Solutions to Problem Set No. 2

1. For a single oscillator in 3-d, the Hamiltonian H is

$$H = \frac{1}{2m} \underset{\sim}{p}^2 + \frac{k}{2} \underset{\sim}{x}^2 \qquad \ldots(1)$$

From Hamilton's eqns., $\dot{p}_\alpha = -\frac{\partial H}{\partial x_\alpha}$, $\alpha = x, y, z$

$\therefore$ $\dot{p}_\alpha = -k x_\alpha$. Similarly, $\dot{x}_\alpha = \frac{\partial H}{\partial p_\alpha}$, so $\dot{x}_\alpha = \frac{1}{m} p_\alpha$, $\alpha = x, y, z$

From these two eqns.,

$$\ddot{x}_\alpha = \frac{1}{m} \dot{p}_\alpha = -\frac{k}{m} x_\alpha \qquad \ldots(2)$$

The solution of (2) is, $x_\alpha(t) = A e^{i\sqrt{k/m}\,t} + B e^{-i\sqrt{k/m}\,t}$ $\quad \ldots(3)$

Applying initial conditions:

$$x_\alpha(0) = A + B \quad \text{and} \quad m\dot{x}_\alpha(0) = p_\alpha(0) = i\sqrt{mk}\,(A - B)$$

$$\therefore A = \frac{1}{2}\left(x_\alpha(0) + \frac{p_\alpha(0)}{i\sqrt{mk}}\right) \text{ and } B = \frac{1}{2}\left(x_\alpha(0) - \frac{p_\alpha(0)}{i\sqrt{mk}}\right)$$

$$\therefore x_\alpha(t) = x_\alpha(0)\cos\sqrt{\frac{k}{m}}\,t + \frac{p_\alpha(0)}{\sqrt{mk}}\sin\sqrt{\frac{k}{m}}\,t \qquad \ldots(4)$$

$$\text{and } \dot{x}_\alpha(t) = v_\alpha(t) = -x_\alpha(0)\sqrt{\frac{k}{m}}\sin\sqrt{\frac{k}{m}}\,t + \frac{p_\alpha(0)}{m}\cos\sqrt{\frac{k}{m}}\,t \qquad \ldots(5)$$

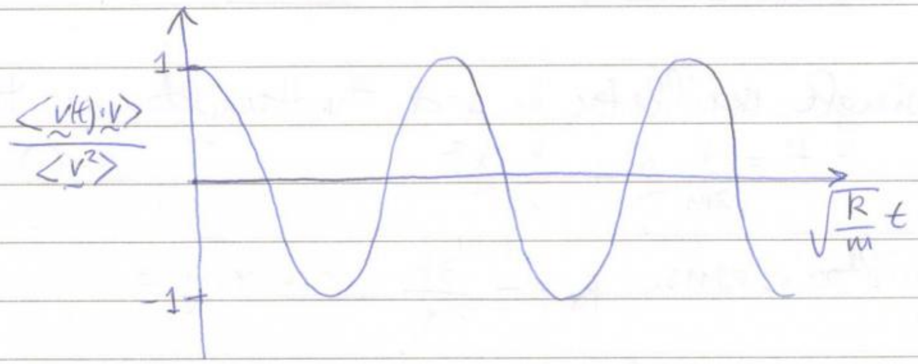
$$\therefore \langle v_\alpha(t)\, v_\alpha(0)\rangle = 0 + \langle v_\alpha^2(0)\rangle \cos\omega t$$

Since the oscillator is assumed to be at const. T, $\langle v_\alpha^2(0)\rangle$ can be calculated in the canonical ensemble, which leads to

$$\langle v_\alpha^2(0)\rangle = \frac{k_B T}{m} \Rightarrow \langle \underset{\sim}{v}^2\rangle = \frac{3k_B T}{m}$$

$$\therefore \langle \underset{\sim}{v}(t)\cdot\underset{\sim}{v}\rangle = \frac{3k_B T}{m}\cos\left(\sqrt{\frac{k}{m}}\,t\right)$$

Graphically, the normalized correlation function is as shown:



2. (i) Given $x_k = \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} q_j\, e^{-2\pi i jk/(2N+1)}$ ...(1)

Multiply (1) by $\exp(2\pi i\, lk/(2N+1))$ and sum over k:

$$\sum_{k=-N}^{N} x_k\, e^{2\pi i k l/(2N+1)} = \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} \sum_{k=-N}^{N} q_j\, e^{2\pi i k(l-j)/(2N+1)} \quad ...(2)$$

Consider

$$S_1 \equiv \sum_{k=-N}^{N} e^{2\pi i k(l-j)/(2N+1)} = 1 + \sum_{k=1}^{N}\left(e^{-2\pi i (l-j)/(2N+1)}\right)^k + \sum_{k=1}^{N}\left(e^{2\pi i (l-j)/(2N+1)}\right)^k \quad ...(3)$$

Using the formula for a geometric series

$$S_1 = 1 + \frac{e^{-2\pi i (l-j)(N+1)/(2N+1)} - e^{-2\pi i(l-j)/(2N+1)}}{e^{-2\pi i (l-j)/(2N+1)} - 1} + \frac{e^{2\pi i (l-j)(N+1)/(2N+1)} - e^{2\pi i (l-j)/(2N+1)}}{e^{2\pi i(l-j)/(2N+1)} - 1} \quad ...(4)$$

After combining the terms together, writing $N+1 = 2N+1-N$, and using the fact that $\exp(\pm 2\pi i(l-j)) = 1$ for $l \neq j$, we see that

Numerator of $S_1 = 0$

Now consider the case $l=j$ in S_1:

$$S_1 = \sum_{k=-N}^{N} e^{2\pi i k(l-j)/(2N+1)} = \sum_{k=-N}^{N} = 2N+1$$

$$\therefore \sum_{k=-N}^{N} e^{2\pi i k(l-j)/(2N+1)} = (2N+1)\delta_{lj} \qquad \ldots (5)$$

Substitute (5) in (2)

$$\sum_{k=-N}^{N} x_k e^{2\pi i k l/(2N+1)} = \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} q_j (2N+1)\delta_{lj}$$

$$\therefore \quad q_l = \frac{1}{\sqrt{2N+1}} \sum_{k=-N}^{N} x_k e^{2\pi i k l/(2N+1)} \qquad \ldots (6)$$

which is the required expression for q_l as an expansion in x_k.

(ii) In class, we showed that

$$[m + (M-m)\delta_{i,0}]\ddot{x}_i(t) = b(x_{i-1}(t) - 2x_i(t) + x_{i+1}(t)) \qquad \ldots (7)$$

Multiply (7) by $e^{2\pi i k l/(2N+1)}$ (replacing index i by k), sum over all k and divide by $\sqrt{2N+1}$

The result is

$$\frac{m}{\sqrt{2N+1}} \sum_{k=-N}^{N} e^{2\pi i k l/(2N+1)} \ddot{x}_k(t) + \frac{1}{\sqrt{2N+1}}(M-m)\sum_{k=-N}^{N} e^{2\pi i k l/(2N+1)} \delta_{k,0}\ddot{x}_0(t)$$

$$= \frac{b}{\sqrt{2N+1}} \sum_{k=-N}^{N} e^{2\pi i k l/(2N+1)} \{x_{k-1}(t) - 2x_k(t) + x_{k+1}(t)\} \qquad \ldots (8)$$

Consider

$$S_2 \equiv \sum_{k=-N}^{N} e^{2\pi i k l/(2N+1)} x_{k-1}$$

$$= \frac{1}{\sqrt{2N+1}} \sum_{k=-N}^{N} e^{2\pi i k l/(2N+1)} \sum_{j=-N}^{N} q_j e^{-2\pi i j(k-1)/(2N+1)}$$

$$= \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} q_j e^{2\pi i j/(2N+1)} \sum_{k=-N}^{N} e^{2\pi i k(l-j)/(2N+1)}$$

$$= \sqrt{2N+1}\; q_\ell\, e^{2\pi i \ell/(2N+1)} \qquad \text{(using (5))} \qquad \ldots(9)$$

iii) Consider $S_3 \equiv \sum_{k=-N}^{N} e^{2\pi i k\ell/(2N+1)} x_{k+1}$

$$= \frac{1}{\sqrt{2N+1}} \sum_{k=-N}^{N} e^{2\pi i k\ell/(2N+1)} \sum_{j=-N}^{N} q_j\, e^{-2\pi i j(k+1)/(2N+1)}$$

$$= \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} q_j\, e^{-2\pi i j/(2N+1)} \sum_{k=-N}^{N} e^{2\pi i k(\ell-j)/(2N+1)}$$

$$= \sqrt{2N+1}\; q_\ell\, e^{-2\pi i \ell/(2N+1)} \qquad \ldots(10)$$

With these results, (8) becomes

$$m\ddot{q}_\ell + \frac{1}{\sqrt{2N+1}}(M-m)\ddot{x}_0 = b\left(q_\ell\, e^{2\pi i\ell/(2N+1)} - 2q_\ell + q_\ell\, e^{-2\pi i \ell/(2N+1)}\right) \qquad \ldots(11)$$

Dividing (11) by m and defining $Q = (M-m)/m$, we get

$$\ddot{q}_\ell(t) + \frac{Q}{\sqrt{2N+1}}\ddot{x}_0(t) = \frac{2b}{m} q_\ell(t)\left(\cos\frac{2\pi\ell}{2N+1} - 1\right)$$

This is the sought-for expression.

3. (i) We showed in class that in the coupled oscillator model

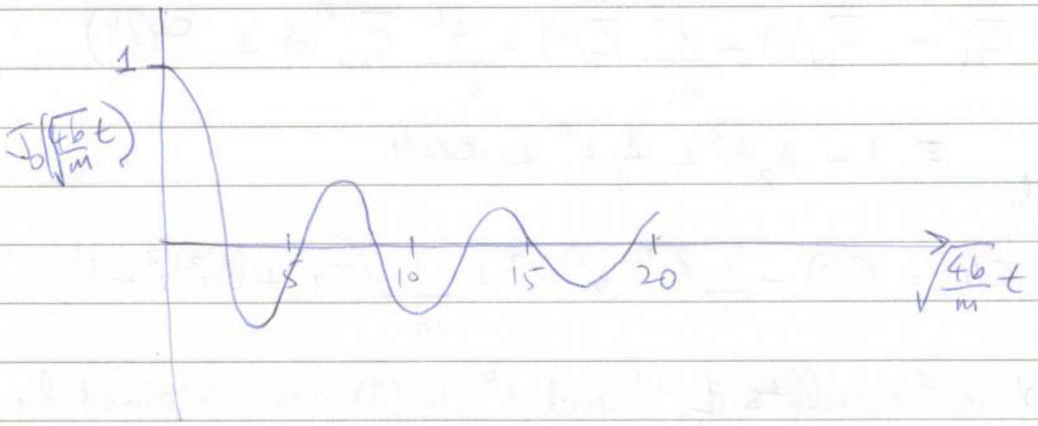
$$v_0(t) = (1+Q)\, v_0(0)\, \mathcal{L}^{-1} \frac{1}{sQ + \sqrt{s^2 + 4b/m}} \qquad \ldots(1)$$

So for $Q=0$

$$\langle v_0(t) v_0\rangle = \langle v_0^2\rangle\, \mathcal{L}^{-1}\frac{1}{\sqrt{s^2+4b/m}} = \langle v_0^2\rangle\, J_0\left(\sqrt{\frac{4b}{m}}\,t\right) \qquad \ldots(2)$$

where J_0 is the Bessel function of order 0.

Plotting $\langle v_0(t) v_0\rangle / \langle v_0^2\rangle$ against $\sqrt{\frac{4b}{m}}\,t$, we got



(ii) From (i), with $Q = 0$

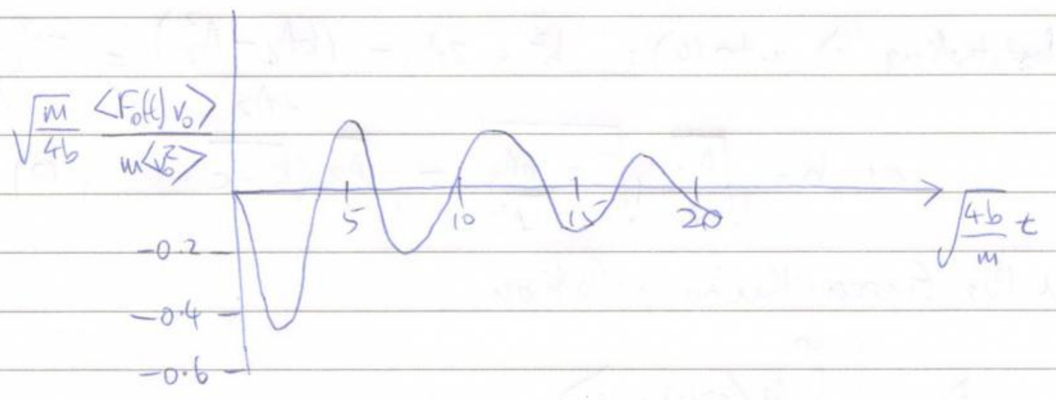
$$\dot{v}_0(t) = v_0(0)\frac{d}{dt}J_0\left(\sqrt{\frac{4b}{m}}\,t\right) \qquad (J_0(x) = \text{Bessel fxn of order } 0)$$

$$= -v_0(0)\sqrt{\frac{4b}{m}}\,J_1\left(\sqrt{\frac{4b}{m}}\,t\right) = \frac{F_0(t)}{m} \qquad \ldots(3)$$

where $F_0(t)$ is the force on particle 0

$$\therefore \langle F_0(t)\,v_0(0)\rangle = -m\langle v_0^2(0)\rangle\sqrt{\frac{4b}{m}}\,J_1\left(\sqrt{\frac{4b}{m}}\,t\right) \qquad \ldots(4)$$

Plotting $\sqrt{\frac{m}{4b}}\dfrac{\langle F_0(t)\,v_0(0)\rangle}{m\langle v_0^2(0)\rangle}$ against $\sqrt{\frac{4b}{m}}t$, we get



4. Given $\bar{C}_{vv}(t) = \dfrac{\langle \underset{\sim}{v}(t)\cdot \underset{\sim}{v}(0)\rangle}{\langle \underset{\sim}{v}(0)\cdot \underset{\sim}{v}(0)\rangle}$ and $C(t) \equiv \operatorname{sech} at \cos bt$,

$$\bar{C}_{vv} = \bar{C}_{vv}(0) - \frac{t^2}{2!}\ddot{\bar{C}}_{v}(0) + \frac{t^4}{4!}\bar{C}_{vv}^{(iv)}(0) + O(t^6) \qquad \ldots(1)$$

$$\equiv 1 - A_2 t^2 + A_4 t^4 + O(t^6) \qquad \ldots(2)$$

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$$C(t) = C(0) - \frac{1}{2}(a^2+b^2)t^2 + \frac{1}{24}(5a^4+6a^2b^2+b^4)t^4 + O(t^6) \quad \ldots(3)$$

where the coeffts of t^2 and t^4 in (3) are obtained by taking the second and fourth derivatives of $C(t)$ with respect to t, and then setting $t=0$

Comparing (2) and (3)

$$A_2 = \frac{1}{2}(a^2+b^2), \text{ or } \quad b^2 = 2A_2 - a^2 \qquad \ldots(4)$$

Also, $A_4 = \frac{1}{24}(5a^4+6a^2b^2+b^4) \qquad \ldots(5)$

Substituting (4) in (5):

$$24A_4 = 5a^4 + 6a^2(2A_2 - a^2) + 4A_2^2 + a^4 - 4A_2a^2$$

$$= 8a^2A_2 + 4A_2^2$$

$$\therefore \ 6A_4 = 2a^2A_2 + A_2^2$$

$$\therefore \ a = \sqrt{\frac{A_2}{2}}\sqrt{\frac{6A_4}{A_2^2} - 1} \equiv \sqrt{\frac{A_2}{2}}\sqrt{c-1} \qquad \ldots(6)$$

Substituting (6) into (4): $b^2 = 2A_2 - \frac{(6A_4 - A_2^2)}{2A_2} = \frac{5A_2^2 - 6A_4}{2A_2}$

$$\text{or } b = \sqrt{\frac{A_2}{2}}\sqrt{5 - \frac{6A_4}{A_2^2}} \equiv \sqrt{\frac{A_2}{2}}\sqrt{5-c} \qquad \ldots(7)$$

From the Green-Kubo relation

$$D = \frac{1}{3}\int_0^\infty dt \langle \underset{\sim}{v}(t)\cdot \underset{\sim}{v} \rangle$$

$$\simeq \frac{\langle \underset{\sim}{v}\cdot\underset{\sim}{v}\rangle}{3}\int_0^\infty dt \ \operatorname{sech} at \cos bt$$

Using a table of integrals or Mathematica,

$$\int_0^\infty dt \operatorname{sech} at \cos bt = \frac{\pi}{2a} \operatorname{sech}\left(\frac{b\pi}{2a}\right) \quad \ldots (8)$$

From equipartition, $\langle \underline{v} \cdot \underline{v} \rangle = \frac{3k_BT}{m}$ $\quad \ldots (9)$

Substituting (8) and (9) into D,

$$D = \frac{\pi k_B T}{2ma} \operatorname{sech} \frac{b\pi}{2a}$$

$$= \frac{\pi k_B T}{m\sqrt{2A_2(c-1)}} \operatorname{sech}\left(\frac{\pi}{2}\sqrt{\frac{5-c}{c-1}}\right) \quad \text{(using (6) and (7))}$$

This is the required expression for D.