\partial r}\left(u(r)\right) = \frac{\partial}{\partial r}\left(4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]\right)$$

$$\overset{!}{=} 4\varepsilon\left[-12\left(\frac{\sigma}{r}\right)^{12}\frac{1}{r} + 6\left(\frac{\sigma}{r}\right)^6\frac{1}{r}\right] = 0$$

$$12\left(\frac{\sigma}{r}\right)^{12}\cancel{\frac{1}{r}} = 6\left(\frac{\sigma}{r}\right)^6\cancel{\frac{1}{r}}$$

$$2\left(\frac{\sigma}{r}\right)^6 = 1$$

$$\hookrightarrow \boxed{r_0 = 2^{1/6}\sigma}$$

$$u(r=r_0) = 4\varepsilon\left[\left(\frac{\sigma}{2^{1/6}\sigma}\right)^{12} - \left(\frac{\sigma}{2^{1/6}\sigma}\right)^{6}\right]$$

$$= 4\varepsilon\left(\frac{1}{4} - \frac{1}{2}\right)$$

$$\boxed{u(r=r_0) = -\varepsilon}$$

c) Show $g(r)$ and $S(k)$ are related.

⇒ Given:

$$S(k) = \frac{1}{N}\left\langle \sum_{i=1}^{N}\sum_{j=1}^{N} e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}\right\rangle$$

→ split $\sum_{i=1}^{N}\sum_{j=1}^{N}$ into cases when $i=j$ and $i\neq j$.

→ we see that if $i=j$, then $e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)} = e^0 = 1$.
since there are N terms, $\sum_{i=j}$ give N.

then $$S(k) = \frac{1}{N}\left\langle\left(N + \sum_{i=1}^{N}\sum_{j=1, i\neq j}^{N} e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\right)\right\rangle$$

→ there are $(N)(N-1)$ $i\neq j$ terms after taking out N- diagonal terms.

$$S(k) = \frac{1}{N}\left(N + (N)(N-1)\left\langle e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\right\rangle\right)$$

Know $$\left\langle e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\right\rangle = \frac{\int d^3r_1 \cdots \int d^3r_N\, e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} e^{-\beta U}}{\int d^3r_1 \cdots \int d^3r_N\, e^{-\beta U}}.$$

Recognizing $\rho^2 g(r) = N(N-1)\dfrac{\int d^3r_3 \cdots \int d^3r_N\, e^{-\beta U}}{\int d^3r_1 \cdots \int d^3r_N\, e^{-\beta U}}$

then $\dfrac{1}{N}\left[N + N(N-1)\int d^3r_1 \int d^3r_2\, e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\dfrac{\int d^3r_3 \cdots \int d^3r_N\, e^{-\beta U}}{\int d^3r_1 \cdots \int d^3r_N\, e^{-\beta U}}\right]$

let $\vec{r} = \vec{r}_1 - \vec{r}_2$

$$\hookrightarrow = \frac{1}{N}\Big[N + \underbrace{\int d^3\vec{r}_1}_{V} \int d^3\vec{r}\ \rho^2 g(r)\, e^{i\vec{k}\cdot\vec{r}}\Big]$$

$$\stackrel{!}{=} 1 + \cancel{\tfrac{1}{\rho}}\int d^3\vec{r}\ \rho^{\cancel{2}}\, g(r)\, e^{i\vec{k}\cdot\vec{r}}$$

$$\stackrel{!}{=} 1 + \rho\int d^3\vec{r}\ e^{i\vec{k}\cdot\vec{r}}\,(g(r)-1) + \rho\underbrace{\int d^3\vec{r}\ e^{i\vec{k}\cdot\vec{r}}}_{(2\pi)^3\delta(k)}$$

This term only contribute when $k=0$, but we neglect $k=0$ term.

$$= 1 + \rho\int d^3\vec{r}\, e^{i\vec{k}\cdot\vec{r}}\,(g(r)-1)$$

$$\stackrel{!}{=} 1 + \rho\underbrace{\int_0^{2\pi} d\phi}_{2\pi} \int_0^\infty \underbrace{\int_0^\pi d\theta\ \sin\theta\, e^{ikr\cos\theta}}_{=\frac{ie^{ikr\cos\theta}}{kr}\Big|_0^\pi = \frac{2\sin kr}{kr}}\,[g(r)-1]\, r^2\, dr$$

$$= 1 + 4\pi\rho\int_0^\infty \left(\frac{\sin kr}{k\cancel{r}}\right) r^{\cancel{2}}\,[g(r)-1]\, dr$$

$$\boxed{S(k) \stackrel{!}{=} 1 + \frac{4\pi\rho}{k}\int_0^\infty dr\ r\sin kr\,[g(r)-1]}$$

Since previously found $S(k)$ is just Fourier Transform of $g(r)$.

$$S(k) = 1 + \rho \int d^3r \left[g(r) - 1\right] e^{i\vec{k}\cdot\vec{r}}$$

rearrange: $$\frac{S(k)-1}{\rho} = \int d^3r \left[g(r) - 1\right] e^{i\vec{k}\cdot\vec{r}}$$

So $$FT\left[g(r) - 1\right] = \frac{S(k)-1}{\rho}$$

then $$FT^{-1}\left[\frac{S(k)-1}{\rho}\right] = g(r) - 1$$

with Inverse FT:

$$g(r) = 1 + \frac{1}{(2\pi)^3} \int d^3k \, e^{-i\vec{k}\cdot\vec{r}} \left[S(k) - 1\right] \frac{1}{\rho}$$

$$\hookrightarrow g(r) = 1 + \frac{1}{(2\pi)^3} \int_0^\infty \underbrace{\int_0^\pi \sin\theta \, e^{-ikr\cos\theta} \, d\theta}_{\frac{2\sin(kr)}{kr}} \, k^2 dk \, \frac{\left[S(k) - 1\right]}{\rho}$$

$$= 1 + \frac{1}{\rho} \frac{4\pi}{(2\pi)^3} \int_0^\infty \frac{\sin(kr)}{kr} k^2 \left[S(k) - 1\right] dk$$

$$\boxed{g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^\infty k \sin(kr) \left[S(k) - 1\right] dk}$$

d-f) See code for plotting.

g) $\langle U\rangle/N = \frac{1}{2}\int_0^\infty 4\pi r^2 \rho g(r) u(r) dr$, integrate numerically.

I get $\frac{\langle U\rangle}{N} = -10^{21}\,eV$

this doesn't make sense.

$\Rightarrow$ If integrate $n(R) = \int_0^R 4\pi r^2 dr\, \rho g(r)$,

then I find that $n(R = 1.03\,\sigma) \sim 1$

and $n(R<\sigma) \ll 1$, so I shouldn't go below σ.

So if I do $\frac{\langle U\rangle}{N} = \frac{1}{2}\int_\sigma^\infty 4\pi r^2 \rho g(r) u(r) dr$

I get $\boxed{\frac{\langle U\rangle}{N} \sim -0.06\,eV}$, comparable to $-\varepsilon = -0.01 eV$

$$\boxed{\frac{\langle E\rangle}{N} = \frac{3}{2}k_B T + \frac{\langle U\rangle}{N} \cong -0.049\,eV}$$

h) Find μ, given $T = 85\,K$, $p = 594$ Torr

for ideal gas: $p = \rho k_B T \Rightarrow V = \frac{N k_B T}{p}$

$$Q = \frac{1}{N!}\left(\frac{V}{(\lambda_{th})^3}\right)^N \qquad \lambda_{th} = \frac{h}{2\pi m k_B T}$$

$$A = -k_B T \ln Q$$

$$\stackrel{!}{=} -k_B T\left[N\left(\ln(V) - 3\ln\lambda_{th}\right) - \ln N!\right]$$

$\ln N! \approx N\ln N - N$

$$\stackrel{!}{=} -k_B T\left[N\left(\ln V - 3\ln\lambda_{th}\right) - N\ln N - N\right]$$

$$\mu = \left(\frac{\partial A}{\partial N}\right)_{T,V} = -k_B T\left[\left(\ln V - 3\ln\lambda_{th}\right) - \ln N\right]$$

$$\stackrel{!}{=} -k_B T \ln\left(\frac{V}{N\left(\frac{h^2}{2\pi m k_B T}\right)^{3/2}}\right)$$

with $V = \frac{N k_B T}{p}$

$$\mu = -k_B T \ln\left[\frac{k_B T}{p\left(\frac{h^2}{2\pi m k_B T}\right)^{3/2}}\right]$$

plug in #'s, $T = 85\,K$, $p = (594 \times 133.3224)\,Pa$

$$\boxed{\mu \cong -0.0968\ eV}$$

i) $\mu_{liquid} = k_B T \ln(\rho_{liquid} \lambda_{th}^3) + \frac{\langle U \rangle}{N}$

from part a) found $\rho_{liquid} \lambda_{th}^3 = 0.00057$

part g) found $\frac{\langle U \rangle}{N} \sim -0.06 \, eV$

Plug in #'s: with $T = 85K$

$$\boxed{\mu_{liquid} = -0.1147 \, eV}$$

indeed lower than $\mu_{gas} = -0.0968 \, eV$

Explain the resolution to this discrepancy:

If we use the reversible work, $w(r) = -k_B T \ln g(r)$ to calculate $\frac{\langle U \rangle}{N}$ instead of $u(r)$, then I get:

$$\frac{\langle U \rangle}{N} \cong -0.0214 \, eV$$

then $\mu_{liquid} \cong -0.076 \, eV$ which is then higher compared to μ_{gas}.

45) Quantum Correlation Functions and second Quantizations

a) Show $g(r) = g(0,r) = 1 \pm \frac{2S+1}{\bar{\rho}^2 (2\pi)^6} \left| \int d^3k \, e^{i\vec{k}\cdot\vec{r}} \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - \mu)} \mp 1} \right|^2$

$$\Rightarrow \hat{n} = \hat{\psi}^+ \hat{\psi} = \sum_{\sigma} \sum_{k} \sum_{k'} \hat{a}^+_{k\sigma} \hat{a}_{k'\sigma} \phi^*_{k\sigma}(\vec{r}) \phi_{k'\sigma}(\vec{r})$$

$$= \underbrace{\sum_{\sigma}}_{2S+1} \Big(\sum_{k=k'} \underbrace{\hat{a}^+_{k\sigma} \hat{a}_{k'\sigma}}_{} \underbrace{|\phi_{k\sigma}|^2}_{} + \sum_{k} \sum_{k', k\neq k'} \hat{a}^+_{k\sigma} \hat{a}_{k'\sigma} \phi^*_{k\sigma}(\vec{r}) \phi_{k'\sigma}(\vec{r}) \Big)$$

given $\hat{a}^+_{i\sigma} \hat{a}_{i\sigma} = \hat{n}_{i\sigma}$

$$|\phi_{k\sigma}|^2 = \langle \sigma | \left(\frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}} \right) \left(\frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \right) | \sigma \rangle = 1/V$$

$$= (2S+1) \Big[\frac{1}{V} \sum_{k} n_{k\sigma} + \sum_{k} \sum_{k', k\neq k'} \hat{a}^+_{k\sigma} \hat{a}_{k'\sigma} \phi^*_{k\sigma}(\vec{r}) \phi_{k'\sigma}(\vec{r}) \Big]$$

$\bar{\rho} = (2S+1) \frac{N}{V}$

$$\hat{n} = \bar{\rho} + (2S+1) \sum_{k} \sum_{k, k\neq k'} \hat{a}^+_{k\sigma} \hat{a}_{k'\sigma} \phi^*_{k\sigma}(\vec{r}) \phi_{k'\sigma}(\vec{r})$$

Since $\langle (\hat{n}(\vec{r}_1) - \bar{\rho})(\hat{n}(\vec{r}_2) - \bar{\rho}) \rangle = \langle \hat{n}(\vec{r}_1)\hat{n}(\vec{r}_2) \rangle - \bar{\rho} \underbrace{\langle \hat{n}(\vec{r}_1) \rangle}_{\sim \bar{\rho}} - \bar{\rho} \underbrace{\langle \hat{n}(\vec{r}_2) \rangle}_{\sim \bar{\rho}} + \bar{\rho}^2$

$$\cong \langle \hat{n}(\vec{r}_1)\hat{n}(\vec{r}_2) \rangle - \bar{\rho}^2$$

then $\langle \hat{n}(\vec{r}_1)\hat{n}(\vec{r}_2) \rangle = \bar{\rho}^2 + \underbrace{\langle (\hat{n}(\vec{r}_1) - \bar{\rho})(\hat{n}(\vec{r}_2) - \bar{\rho}) \rangle}_{\text{off-diagonal term.}}$

then

$$\langle(\hat{n}(\vec{r}_1)-\bar{\rho})(\hat{n}(\vec{r}_2)-\bar{\rho})\rangle = (2s+1)\sum_{k_1}\sum_{\substack{k_2\\k_1\neq k_2}}\sum_{k_3}\sum_{\substack{k_4\\k_3\neq k_4}} a^{+}_{k_1} a_{k_2} a^{+}_{k_3} a_{k_4} \psi^{*}_{k_1}(r_1)\psi_{k_2}(r_1)\psi^{*}_{k_3}(r_2)\psi_{k_4}(r_2)$$

However, we must have $k_2 = k_3$ and $k_1 = k_4$ for non-zero expectations, otherwise we would have different k for different ψ. Since ψ with different r is orthogonal to each other when k is different, this requires $k_1 = k_4$, $k_2 = k_3$.

then $$\langle(\hat{n}(\vec{r}_1)-\bar{\rho})(\hat{n}(\vec{r}_2)-\bar{\rho})\rangle = (2s+1)\sum_{k_1}\sum_{\substack{k_2\\k_1\neq k_2}} \hat{a}^{+}_{k_1}\hat{a}_{k_2}\hat{a}^{+}_{k_2}\hat{a}_{k_1} \phi^{*}_{k_1}(\vec{r}_1)\phi_{k_2}(\vec{r}_1)\phi^{*}_{k_2}(\vec{r}_2)\phi_{k_1}(\vec{r}_2)$$

Since $\hat{a}$ follow the same commutation relation,

i.e. $$[\hat{a}_\alpha, \hat{a}^{+}_\beta] = \hat{a}_\alpha\hat{a}^{+}_\beta - \hat{a}^{+}_\beta\hat{a}_\alpha = \delta_{\alpha\beta} \quad \text{for bosons}$$
$$\{\hat{a}_\alpha, \hat{a}^{+}_\beta\} = \hat{a}_\alpha\hat{a}^{+}_\beta + \hat{a}^{+}_\beta\hat{a}_\alpha = \delta_{\alpha\beta} \quad \text{for fermions.}$$

then $$\hat{a}_{k_2}\hat{a}^{+}_{k_2} = 1 \pm \underbrace{\hat{a}^{+}_{k_2}\hat{a}_{k_2}}_{=\hat{n}_{k_2}} = 1 \pm \hat{n}_{k_2}$$

+ for bosons

− for fermions

then

$$\langle(\hat{n}(\vec{r}_1)-\bar{\rho})(\hat{n}(\vec{r}_2)-\bar{\rho})\rangle =$$

$$\hookrightarrow = (2s+1)\sum_{k_1}\sum_{\substack{k_2\\k_1\neq k_2}} (1\pm\hat{n}_{k_2})\hat{n}_{k_1}\frac{1}{V^2}\left(\langle 0|e^{-i\vec{k}_1\cdot\vec{r}_1}\right)\left(e^{i\vec{k}_2\cdot\vec{r}_1}|0\rangle\right)\left(\langle 0|e^{-i\vec{k}_1\cdot\vec{r}_2}\right)\left(e^{i\vec{k}_2\cdot\vec{r}_2}|0\rangle\right)$$

$$\hookrightarrow = (2s+1)\sum_{k_1}\sum_{\substack{k_2\\k_1\neq k_2}} (1\pm\hat{n}_{k_2})\hat{n}_{k_1}\frac{1}{V^2} e^{-i(\vec{k}_1-\vec{k}_2)\vec{r}_1}\, e^{i(\vec{k}_1-\vec{k}_2)\vec{r}_2}$$

$$\stackrel{!}{=} (2s+1)\sum_{k_1}\sum_{\substack{k_2\\k_1\neq k_2}} (1\pm\hat{n}_{k_2})\hat{n}_{k_1}\frac{1}{V^2} e^{i\vec{k}_1\cdot(\vec{r}_2-\vec{r}_1)}\, e^{-i\vec{k}_2\cdot(\vec{r}_2-\vec{r}_1)}$$

Since quantum states behave independently, let

$$\langle (1 \pm \hat{n}_{k_2}) \hat{n}_{k_1} \rangle = (1 \pm \langle \hat{n}_{k_2} \rangle) \langle \hat{n}_{k_1} \rangle$$

change summation to integral. by multiplying $\frac{V d^3k_1}{(2\pi)^3} \frac{V}{(2\pi)^3} d^3k_2$

$$\Rightarrow \frac{2S+1}{(2\pi)^6} \iint (1 \pm \langle \hat{n}_{k_2} \rangle) \langle \hat{n}_{k_1} \rangle e^{i\vec{k}_1 \cdot (\vec{r}_2 - \vec{r}_1)} e^{-i\vec{k}_2 \cdot (\vec{r}_2 - \vec{r}_1)} d^3k_1 d^3k_2$$

$$\Rightarrow = \frac{2S+1}{(2\pi)^6} \Big[\underbrace{\iint \langle \hat{n}_{k_1} \rangle e^{i\vec{k}_1 \cdot (\vec{r}_2 - \vec{r}_1)} e^{-i\vec{k}_2 \cdot (\vec{r}_2 - \vec{r}_1)} d^3k_1 d^3k_2}_{1} \pm \underbrace{\iint \langle \hat{n}_{k_2} \rangle \langle \hat{n}_{k_1} \rangle e^{i\vec{k}_1 \cdot (\vec{r}_2 - \vec{r}_1)} e^{-i\vec{k}_2 \cdot (\vec{r}_2 - \vec{r}_1)} d^3k_1 d^3k_2}_{2}$$

Calculate term 1:

Since $\int e^{i\vec{k} \cdot \vec{r}} d^3\vec{k} = (2\pi)^3 \delta(r)$

$$\Rightarrow = \frac{2S+1}{(2\pi)^6} \underbrace{\int e^{-ik_2(\vec{r}_2 - \vec{r}_1)} d^3k_2}_{(2\pi)^3 \delta(\vec{r}_1 - r_2)} \underbrace{\int \langle \hat{n}_{k_1} \rangle e^{i\vec{k}_1(\vec{r}_2 - \vec{r}_1)}} d^3k_1$$

$$\stackrel{!}{=} \frac{(2S+1)}{(2\pi)^3} \int e^{i\vec{k}_1(\vec{r}_2 - \vec{r}_1)} \langle \hat{n}_{k_1} \rangle \delta(\vec{r}_1 - \vec{r}_2) \, d^3k_1$$

$$\stackrel{!}{=} (2S+1) \bar{\rho} \, \delta(\vec{r}_2 - \vec{r}_1)$$

$$\stackrel{!}{=} 0 \quad \text{if } \vec{r}_2 \neq \vec{r}_1$$

Calculate ② term.

$$\hookrightarrow \pm \frac{2S+1}{(2\pi)^6} \iint \langle \hat{n}_{k_2} \rangle \langle \hat{n}_{k_1} \rangle e^{i\vec{k}_1 \cdot (\vec{r}_2 - \vec{r}_1)} e^{-i\vec{k}_2 (\vec{r}_2 - \vec{r}_1)} d^3k_1 d^3k_2$$

let $\vec{r}_1 = 0$, $\vec{r}_2 - \vec{r}_1 \to \vec{r}$ and $\vec{k}_2 = 0$, $\vec{k}_1 - \vec{k}_2 = \vec{k}$

$$\hookrightarrow \pm \frac{2S+1}{(2\pi)^6} \left| \int \langle n_k \rangle e^{i\vec{k}\cdot\vec{r}} d^3k \right|^2$$

use $\langle n_k \rangle$ from bose-eistein and fermi-dirac statistics:

$$\langle n_k \rangle = \frac{1}{e^{\beta(\varepsilon - \mu)} \mp 1}$$ where $-$ for boson, $+$ for fermion.

and $\varepsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

then ② term is:

$$\hookrightarrow = \pm \frac{(2S+1)}{(2\pi)^6} \left| \int e^{i\vec{k}\cdot\vec{r}} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} \mp 1} d^3k \right|^2$$

All together:

$$g(r) = \frac{1}{\bar{\rho}^2} \langle \hat{n}(\vec{r}_1) \hat{n}(\vec{r}_2) \rangle = \frac{1}{\bar{\rho}^2} \left(\bar{\rho}^2 + \langle (\hat{n}(\vec{r}_1) - \bar{\rho})(\hat{n}(\vec{r}_2) - \bar{\rho}) \rangle \right)$$

$$\stackrel{!}{=} \frac{1}{\bar{\rho}^2} \left(\bar{\rho}^2 \pm \frac{2S+1}{(2\pi)^6} \left| \int e^{i\vec{k}\cdot\vec{r}} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} \mp 1} d^3k \right|^2 \right)$$

$$\boxed{g(r) \stackrel{!}{=} 1 \pm \frac{2S+1}{(2\pi)^6} \left| \int e^{i\vec{k}\cdot\vec{r}} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} \mp 1} d^3k \right|^2}$$

b) Show with classical limit:

$$g(r) \to 1 \pm \frac{1}{2S+1} e^{-2\pi r^2/\lambda_{th}^2} \quad , \quad \lambda_{th} = \sqrt{\frac{2\pi\beta\hbar^2}{m}}$$

$$\xrightarrow{\quad} e^{\frac{-mr^2}{\beta\hbar^2}}$$

Classical limit, μ is large and negative.

$$\langle n \rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} \mp 1} \ll 1$$

$$\cong e^{-\beta\varepsilon} e^{\beta\mu}$$

$$= e^{-\frac{\beta\hbar^2 k^2}{2m}} e^{\beta\mu}$$

If classical limit, then we know $\mu = k_B T \ln\left(\frac{N}{V}\lambda_{th}^3\right)$

and from part a) we know $\bar{\rho} = (2S+1)\frac{N}{V}$

then

$$g(r) = 1 \pm \frac{1}{(2S+1)\left(\frac{N}{\cancel{V}}\right)^2 (2\pi)^6} \left| \iint k^2 \sin\theta \, d\theta \, dk \; e^{-\frac{\beta\hbar^2 k^2}{2m}} \left(\frac{\cancel{N}}{\cancel{V}} \lambda_{th}\right)^3 e^{ikr\cos\theta} \int_0^{2\pi} d\phi \right|^2$$

$$= 1 \pm \frac{1}{(2S+1)(2\pi)^6} \left| \int_0^\infty \underbrace{\int_0^\pi \sin\theta \, e^{ikr\cos\theta} d\theta}_{= \frac{2\sin(kr)}{kr}} \, e^{-\frac{\beta\hbar^2 k^2}{2m}} (\lambda_{th})^3 k^2 \, 2\pi \right|^2$$

$$= 1 \pm \frac{\lambda_{th}^6}{(2S+1)(2\pi)^6} \left| \underbrace{\int_0^\infty 4\pi \frac{\sin(kr)}{\cancel{k}r} k^{\cancel{2}} e^{-\frac{\beta\hbar^2 k^2}{2m}}}\right|^2$$

$$= 1 \pm \frac{(\lambda_{th})^6}{(2S+1)(2\pi)^6} \left(\frac{\cancel{4}\pi}{\cancel{r}} \frac{\sqrt{\pi}\,\cancel{r}}{\cancel{4}\left(\frac{\beta\hbar^2}{2m}\right)^{3/2}} \exp\left\{ \frac{-r^2}{4\left(\frac{\beta\hbar^2}{2m}\right)} \right\} \right)^2$$

$$= 1 \pm \frac{\lambda_{th}^6}{(2s+1)(2\pi)^6} \underbrace{\left(\frac{2\pi m}{\beta\hbar^2}\right)^3}_{\left[(2\pi)^2 \frac{m}{2\pi\beta\hbar^2}\right]^3 = (2\pi)^6 \frac{1}{\lambda_{th}^6}} \exp\left\{\frac{-mr^2}{\beta\hbar^2}\right\}$$

$$\boxed{g(r) = 1 \pm \frac{1}{2s+1} \exp\left\{\frac{-2\pi r^2}{\lambda_{th}^2}\right\} \quad \text{for} \quad \lambda_{th} = \sqrt{\frac{2\pi\beta\hbar^2}{m}}}$$

4b) Stochastically Driven Oscillator:

$$m\ddot{q} + \eta\dot{q} + m\omega_0^2 q = \Delta F_{env}(t)$$

Let $q(t) = q_\omega e^{-i\omega t}$ and consider driving force $F_\omega e^{-i\omega t}$

then $\dot{q} = -i\omega q \qquad \ddot{q} = -\omega^2 q$

Substitute in:

$$-\omega^2 m q_\omega \cancel{e^{-i\omega t}} - i\omega\eta q_\omega \cancel{e^{-i\omega t}} + m\omega_0^2 q_\omega \cancel{e^{-i\omega t}} = F_\omega \cancel{e^{-i\omega t}}$$

$$\hookrightarrow \; -\omega^2 m q_\omega - i\omega\eta q_\omega + m\omega_0^2 q_\omega = F_\omega$$

$$\hookrightarrow \; q_\omega = \frac{F_\omega}{(-\omega^2 m - i\omega\eta + m\omega_0^2)} \; \frac{-\omega^2 m + i\omega\eta + m\omega_0^2}{-\omega^2 m + i\omega\eta + m\omega_0^2}$$

$$q_\omega = \frac{[m(\omega_0^2 - \omega^2) + i\omega\eta]\, F_\omega}{(m(\omega_0^2 - \omega^2))^2 + (\omega\eta)^2}$$

In order to account for the actual stochastic force, we need to use S_F.

$$\langle q_\omega^* q_\omega \rangle = \left\langle \frac{[m(\omega_0^2-\omega^2) - i\omega\eta] F_\omega^*}{(m(\omega_0^2-\omega^2))^2 + (\omega\eta)^2} \; \frac{[m(\omega_0^2-\omega^2) + i\omega\eta] F_\omega}{(m(\omega_0^2-\omega^2))^2 + (\omega\eta)^2} \right\rangle$$

$$= \frac{\langle F_\omega^* F_\omega \rangle}{(m(\omega_0^2-\omega^2))^2 + (\omega\eta)^2}$$

① $S_q = \langle q_\omega^* q_\omega \rangle = \dfrac{S_F(\omega)}{(m(\omega_0^2-\omega^2))^2+(\omega\eta)^2}$

We also know Fluctuation dissipation theorem says:

$$S_q = \frac{2k_BT}{\omega} \, Im(\chi)$$

Since $\chi = \dfrac{q_\omega}{F_\omega} = \dfrac{m(\omega_0^2-\omega^2)+i\omega\eta}{(m(\omega_0^2-\omega^2))^2+(\omega\eta)^2}$

then

$$Im(\chi) = \frac{\omega\eta}{(m(\omega_0^2-\omega^2))^2+(\omega\eta)^2}$$

② $\therefore$ $S_q = \dfrac{2k_BT}{\cancel{\omega}} \dfrac{\cancel{\omega}\eta}{[m(\omega_0^2-\omega^2)]^2+(\omega\eta)^2}$

by comparing two expression we get for S_q,

we see that $\underline{\underline{S_F = 2k_BT\eta}}$

Now we can solve for $\langle q(t)q(t-\tau)\rangle$ by taking inverse Fourier Transform of S_q using Wiener-Khinchin Thm:

$$K(\tau) = \int_{-\infty}^{\infty} d\omega \, e^{-i\omega\tau} S_q$$

$$K(\tau) \overset{!}{=} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega\tau} \frac{2k_BT\eta}{[m(\omega_0^2-\omega^2)]^2+(\omega\eta)^2}$$