(1) Self Interactions

Solution: We have given a Hamiltonian with nearest neighbor interaction,

$$H = \sum_j \left\{ \frac{D}{2} Q_j Q_j + \frac{1}{2M} P_j P_j \right\}. \tag{1}$$

Now we add a so-called self-interaction term, i. e. an interaction at the same lattice site:

$$H_{self} = \sum_j \lambda Q_j Q_j Q_j Q_j = \sum_j \frac{\lambda}{4DM} (a_j + a_j^\dagger)^4 \tag{2}$$

Now we want to express H_{self} in terms of annihilation and creation operators in Fourier space. Therefore, we express Q_j in terms of annihilation and creation operators in position space and make the Fourier transformation.

$$\begin{aligned}
H_{self} &= \sum_j \lambda Q_j Q_j Q_j Q_j = \sum_j \frac{\lambda}{4DM} (a_j + a_j^\dagger)^4 && (3)\\
&= \frac{\lambda}{4DMN^2} \sum_{j,q_1,q_2,q_3,q_4} \left(e^{iaq_1 j} a_{q_1} + e^{-iaq_1 j} a_{q_1}^\dagger \right) \left(e^{iaq_2 j} a_{q_2} + e^{-iaq_2 j} a_{q_2}^\dagger \right) \dots \\
&\quad \dots \left(e^{iaq_4 j} a_{q_4} + e^{-iaq_4 j} a_{q_4}^\dagger \right) && (4)\\
&= \frac{\lambda}{4DMN^2} \sum_{j,q_1,q_2,q_3,q_4} \left(e^{iaq_1 j} a_{q_1} + e^{iaq_1 j} a_{-q_1}^\dagger \right) \dots \left(e^{iaq_4 j} a_{q_4} + e^{iaq_4 j} a_{-q_4}^\dagger \right) && (5)\\
&= \frac{\lambda}{4DMN^2} \sum_{j,q_1,q_2,q_3,q_4} e^{iaj(q_1+q_2+q_3+q_4)} \left(a_{q_1} + a_{-q_1}^\dagger \right) \dots \left(q_{q_4} + a_{-q_4}^\dagger \right) && (6)\\
&= \frac{\lambda}{4DMN} \sum_{q_1,q_2,q_3,q_4} \delta_{0,q_1+q_2+q_3+q_4} \left(a_{q_1} + a_{-q_1}^\dagger \right) \dots \left(q_{q_4} + a_{-q_4}^\dagger \right). && (7)
\end{aligned}$$

In the last line we have used the identity $\frac{1}{N} \sum_j e^{iajq} = \delta_{0,q}$ for our periodic lattice. This Kronecker-Delta corresponds to conservation of momentum.

(2) One-Phonon States

Solution: (a) Uncoupled phonon state:
For uncoupled phonons on our one-dimensional grid, we want to compute the mean square displacement for a one-phonon state, i. e. $\langle j | Q_j^2 | j \rangle$. First we express Q_j in terms of annihilation and creation operators. Therefore

$$\langle j | Q_j^2 | j \rangle = \frac{1}{2(DM)^{1/2}} \langle j | a_j^2 + a_j a_j^\dagger + a_j^\dagger a_j + {a_j^\dagger}^2 | j \rangle. \tag{1}$$

Now a_j^2 acting on $|j\rangle$ gives zero ($a_j^2|j\rangle = a_j|0\rangle = 0$), as well as ${a_j^\dagger}^2$ acting on $\langle j|$. Now we remember $\hat{n}_q = a_q^\dagger a_q$ and use the commutator $[a_q, a_q^\dagger] = 1$. Then we get

$$\langle j|Q_j^2|j\rangle = \frac{1}{2(DM)^{1/2}}\langle j|(1 + a_j^\dagger a_j) + a_q^\dagger a_q|j\rangle = \frac{3}{2(DM)^{1/2}} \tag{2}$$

(b) Phonon state with nearest-neighbor interaction:
In a phonon state with nearest-neighbor interaction, the physical creation and annihilation operators in Fourier space are given by

$$A_q = \alpha a_q - \beta_{-q}^\dagger \tag{3}$$
$$A_q^\dagger = \alpha a_q^\dagger - \beta a_{-q}. \tag{4}$$

Now we transform back to position space by

$$A_j = \frac{1}{\sqrt{N}}\sum_q e^{iaqj}A_q = \frac{1}{\sqrt{N}}\sum_q e^{iaqj}(\alpha a_q - \beta a_{-q})$$
$$= \frac{1}{\sqrt{N}}\sum_q e^{iaqj}\alpha a_q + \frac{1}{\sqrt{N}}\sum_q e^{iaqj}(-\beta a_{-q})) \tag{5}$$
$$A_j = \frac{1}{\sqrt{N}}\sum_q e^{iaqj}\alpha a_q + \frac{1}{\sqrt{N}}\sum_q e^{-iaqj}(-\beta a_q)) = \alpha a_j^\dagger - \beta a_j. \tag{6}$$

In the same way

$$A_j^\dagger = \alpha a_j^\dagger - \beta a_j \tag{7}$$

Adding (6) and (7) gives

$$A_j + A_j^\dagger = (\alpha - \beta)(a_j + a_j^\dagger). \tag{8}$$

So

$$Q_j = \frac{1}{\sqrt{2}(DM)^{1/4}(\alpha - \beta)}. \tag{9}$$

Doing the same calculation as in 2.1, it follows that

$$\langle j|Q_j^2|j\rangle = \frac{3}{2(DM)^{1/2}(\alpha - \beta)^2}. \tag{10}$$

So in the special case $\alpha = 1$ and $\beta = 0$, we get the same result as in 2.1.

(3) Two Point Function

Solution: (a) We first write Q_j and $Q_{j+\Delta j}$ in terms of a_q and $a^\dagger_{-q}$:

$$Q_j =\sqrt{\frac{1}{2\mathcal{N}}}\left(a_j + a_j^\dagger\right) = \sqrt{\frac{1}{2\mathcal{N}}}\sum_q e^{iajq}\left(a_q + a^\dagger_{-q}\right) \tag{1}$$

$$Q_{j+\Delta j} =\sqrt{\frac{1}{2\mathcal{N}}}\left(a_j + a_j^\dagger\right) = \sqrt{\frac{1}{2\mathcal{N}}}\sum_q e^{ia(j+\Delta j)q}\left(a_q + a^\dagger_{-q}\right) \tag{2}$$

Then we wish to change to equation with A_q and $A_q^\dagger$. For this we use the transformation

$$a_q =\alpha_q A_q + \beta_q A^\dagger_{-q}, \tag{3}$$

$$a^\dagger_{-q} =\alpha_{-q} A^\dagger_{-q} + \beta_{-q} A_q = \alpha_q A^\dagger_{-q} + \beta_q A_q, \tag{4}$$

and find

$$Q_j =\sqrt{\frac{1}{2\mathcal{N}}}\sum_q e^{iqaj}\left(\alpha_q + \beta_q\right)\left(A_q + A^\dagger_{-q}\right), \tag{5}$$

$$Q_{j+\Delta j} =\sqrt{\frac{1}{2\mathcal{N}}}\sum_q e^{iq'a(j+\Delta j)}\left(\alpha_{q'} + \beta_{q'}\right)\left(A_{q'} + A^\dagger_{-q'}\right). \tag{6}$$

Then we calculate the product of the two,

$$Q_j Q_{j+\Delta j} = \frac{1}{2\mathcal{N}}\sum_{qq'} e^{iaj(q+q')}e^{iq'a\Delta j}\left(\alpha_q + \beta_q\right)\left(\alpha_{q'} + \beta_{q'}\right)\left(A_q A_{q'} + A_q A^\dagger_{-q'} + A^\dagger_{-q} A_{q'} + A^\dagger_{-q} A^\dagger_{-q'}\right). \tag{7}$$

When calculating $\langle 0|Q_j Q_{j+\Delta j}|0\rangle$ we see, that only the $A_q A^\dagger_{-q'}$ term survives. Through the commutator relation, we get a $\delta_{q,-q'}$ function,

$$\langle 0|Q_j Q_{j+\Delta j}|0\rangle =\frac{1}{2\mathcal{N}}\sum_{qq'} e^{iaj(q+q')}e^{iq'a\Delta j}\left(\alpha_q + \beta_q\right)\left(\alpha_{q'} + \beta_{q'}\right)\delta_{q,-q'}. \tag{8}$$

The result is

$$\langle 0|Q_j Q_{j+\Delta j}|0\rangle = \frac{1}{2\mathcal{N}}\sum_q \left(\alpha_q + \beta_q\right)^2 e^{iqa\Delta j}. \tag{9}$$

(b) Without nearest neighbour interaction, $\alpha_q = 1$ and $\beta_q = 0$. Using the result from (a) we then have

$$\langle 0|Q_j Q_{j+\Delta j}|0\rangle = \frac{1}{2\mathcal{N}}\delta_{\Delta j,0}. \tag{10}$$

(4) Operator Gymnastics

Solution: (a) We use the commutator relation $\left[\hat{\phi}(\vec{x}), \hat{\phi}^\dagger(\vec{y})\right] = \delta(\vec{x}-\vec{y})$. This leads directly to the result:

$$\langle 0|\hat{\phi}(\vec{x})\hat{\phi}^\dagger(\vec{y})|0\rangle = \delta(\vec{x}-\vec{y}) \tag{1}$$

(b) We use the hint in the form

$$\hat{\phi}(\vec{x}_2)\hat{\phi}^\dagger(\vec{x}_3)\hat{\phi}^\dagger(\vec{x}_4) = \hat{\phi}^\dagger(\vec{x}_3)\hat{\phi}^\dagger(\vec{x}_4)\hat{\phi}(\vec{x}_2) + \left[\hat{\phi}(\vec{x}_2), \hat{\phi}^\dagger(\vec{x}_3)\right]\hat{\phi}^\dagger(\vec{x}_4) + \hat{\phi}^\dagger(\vec{x}_3)\left[\hat{\phi}(\vec{x}_2), \hat{\phi}^\dagger(\vec{x}_4)\right]. \tag{2}$$

When calcultating the 4 point correlation function, the first term on the right above vanishes. One then replaces the commutors by their delta functions, and uses then the result from (a) twice, yielding

$$\langle 0|\hat{\phi}(\vec{x}_1)\hat{\phi}(\vec{x}_2)\hat{\phi}^\dagger(\vec{x}_3)\hat{\phi}^\dagger(\vec{x}_4)|0\rangle = \delta(\vec{x}_2-\vec{x}_3)\delta(\vec{x}_1-\vec{x}_4) + \delta(\vec{x}_2-\vec{x}_4)\delta(\vec{x}_1-\vec{x}_3). \tag{3}$$

(5) Matrix Elements

Solution: (a) We express $\langle x|$ and $|q\rangle$ with the creation and annihilation operators:

$$\langle x|q\rangle = \langle 0|\hat{\phi}(x)\hat{\phi}^\dagger(q)|0\rangle. \tag{1}$$

Using $\hat{\phi}^\dagger(q) = \int_y e^{iqy}\hat{\phi}^\dagger(y)$ we obtain

$$\int_y e^{iqy}\langle 0|\hat{\phi}(x)\hat{\phi}^\dagger(y)|0\rangle = \int_y e^{iqy}\delta(x-y) = e^{iqx}. \tag{2}$$

(b) We can write

$$\begin{aligned}\langle\vec{q}|\hat{\phi}(\vec{x})\hat{\phi}^\dagger(\vec{y})|\vec{p}\rangle =& \langle 0|\hat{\phi}(\vec{q})\hat{\phi}(\vec{x})\hat{\phi}^\dagger(\vec{y})\hat{\phi}^\dagger(\vec{p})|0\rangle \\ =& \int_{\vec{x}_1,\vec{x}_2} e^{i(\vec{p}\vec{x}_2-\vec{q}\vec{x}_1)}\langle 0|\hat{\phi}(\vec{x}_1)\hat{\phi}(\vec{x})\hat{\phi}^\dagger(\vec{y})\hat{\phi}^\dagger(\vec{x}_2)|0\rangle.\end{aligned} \tag{3}$$

For the second equation, we can use the result from Problem 4(b):

$$= \int_{\vec{x}_1,\vec{x}_2} e^{i(p\vec{x}_2-q\vec{x}_1)}\left(\delta(\vec{x}_1-\vec{y})\delta(\vec{x}-\vec{x}_2) + \delta(\vec{x}_1-\vec{x}_2)\delta(\vec{x}-\vec{y})\right). \tag{4}$$

The second term vanishes, since $\vec{x} \neq \vec{y}$. We finally get

$$lim_{\vec{q}\to\vec{p}} \langle \vec{q}|\hat{\phi}(\vec{x})\hat{\phi}^\dagger(\vec{y})|\vec{p}\rangle = lim_{\vec{q}\to\vec{p}}\, e^{i(\vec{p}\vec{x}-\vec{q}\vec{y})} = e^{i\vec{p}(\vec{x}-\vec{y})}. \quad (5)$$

(6) Atom Propagator

Solution: (a)

$$\langle x|x_0\rangle = \langle 0|\hat{\phi}(x)\hat{\phi}^\dagger(x_0)|0\rangle \quad (1)$$

(b)

$$P(x-x_0) = \theta(t-t_0)\langle x|x_o\rangle \quad (2)$$

Apart from ∂_t, all the operators in $D = i\partial_t + \frac{\Delta}{2M} - \mu$ commute with $\theta(t-t_0)$. Therefore we can compute

$$\begin{aligned} D\theta(t-t_0)\langle x|x_o\rangle &= i\delta(t-t_0)\langle 0|\phi(x)\phi^\dagger(x_0)|0> \\ &+ i\theta(t-t_0)\langle 0|\frac{\partial\phi}{\partial t}(x)\phi^\dagger(x_0)|0\rangle + (\frac{\Delta}{2M}-\mu)P(x-x_0) \\ &= i\delta(t-t_0)\delta(x-x_0). \end{aligned} \quad (3)$$

In the last step we have used the equation of motion for $\phi(x)$.
(c) We go to energy-momentum space with($p = (E,\vec{p})$) by

$$P(x-x_0) = \int_{\vec{p},E} \tilde{P}(p)e^{-ip(x-x_0)}. \quad (4)$$

Using the result of (b) and remembering the Fourier transform of the delta-function, as well as the translation of ∂_t and Δ in Fourier space, we find that

$$DP(x-x_0) = \int_p (\omega - \frac{\vec{p}^2}{2M} - \mu)\tilde{P}(p)e^{-ip(x-x_0)} = i\delta(x-x_0) \quad (5)$$

$$\Rightarrow \tilde{P} = \frac{i}{\omega - \frac{\vec{p}^2}{2M} - \mu} \quad (6)$$

(d) Now we transform back to position space to get an explicit result for $P(x-x_0)$.

$$\begin{aligned} P(x-x_0) &= \int_p \tilde{P}(p)e^{ip(x-x_0)} = \int_p \frac{i}{\omega - \frac{\vec{p}^2}{2M} - \mu} e^{ip(x-x_0)} \\ &= \int_{\tilde{\omega},\vec{p}} \frac{i}{\tilde{\omega}} e^{i((\tilde{\omega}+\frac{\vec{p}^2}{2M}+\mu)(t-t_0) - \vec{p}(\vec{x}-\vec{x_0}))} \\ &= i\int_{\tilde{\omega},\vec{p}} \left(\frac{e^{-i\tilde{\omega}(t-t_0)}}{\tilde{\omega}}\right) e^{-i((\frac{\vec{p}^2}{2M}+\mu)(t-t_0)-\vec{p}(\vec{x}-\vec{x_0}))} \\ &= \theta(t-t_0)e^{-i\mu(t-t_0)} \int_{\vec{p}} e^{-\frac{\tau}{2M}\vec{p}^2} e^{-\frac{M}{2\tau}(\vec{x}-\vec{x_0})^2}, \end{aligned} \quad (7)$$

where we introduced $\tilde{\omega} = \omega - \frac{\vec{p}^2}{2M} - \mu$, $\tau = i(t - t_0)$ and $\tilde{p} = \vec{p} + \frac{M}{t-t_0}(\vec{x} - \vec{x_0})$. The remaining 3-dimensional momentum integration can be done by defining $a = \frac{\tau}{2M}$ and going to polar coordinates. The integrand is spherically symmetric, therefore we can evaluate the integral by

$$\frac{4\pi}{(2\pi)^3}\int_0^\infty dx x^2 e^{-ax^2} = -\partial_a \frac{1}{2\pi^2}\int_0^\infty dx e^{-ax^2} = \left(\frac{M}{2\pi\tau}\right)^{3/2}, \tag{8}$$

where we renamed the integration variable. So the propagator in position space is given by

$$P(x - x_0) = \theta(t - t_0)e^{-\mu\tau}\left(\frac{M}{2\pi\tau}\right)^{3/2} e^{-\frac{M}{2\tau}(\vec{x}-\vec{x_0})^2}. \tag{9}$$

(7) Potential Energy

Solution: (a) The interaction energy in classical theories is often given by some density at place $\vec{x}$ times some density at place $\vec{y}$ times some factor, like for instance in the Newtonian theory of gravity. Therefore, one could write down a term like $V(|\vec{x} - \vec{y}|)\hat{n}(\vec{x}\hat{n}(\vec{y}) = V(\vec{x} - \vec{y})a^\dagger(\vec{x})a(\vec{x})a^\dagger(\vec{y})a(\vec{y})$. This expression makes sense if $\vec{x} \neq \vec{y}$. Then we have an interaction if there is at least one particle at both positions. If $\vec{x} = \vec{y}$, it also gives a contribution, also if there is only one particle at this position. However, we do not want such a behaviour, since we only want to describe interactions between particles. This can be done if we change the order of the operators, leading to the following expression: $V(|\vec{x}-\vec{y}|)a^\dagger(\vec{x})a^\dagger(\vec{y})a(\vec{x})a(\vec{y})$. This term gives the same result if $\vec{x} \neq \vec{y}$, since in this case the operators just commute. However if $\vec{x} = \vec{y}$ and there is just one particle at this position, the result is zero. For convenience, I will now suppress arrows above x and y, though of course they are 3-vectors. Now after the previous considerations, we can write down the interaction Hamiltonian:

$$H_{int} = \frac{1}{2}\int_{x,y} V(|\vec{x} - \vec{y}|)a^\dagger(\vec{x})a^\dagger(\vec{y})a(\vec{x})a(\vec{y}) \tag{1}$$

(b)i)To rewrite H_{int} in terms of the number operator, we do the following calculation:

$$\begin{aligned} a^\dagger(\vec{x})a^\dagger(\vec{y})a(\vec{x})a(\vec{y}) &= a^\dagger(x)(-\delta(x - y) + a(x)a^\dagger(y))a(y) \\ &= -\hat{n}(x)\delta(x - y) + \hat{n}(x)\hat{n}(y), \end{aligned} \tag{2}$$

where we just used the definition of the number operator, as well as the canonical commutator relations. Now the interaction Hamiltonian reads

$$H_{int} = \frac{1}{2}\int_{x,y} V(|\vec{x} - \vec{y}|)(-\hat{n}(x)\delta(x - y) + \hat{n}(x)\hat{n}(y)). \tag{3}$$

ii)We calculate the action of the number operator on a three-particle state:

$$\begin{aligned}
\hat{n}(x)|x_1x_2x_3\rangle &= \hat{n}a^\dagger(x_1)a^\dagger(x_2)a^\dagger(x_3)|0\rangle \\
&= a^\dagger(x)(\delta(x_1-x)+a^\dagger(x_1)a(x))a^\dagger(x_2)a^\dagger(x_3)|0\rangle \\
&= \delta(x_1-x)|x_1x_2x_3\rangle + a^\dagger(x)a^\dagger(x_1)(\delta(x-x_2)+a^\dagger(x_2)a(x))a^\dagger(x_3)|0\rangle \\
&= (\delta(x_1-x)+\delta(x_2-x))|x_1x_2x_3\rangle + a^\dagger(x)a^\dagger(x_1)a^\dagger(x_2)(\delta(x-x_3)+a^\dagger(x_3)a(x))|0\rangle \\
&= (\delta(x_1-x)+\delta(x_2-x)+\delta(x_3-x))|x_1x_2x_3\rangle, \qquad (4)
\end{aligned}$$

where we have used the definition of the number operator and the canonical commutator relations.
iii)Normalization:

$$\langle x_1x_2x_3|x_1x_2x_3\rangle = [\delta(0)]^3 = V_0^3, \qquad (5)$$

where V_0 is the space volume of our field theory. If we only consider fields in a finite box, this volume will also be finite.
iv) Now we compute the interaction energy for a three-particle state:

$$\begin{aligned}
H_{int} &= \frac{1}{2}\int_{x,y} V(|x-y|)\langle x_1x_2x_3|n(x)n(y)-n(x)\delta(x-y)|x_1x_2x_3\rangle \\
&= -\frac{1}{2}\int_x V(0)\langle x_1x_2x_3|n(x)|x_1x_2x_3\rangle + \frac{1}{2}\int_{x,y} V(|x-y|)\langle x_1x_2x_3|n(x)n(y)|x_1x_2x_3\rangle \\
&= -\frac{1}{2}\int_x V(0)\langle x_1x_2x_3|\delta(x-x_1)+\delta(x-x_2)+\delta(x-x_3)|x_1x_2x_3\rangle \\
&+ \frac{1}{2}\int_{x,y} V(x-y)\langle x_1x_2x_3|(\delta(x-x_1)+\delta(x-x_2)+\delta(x-x_3))(\delta(y-x_1)+\delta(y-x_2)+\delta(y-x_3))|x_1x_2 \\
&= -\frac{3}{2}V(0)[\delta(0)]^3 + \frac{1}{2}\sum_{i,j=1}^{3} V(|x_i-x_j|)[\delta(0)]^3 \\
&= \frac{1}{2}\sum_{i\neq j} V(|x_i-x_j|)[\delta(0)]^3 \qquad (6)
\end{aligned}$$