Coherent State Phonon Dynamics

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Introduction

This note records the derivation developed in my meeting with David on last Tuesday.

Part I formulates the problem; Part II carries out the analysis in the coherent-state representation. The core argument is due to David; I have transcribed and expanded it with proofs and supporting details.

Part I

The model Hamiltonian is

$$H = \sum_{j=1}^{N}\Big(\frac{p_j^2}{2} + V(q_j)\Big) + \frac{1}{2}\omega_0^2\sum_{j=1}^{N}(q_j - q_{j+1})^2 \tag{I.1}$$

where j labels the atom and cyclic boundary condition implies $q_{N+1} \equiv q_1$. We have set $m = 1$ and $\hbar = 1$.

The Hamiltonian can be rewritten as

$$H = \sum_{j=1}^{N}\Big(\frac{p_j^2}{2} + U(q_j)\Big) - \omega_0^2\sum_{j=1}^{N} q_j q_{j+1} \tag{I.2}$$

where $U(q_j)$ is the Feynman-Kleinert effective potential.

Provided that the temperature is low, we can apply the harmonic approximation to the effective on-site potential

$$U(q_j) \approx U_0 + \frac{1}{2}\omega_\beta^2 q_j^2 \tag{I.3}$$

hence

$$\begin{aligned} H &= \sum_{j=1}^{N}\Big(\frac{p_j^2}{2} + \frac{1}{2}\omega_\beta^2 q_j^2\Big) - \omega_0^2\sum_{j=1}^{N} q_j q_{j+1} \\ &= \sum_{j=1}^{N}\Big(\frac{p_j^2}{2} + \frac{1}{2}\omega_\beta^2 q_j^2\Big) - \frac{1}{2}\omega_0^2\sum_{j=1}^{N} q_{j-1}q_j + q_j q_{j+1}) \\ &= \frac{\mathbf{p}^\mathsf{T}\mathbf{p}}{2} + \frac{1}{2}\mathbf{q}^\mathsf{T}\mathbf{\Omega}^2\mathbf{q} \end{aligned} \tag{I.4}$$

where we have used the cyclic boundary condition on line 2, $\mathbf{q}$ is a vector of dimension N, holding the positions of all atoms, similarly for $\mathbf{p}$, and we have also defined

$$\Omega_{ij}^2 \equiv \omega_\beta^2 \delta_{ij} - \omega_0^2(\delta_{i,j-1} + \delta_{i,j+1}) \tag{I.5}$$

we wish to diagonalise $\mathbf{\Omega}^2$ which is equivalent to finding the normal modes, the eigenvalue equation is

$$\mathbf{\Omega}^2 \mathbf{c} = \omega^2 \mathbf{c} \tag{I.6}$$

which can be rewritten in index notation as

$$\sum_k \Omega_{jk}^2 c_k = \omega^2 c_j \tag{I.7}$$

using Eq. (I.5) yields

$$\sum_k (\omega_\beta^2 \delta_{jk} - \omega_0^2(\delta_{j,k-1} + \delta_{j,k+1}))c_k = \omega^2 c_j \tag{I.8}$$

$$\omega_\beta^2 c_j - \omega_0^2 (c_{j+1} + c_{j-1}) = \omega^2 c_j \tag{I.9}$$

Let $c_j = \frac{1}{\sqrt{N}} e^{ij\theta}$, then substitute into Eq. (I.9) yields the eigenvalue

$$\omega_k^2 = \omega_\beta^2 - 2\omega_0^2 \cos\Big(\frac{2\pi k}{N}\Big) \tag{I.10}$$

where we have required $c_{N+1} = c_1$ so $\theta_k = 2\pi k/N$ and k is an integer.

Same result can be obtained if we let $c_j = e^{-ij\theta}$, thus we take the linear combination of these eigenvectors to ensure $\mathbf{C}^\mathsf{T}\mathbf{C} = \mathbf{1}$

$$c_{jk} = \sqrt{\frac{2}{N}} \cos\Big(\frac{2\pi jk}{N}\Big) \tag{I.11}$$

Eq. (I.6) becomes

$$\mathbf{\Omega}^2 = \mathbf{C}\boldsymbol{\omega}^2\mathbf{C}^\mathsf{T} \tag{I.12}$$

where $\boldsymbol{\omega}^2$ is diagonal with eigenvalue ω_k^2 as entries

substitute into Eq. (I.4) yields

$$H = \frac{\tilde{\mathbf{p}}^\mathsf{T}\tilde{\mathbf{p}}}{2} + \frac{1}{2}\tilde{\mathbf{q}}^\mathsf{T}\boldsymbol{\omega}^2\tilde{\mathbf{q}} \tag{I.13}$$

where we have defined $\tilde{\mathbf{q}} \equiv \mathbf{C}^\mathsf{T}\mathbf{q}$, $\tilde{\mathbf{q}}^\mathsf{T} \equiv \mathbf{q}^\mathsf{T}\mathbf{C}$ and similarly for $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{p}}^\mathsf{T}$

Now we move on to consider some commutation relations

$$[\tilde{q}_k, \tilde{q}_{k'}] = 0 \tag{I.14}$$

$$[\tilde{p}_k, \tilde{p}_{k'}] = 0 \tag{I.15}$$

and

$$[\tilde{q}_k, \tilde{p}_{k'}] = i\delta_{kk'} \tag{I.16}$$

from the diagonalisation of $\mathbf{\Omega}^2$ earlier
we now define the dimensionless position and momentum operators

$$\hat{q}_k \equiv \sqrt{\omega_k}\tilde{q}_k \tag{I.17}$$

$$\hat{p}_k \equiv \frac{\tilde{p}_k}{\sqrt{\omega_k}} \tag{I.18}$$

and the dimensionless ladder operators

$$\hat{a}_k \equiv \frac{1}{\sqrt{2}}\Big(\hat{q}_k + i\hat{p}_k\Big) \tag{I.19}$$

$$\hat{a}_k^\dagger = \frac{1}{\sqrt{2}}\Big(\hat{q}_k - i\hat{p}_k\Big) \tag{I.20}$$

which have the commutation relation

$$[\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{kk'} \tag{I.21}$$

Hamiltonian becomes

$$H = \sum_k \omega_k \Big(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2}\Big) \tag{I.22}$$

From this point we will drop all the superscripts, subscripts and bold fonts as we will only consider one γ component of a single k mode. In addition, we will drop the shift in energy scale by the zero-point-energy.

Hence the Hamiltonian under consideration becomes

$$H = \omega \hat{a}^\dagger \hat{a} \tag{I.23}$$

this completes the set up.

Part II

It can be shown that

$$e^{-\lambda \hat{a}^\dagger \hat{a}+\mu \hat{a}^\dagger+\nu \hat{a}} = \frac{1}{\pi}\int d^2\alpha\, |\alpha\rangle e^{\lambda+\frac{\mu\nu}{\lambda}-(e^\lambda-1)(\alpha^*-\frac{\nu}{\lambda})(\alpha-\frac{\mu}{\lambda})}\langle\alpha| \tag{II.1}$$

(Proof: Appendix B)
set $\mu=\nu=0$
The Gibbs operator can be expressed in its diagonal coherent state representation as

$$\boxed{e^{-\beta H} = \frac{1}{\pi}\int d^2\alpha|\alpha\rangle e^{\lambda-(e^\lambda-1)|\alpha|^2}\langle\alpha|} \tag{II.2}$$

where $\beta \equiv 1/k_BT$, $\lambda\equiv\beta\omega$ and $|\alpha\rangle$ is a coherent state. (A more detailed description of coherent state: Appendix A)
The partition function is

$$\begin{aligned} Z &\equiv \mathrm{tr}[e^{-\beta H}] \\ &= \frac{1}{\pi}\int d^2\alpha\, e^{\lambda-(e^\lambda-1)|\alpha|^2} \\ &= \frac{1}{2\pi}\int dp\int dq\, e^{\lambda-(e^\lambda-1)(p^2+q^2)/2} \\ &= \frac{1}{2\pi}e^\lambda\frac{2\pi}{e^\lambda-1} \\ &= \frac{1}{1-e^{-\beta\omega}} \end{aligned} \tag{II.3}$$

where we have used $\alpha=\frac{1}{\sqrt{2}}(q+ip)$, $\alpha^*=\frac{1}{\sqrt{2}}(q-ip)$, $q=\langle\alpha|\hat{q}|\alpha\rangle$ and $p=\langle\alpha|\hat{p}|\alpha\rangle$ and the standard Gaussian integral

$$\int_{-\infty}^{\infty} dt\, t^{2n}e^{-st^2} = \sqrt{\frac{\pi}{s}}\frac{(2n-1)!!}{(2s)^n} \tag{II.4}$$

where n is a positive integer.
The form of the partition function is as expected.
We will now find the diagonal coherent state representation of the Kubo-transformed velocity operator

$$\hat{p}_\beta \equiv \frac{1}{\beta}\int_0^\beta d\eta\, e^{-(\beta-\eta)H}\hat{p}e^{-\eta H} \tag{II.5}$$

Return to Eq. (II.1) then let $\nu=-\mu$

$$e^{-\lambda\hat{a}^\dagger\hat{a}+\mu(\hat{a}^\dagger-\hat{a})} = \frac{1}{\pi}\int d^2\alpha\,|\alpha\rangle e^{\lambda-\frac{\mu^2}{\lambda}-(e^\lambda-1)(\alpha^*+\frac{\mu}{\lambda})(\alpha-\frac{\mu}{\lambda})}\langle\alpha| \tag{II.6}$$

$$
\begin{aligned}
\left.\frac{\partial}{\partial\mu}e^{-\lambda\hat{a}^\dagger\hat{a}+\mu(\hat{a}^\dagger-\hat{a})}\right|_{\mu=0} &= \left.\frac{\partial}{\partial\mu}\frac{1}{\pi}\int d^2\alpha\,|\alpha\rangle e^{\lambda-\frac{\mu^2}{\lambda}-(e^\lambda-1)(\alpha^*+\frac{\mu}{\lambda})(\alpha-\frac{\mu}{\lambda})}\langle\alpha|\right|_{\mu=0} \\
&= \left.\frac{1}{\pi}\int d^2\alpha\,|\alpha\rangle\Big[-\frac{2\mu}{\lambda}-\frac{e^\lambda-1}{\lambda}\Big(\alpha-\alpha^*-\frac{2\mu}{\lambda}\Big)\Big]e^{\lambda-\frac{\mu^2}{\lambda}-(e^\lambda-1)(\alpha^*+\frac{\mu}{\lambda})(\alpha-\frac{\mu}{\lambda})}\langle\alpha|\right|_{\mu=0} \\
&= \frac{\sqrt{2}}{i\pi\lambda}\int d^2\alpha\,|\alpha\rangle(e^\lambda-1)pe^{\lambda-(e^\lambda-1)|\alpha|^2}\langle\alpha| \qquad \text{(II.7)}
\end{aligned}
$$

Consider

$$
\frac{\partial}{\partial\mu}e^{\hat{A}(\mu)} = \int_0^1 d\tau\,e^{(1-\tau)\hat{A}(\mu)}\frac{\partial\hat{A}(\mu)}{\partial\mu}e^{\tau\hat{A}(\mu)} \qquad \text{(II.8)}
$$

(Proof: Appendix C)
let $\hat{A}(\mu) = -\lambda\hat{a}^\dagger\hat{a} + \mu(\hat{a}^\dagger - \hat{a})$

$$
\begin{aligned}
\left.\frac{\partial}{\partial\mu}e^{-\lambda\hat{a}^\dagger\hat{a}+\mu(\hat{a}^\dagger-\hat{a})}\right|_{\mu=0} &= \left.\int_0^1 d\tau\,e^{(1-\tau)[-\lambda\hat{a}^\dagger\hat{a}+\mu(\hat{a}^\dagger-\hat{a})]}(\hat{a}^\dagger-\hat{a})e^{\tau[-\lambda\hat{a}^\dagger\hat{a}+\mu(\hat{a}^\dagger-\hat{a})]}\right|_{\mu=0} \\
&= \int_0^1 d\tau\,e^{-\lambda(1-\tau)\hat{a}^\dagger\hat{a}}(\hat{a}^\dagger-\hat{a})e^{-\lambda\tau\hat{a}^\dagger\hat{a}} \\
&= \frac{1}{\beta}\int_0^\beta d\eta\,e^{-(\beta-\eta)H}(\hat{a}^\dagger-\hat{a})e^{-\eta H} \\
&= \frac{\sqrt{2}}{i\beta}\int_0^\beta d\eta\,e^{-(\beta-\eta)H}\hat{p}e^{-\eta H} \\
&\equiv \frac{\sqrt{2}}{i}\hat{p}_\beta \qquad \text{(II.9)}
\end{aligned}
$$

where we have used Eq. (II.8) on line 1, $\tau = \eta/\beta$ and $\lambda = \beta\omega$ on line 2, $\hat{p} = \frac{i}{\sqrt{2}}(\hat{a}^\dagger - \hat{a})$ on line 3 and definition Eq. (II.5) on line 4

Equate (II.7) and (II.9) to obtain the diagonal coherent state representation of the Kubo-transformed velocity operator

$$
\boxed{\hat{p}_\beta = \frac{1}{\pi\lambda}\int d^2\alpha\,|\alpha\rangle(e^\lambda-1)pe^{\lambda-(e^\lambda-1)|\alpha|^2}\langle\alpha|} \qquad \text{(II.10)}
$$

Let us now use it to evaluate the Kubo-transformed normal mode velocity correlation function

$$
\begin{aligned}
C(t) &\equiv \frac{1}{Z}\,\mathrm{tr}\big[\hat{p}_\beta(0)\hat{p}(t)\big] \\
&= \frac{1}{\pi Z\lambda}\int d^2\alpha\,(e^\lambda-1)pe^{\lambda-(e^\lambda-1)|\alpha|^2}\langle\alpha|\hat{p}(t)|\alpha\rangle \\
&= \frac{1}{2\pi Z\lambda}\int dp\int dq\,(e^\lambda-1)e^{\lambda-(e^\lambda-1)(p^2+q^2)/2}(p^2\cos\omega t-pq\sin\omega t) \\
&= \frac{(e^\lambda-1)\displaystyle\int dp\int dq\,e^{\lambda-(e^\lambda-1)(p^2+q^2)/2}p^2}{\lambda\displaystyle\int dp\int dq\,e^{\lambda-(e^\lambda-1)(p^2+q^2)/2}}\cos\omega t \\
&= \frac{(e^\lambda-1)\displaystyle\int dp\,e^{-(e^\lambda-1)p^2/2}p^2}{\lambda\displaystyle\int dp\,e^{-(e^\lambda-1)p^2/2}}\cos\omega t
\end{aligned}
\tag{II.11}
$$

where we have noticed the part of the integrand multiplied by $-pq\sin\omega t$ is odd, thus vanishes and the integral with respect to dq are the same for both the numerator and denominator.

Recall we have scaled momentum in Eq. (I.18), this should now be scaled back to the correct dimension via $p^2\to\omega p^2$, so we have

$$
C(t) = \frac{(e^\lambda-1)\omega\displaystyle\int dp\,e^{-(e^\lambda-1)p^2/2}p^2}{\lambda\displaystyle\int dp\,e^{-(e^\lambda-1)p^2/2}}\cos\omega t \tag{II.12}
$$

using Eq. (II.4) yields

$$
C(t) = \frac{e^\lambda-1}{\lambda}\frac{\omega}{e^\lambda-1}\cos\omega t \tag{II.13}
$$

after simplifying

$$
C(t) = \frac{1}{\beta}\cos\omega t \tag{II.14}
$$

which is expected.

Appendix A

Coherent state is defined as the eigenstate of the annihilation operator $\hat{a}$ for a harmonic oscillator

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{A1}$$

α in general is a complex number $\alpha = |\alpha|e^{i\phi}$.
where

$$\hat{a} \equiv \frac{m\omega\hat{x} + i\hat{p}}{\sqrt{2m\hbar\omega}} \tag{A2}$$

$$\hat{a}^\dagger = \frac{m\omega\hat{x} - i\hat{p}}{\sqrt{2m\hbar\omega}} \tag{A3}$$

$$[\hat{a}, \hat{a}^\dagger] = 1 \tag{A4}$$

Projection into the position basis yields a linear first-order ODE, solved by seperation of variables

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\right)\langle x|\alpha\rangle = \alpha\langle x|\alpha\rangle \tag{A5}$$

the solution is

$$\langle x|\alpha\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}}e^{-x^2/4\sigma^2}e^{\alpha x/\sigma} \tag{A6}$$

which can be rewritten as

$$\langle x|\alpha\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}}e^{-(x-x_\alpha)^2/4\sigma^2}e^{ip_\alpha x/\hbar}e^{i\theta_\alpha} \tag{A7}$$

where $\theta_\alpha \equiv -\Re\alpha\Im\alpha$, $\sigma \equiv \sqrt{\frac{\hbar}{2m\omega}}$ and

$$x_\alpha \equiv \langle\alpha|\hat{x}|\alpha\rangle = \sigma\langle\alpha|\hat{a} + \hat{a}^\dagger|\alpha\rangle = \sigma(\alpha + \alpha^*) = \sigma|\alpha|(e^{i\phi} + e^{-i\phi}) = 2\sigma|\alpha|\cos\phi \tag{A8}$$

$$p_\alpha \equiv \langle\alpha|\hat{p}|\alpha\rangle = -\frac{i\hbar}{2\sigma}\langle\alpha|\hat{a} - \hat{a}^\dagger|\alpha\rangle = -\frac{i\hbar}{2\sigma}(\alpha - \alpha^*) = \frac{\hbar}{\sigma}|\alpha|\sin\phi \tag{A9}$$

$$\begin{aligned}
\Delta x^2 &\equiv \langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2 \\
&= \sigma^2\big(\langle\alpha|(\hat{a} + \hat{a}^\dagger)^2|\alpha\rangle - \langle\alpha|\hat{a} + \hat{a}^\dagger|\alpha\rangle^2\big) \\
&= \sigma^2\big(\langle\alpha|\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}|\alpha\rangle - (\alpha + \alpha^*)^2\big) \\
&= \sigma^2\big(\langle\alpha|\hat{a}^2 + 2\hat{a}^\dagger\hat{a} + 1 + \hat{a}^{\dagger 2}|\alpha\rangle - (\alpha + \alpha^*)^2\big) \\
&= \sigma^2\big(\alpha^2 + 2|\alpha|^2 + 1 + \alpha^{*2} - \alpha^2 - 2|\alpha|^2 - \alpha^{*2}\big) \\
&= \sigma^2
\end{aligned} \tag{A10}$$

similarly

$$\Delta p^2 = \frac{\hbar^2}{4\sigma^2} \tag{A11}$$

hence

$$\Delta x \Delta p = \frac{\hbar}{2} \tag{A12}$$

therefore coherent state is a state of minimum uncertainty.
Another equivalent definition of coherent state is in terms of displacement operator

$$|\alpha\rangle \equiv \hat{D}|0\rangle \tag{A13}$$

where

$$\hat{D}(\alpha) \equiv e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} \tag{A14}$$

where an Baker-Campbell-Hausdorff formula is used for the second equality

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A},\hat{B}]/2} \tag{A15}$$

provided that $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$
It is easy to show the following properties using Eq. (A14)

$$\hat{D}^\dagger(\alpha)\hat{D}(\alpha) = \hat{1} \tag{A16}$$

$$\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha) \tag{A17}$$

$$[\hat{a}, \hat{D}(\alpha)] = \alpha \hat{D}(\alpha) \tag{A18}$$

therefore

$$\begin{aligned} \hat{a}\hat{D}(\beta)|\alpha\rangle &= \hat{D}(\beta)\hat{a}|\alpha\rangle + [\hat{a}, \hat{D}(\beta)]|\alpha\rangle \\ &= (\alpha + \beta)\hat{D}(\beta)|\alpha\rangle \end{aligned} \tag{A19}$$

hence

$$\hat{D}(\alpha)|\beta\rangle = |\alpha + \beta\rangle \tag{A20}$$

Consider

$$
\begin{aligned}
\langle x|\alpha\rangle &= \langle x|\hat{D}(\alpha)|0\rangle \\
&= \langle x|e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}|0\rangle \\
&= \langle x|e^{\alpha\left(\frac{m\omega\hat{x}-i\hat{p}}{\sqrt{2m\hbar\omega}}\right)-\alpha^*\left(\frac{m\omega\hat{x}+i\hat{p}}{\sqrt{2m\hbar\omega}}\right)}|0\rangle \\
&= \langle x|e^{\sqrt{\frac{m\omega}{2\hbar}}(\alpha-\alpha^*)\hat{x}-\frac{i}{\sqrt{2m\hbar\omega}}(\alpha+\alpha^*)\hat{p}}|0\rangle \\
&= \langle x|e^{\sqrt{\frac{m\omega}{2\hbar}}(\alpha-\alpha^*)\hat{x}}e^{-\frac{i}{\sqrt{2m\hbar\omega}}(\alpha+\alpha^*)\hat{p}}e^{-\frac{1}{2}\left[\sqrt{\frac{m\omega}{2\hbar}}(\alpha-\alpha^*)\hat{x},-\frac{i}{\sqrt{2m\hbar\omega}}(\alpha+\alpha^*)\hat{p}\right]}|0\rangle \\
&= \langle x|e^{\sqrt{\frac{m\omega}{2\hbar}}(\alpha-\alpha^*)\hat{x}}e^{-\frac{i}{\sqrt{2m\hbar\omega}}(\alpha+\alpha^*)\hat{p}}e^{-\frac{1}{4}(\alpha^2-\alpha^{*2})}|0\rangle \\
&= e^{-\frac{1}{4}(\alpha^2-\alpha^{*2})}e^{\sqrt{\frac{m\omega}{2\hbar}}(\alpha-\alpha^*)x}\langle x|e^{-\frac{i}{\sqrt{2m\hbar\omega}}(\alpha+\alpha^*)\hat{p}}|0\rangle \\
&= e^{i\theta_\alpha}e^{ip_\alpha x/\hbar}\langle x|e^{-\frac{ix_\alpha}{\hbar}\hat{p}}|0\rangle \\
&= e^{i\theta_\alpha}e^{ip_\alpha x/\hbar}\langle x|\hat{T}(x_\alpha)|0\rangle \\
&= e^{i\theta_\alpha}e^{ip_\alpha x/\hbar}\langle x-x_\alpha|0\rangle
\end{aligned} \tag{A21}
$$

where we have recognised the translation operator as

$$\hat{T}(q) = e^{-iqp/\hbar} \tag{A22}$$

which is unitary

$$\hat{T}^\dagger(q)\hat{T}(q) = \hat{1} \tag{A23}$$

and has the effect on position eigenstates

$$\hat{T}(q)|x\rangle = |x+q\rangle \tag{A24}$$

these results can be easily proven using Eq. (A22)

therefore Eq. (A21) suggests the effect of displacement operator is displacement of the position by x_α and boost in momentum by p_α, this is consistent with Eq. (A7)

We now express the coherent state in energy basis

$$|\alpha\rangle = \sum_{n=1}^{\infty} c_n|n\rangle \tag{A25}$$

where c_n is to be determined

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_n\hat{a}|n\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle \tag{A26}$$

but also

$$\hat{a}|\alpha\rangle = \alpha\sum_{n=1}^{\infty} c_n|n\rangle \tag{A27}$$

therefore

$$c_{n+1} = \frac{\alpha}{\sqrt{n+1}}c_n \tag{A28}$$

repeated substitution of this recurrence relation into itself yields

$$c_n = \frac{\alpha^n}{\sqrt{n!}} c_0 \tag{A29}$$

c_0 is determined by normalisation

$$\langle\alpha|\alpha\rangle = \sum_n |c_n|^2 = c_0^2 \sum_n \frac{|\alpha|^2}{n!} = c_0^2 e^{|\alpha|^2} \tag{A30}$$

hence

$$c_0 = e^{-|\alpha|^2/2} \tag{A31}$$

so that

$$\langle\alpha|\alpha\rangle = 1 \tag{A32}$$

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{A33}$$

It is easy to show using Eq. (A33)

$$\langle\beta|\alpha\rangle = e^{-\frac{1}{2}|\beta|^2 - \frac{1}{2}|\alpha|^2 + \beta^*\alpha} \tag{A34}$$

therefore different coherent states are not orthogonal.
The expectation value and variance of the number of excitation are the same

$$n_\alpha = \sigma_{n,\alpha}^2 = |\alpha|^2 \tag{A35}$$

$$|\langle n|\alpha\rangle|^2 = \frac{n_\alpha^n e^{-n_\alpha}}{n!} \tag{A36}$$

where $n_\alpha \equiv \langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle$ and $\sigma_{n,\alpha}^2 \equiv \langle\alpha|\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}|\alpha\rangle - \langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle^2$ therefore the number of excitation in a coherent state follows a Poisson distribution.

We shall now consider the time evolution of a coherent state

$$\begin{aligned}
|\alpha(t)\rangle &= e^{-iHt}|\alpha\rangle \\
&= e^{-iHt} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\
&= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-iHt} |n\rangle \\
&= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-iE_n t} |n\rangle \\
&= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i(n+1/2)\omega t} |n\rangle \\
&= e^{-i\omega t/2} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} |n\rangle \\
&= e^{-i\omega t/2} |\alpha e^{-i\omega t}\rangle
\end{aligned} \tag{A37}$$

Therefore coherent state stays coherent under time evolution.

Using Eq. (A8), (A9) and angle difference identity $\cos(A-B) \equiv \cos A\cos B + \sin A\sin B$, $\sin(A-B) \equiv \cos A\sin B - \sin A\cos B$, we obtain the time evolution of expecation values of observables

$$\langle\alpha|\hat{x}(t)|\alpha\rangle = 2\sigma|\alpha|\cos(\phi-\omega t) = x_\alpha\cos\omega t + \frac{2\sigma^2}{\hbar}p_\alpha\sin\omega t \tag{A38}$$

$$\langle\alpha|\hat{p}(t)|\alpha\rangle = \frac{\hbar}{\sigma}|\alpha|\sin(\phi-\omega t) = p_\alpha\cos\omega t - \frac{\hbar}{2\sigma^2}x_\alpha\sin\omega t \tag{A39}$$

Consider the integral

$$\begin{aligned}
\int d^2\alpha\langle m|\alpha\rangle\langle\alpha|n\rangle &= \int d^2\alpha\, e^{-|\alpha|^2}\frac{\alpha^{*m}}{\sqrt{m!}}\frac{\alpha^n}{\sqrt{n!}} \\
&= \frac{1}{\sqrt{m!n!}}\iint |\alpha|d|\alpha|\, d\phi\, e^{-|\alpha|^2}|\alpha|^m e^{-im\phi}|\alpha|^n e^{in\phi} \\
&= \frac{1}{\sqrt{m!n!}}\int_0^\infty d|\alpha|\, |\alpha|^{m+n+1}e^{-|\alpha|^2}\int_0^{2\pi} d\phi\, e^{i(n-m)\phi} \\
&= \frac{1}{\sqrt{m!n!}}\frac{1}{2}\Big(\frac{m+n}{2}\Big)!2\pi\delta_{nm} \\
&= \pi\delta_{nm}
\end{aligned} \tag{A40}$$

where we have used the Gamma function

$$\Gamma(n) \equiv \int_0^\infty dt\, t^{n-1}e^{-t} = (n-1)! \tag{A41}$$

for integer n.

Therefore we have a resolution of identity in the coherent state representation

$$\hat{1} = \frac{1}{\pi}\int d^2\alpha|\alpha\rangle\langle\alpha| \tag{A42}$$

due to Eq. (A34), the coherent basis set is known as overcomplete.

Appendix B

Proof.

Consider

$$
\begin{aligned}
\hat{a}^{\dagger r}\hat{a}^{r}|n\rangle &= \hat{a}^{\dagger r}\sqrt{n(n-1)\cdots(n-r+1)}|n-r\rangle \\
&= \sqrt{\frac{n!}{(n-r)!}}\hat{a}^{\dagger r}|n-r\rangle \\
&= \sqrt{\frac{n!}{(n-r)!}}\sqrt{\frac{n!}{(n-r)!}}|n\rangle \\
&= \frac{n!}{(n-r)!}|n\rangle
\end{aligned}
\tag{B1}
$$

for $r > n$, RHS vanishes
normal order operation is defined as

$$
:(\hat{a}^{\dagger}\hat{a})^{r}:\equiv \hat{a}^{\dagger r}\hat{a}^{r}
\tag{B2}
$$

consider

$$
\begin{aligned}
:e^{(e^{\lambda}-1)\hat{a}^{\dagger}\hat{a}}:|n\rangle &= \sum_{r=0}^{\infty}\frac{(e^{\lambda}-1)^{r}}{r!}:(\hat{a}^{\dagger}\hat{a})^{r}:|n\rangle \\
&= \sum_{r=0}^{\infty}\frac{(e^{\lambda}-1)^{r}}{r!}\hat{a}^{\dagger r}\hat{a}^{r}|n\rangle \\
&= \sum_{r=0}^{n}\frac{(e^{\lambda}-1)^{r}}{r!}\frac{n!}{(n-r)!}|n\rangle \\
&= \sum_{r=0}^{n}\binom{n}{r}(e^{\lambda}-1)^{r}1^{n-r}|n\rangle \\
&= e^{\lambda n}|n\rangle
\end{aligned}
\tag{B3}
$$

but we also have

$$
e^{\lambda\hat{a}^{\dagger}\hat{a}}|n\rangle = e^{\lambda n}|n\rangle
\tag{B4}
$$

as $\{|n\rangle\}$ is a complete set, therefore

$$
e^{\lambda\hat{a}^{\dagger}\hat{a}} =: e^{(e^{\lambda}-1)\hat{a}^{\dagger}\hat{a}}:
\tag{B5}
$$

it is worth noting the general rule

$$
\langle\iota|:f(\hat{a}^{\dagger},\hat{a}):|\alpha\rangle = f(\iota^{*},\alpha)\langle\iota|\alpha\rangle
\tag{B6}
$$

as $\{|\alpha\rangle\}$ is an overcomplete set, any operator can be written in a diagonal coherent state representation

$$\hat{\rho} = \int d^2\alpha\, |\alpha\rangle \varphi(\alpha) \langle\alpha| \tag{B7}$$

to determine the form of $\varphi(\alpha)$, left multiply Eq. (B7) by $\langle -\iota|$ and right multiply by $|\iota\rangle e^{|\iota|^2}$

$$\begin{aligned}
\langle -\iota|\hat{\rho}|\iota\rangle e^{|\iota|^2} &= \int d^2\alpha\, \varphi(\alpha) \langle -\iota|\alpha\rangle\langle\alpha|\iota\rangle e^{|\iota|^2} \\
&= \int d^2\alpha\, \varphi(\alpha) e^{|\iota|^2} e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\iota|^2 + \alpha^*\iota} e^{-\frac{1}{2}|\iota|^2 - \frac{1}{2}|\alpha|^2 - \iota^*\alpha} \\
&= \int d^2\alpha\, \varphi(\alpha) e^{-|\alpha|^2} e^{\alpha^*\iota - \alpha\iota^*}
\end{aligned} \tag{B8}$$

as $\alpha^*\iota - \iota^*\alpha = 2i\Im(\alpha^*\iota)$, Eq. (B8) is a Fourier transform in two dimensions.
Now consider the Dirac delta in 2D, for a complex number $z = x + iy$

$$\delta^{(2)}(z) = \delta(x)\delta(y) = \frac{1}{(2\pi)^2} \int dk_x e^{ik_x x} \int dk_y\, e^{ik_y y} \tag{B9}$$

or equivalently

$$\delta^{(2)}(\mathbf{r}) = \frac{1}{4\pi^2} \int d^2\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}} \tag{B10}$$

where $\mathbf{r} = (x, y)$ and $\mathbf{k} = (k_x, k_y)$
let $\iota = \frac{k_x + ik_y}{2}$, then notice that

$$\mathbf{k}\cdot\mathbf{r} = k_x x + k_y y = \iota^* z - \iota z^* \tag{B11}$$

and

$$d^2\iota = d\Re\iota\, d\Im\iota = \frac{1}{4} d^2\mathbf{k} \tag{B12}$$

therefore

$$\delta^{(2)}(z) = \frac{1}{\pi^2} \int d^2\iota\, e^{\iota^* z - \iota z^*} \tag{B13}$$

apply the inverse transform by multiplying both sides of Eq. (B8) by $\pi^{-2} e^{\iota^*\alpha' - \iota\alpha'^*}$, then integrate over all ι

$$\begin{aligned}
\frac{1}{\pi^2} \int d^2\iota\, \langle -\iota|\hat{\rho}|\iota\rangle e^{|\iota|^2} e^{\iota^*\alpha' - \iota\alpha'^*} &= \frac{1}{\pi^2} \int d^2\alpha\, \varphi(\alpha) e^{-|\alpha|^2} \int d^2\iota\, e^{\alpha^*\iota - \alpha\iota^*} e^{\iota^*\alpha' - \iota\alpha'^*} \\
&= \frac{1}{\pi^2} \int d^2\alpha\, \varphi(\alpha) e^{-|\alpha|^2} \int d^2\iota\, e^{\iota^*(\alpha' - \alpha) - \iota(\alpha' - \alpha)^*} \\
&= \int d^2\alpha\, \varphi(\alpha) e^{-|\alpha|^2} \delta^{(2)}(\alpha' - \alpha) \\
&= \varphi(\alpha') e^{-|\alpha'|^2}
\end{aligned} \tag{B14}$$

hence

$$\varphi(\alpha) = \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, \langle -\iota|\hat{\rho}|\iota\rangle e^{|\iota|^2} e^{\iota^*\alpha - \iota\alpha^*} \tag{B15}$$

Now onto the specific case of

$$\hat{\rho} = e^{\lambda \hat{a}^\dagger \hat{a} + \mu \hat{a}^\dagger + \nu \hat{a}} = e^{-\lambda\left(\hat{a}^\dagger - \frac{\nu}{\lambda}\right)\left(\hat{a} - \frac{\mu}{\lambda}\right) + \frac{\mu\nu}{\lambda}} \tag{B16}$$

make the replacements of $\hat{a} \to \hat{a} - \mu/\lambda$, $\hat{a}^\dagger \to \hat{a}^\dagger - \nu/\lambda$ and $\lambda \to -\lambda$ in Eq. (B5) yields

$$e^{-\lambda\left(\hat{a}^\dagger - \frac{\nu}{\lambda}\right)\left(\hat{a} - \frac{\mu}{\lambda}\right)} =: e^{-(1-e^{-\lambda})\left(\hat{a}^\dagger - \frac{\nu}{\lambda}\right)\left(\hat{a} - \frac{\mu}{\lambda}\right)} : \tag{B17}$$

the replacement is allowed due to the only requirement for Eq. (B5) is $[\hat{a}, \hat{a}^\dagger] = 1$ which is invariant under additive constants in the both arguments of the commutator.

Left multiply Eq. (B16) by $\langle -\iota|$ and right multiply by $|\iota\rangle$ and using Eq. (B17) and Eq. (B6) yields

$$\langle -\iota|\hat{\rho}|\iota\rangle = e^{(1-e^{-\lambda})\left(\iota^* + \frac{\nu}{\lambda}\right)\left(\iota - \frac{\mu}{\lambda}\right) - 2|\iota|^2 + \frac{\mu\nu}{\lambda}} \tag{B18}$$

therefore

$$\begin{aligned}
\varphi(\alpha) &= \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, e^{(1-e^{-\lambda})\left(\iota^* + \frac{\nu}{\lambda}\right)\left(\iota - \frac{\mu}{\lambda}\right) - 2|\iota|^2 + \frac{\mu\nu}{\lambda}} e^{|\iota|^2} e^{\iota^*\alpha - \iota\alpha^*} \\
&= \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, e^{(1-e^{-\lambda})\left(\iota^* + \frac{\nu}{\lambda}\right)\left(\iota - \frac{\mu}{\lambda}\right) - |\iota|^2 + \frac{\mu\nu}{\lambda}} e^{\iota^*\alpha - \iota\alpha^*} \\
&= \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, e^{(1-e^{-\lambda})|\iota|^2 - (1-e^{-\lambda})\frac{\mu}{\lambda}\iota^* + (1-e^{-\lambda})\frac{\nu}{\lambda}\iota - \frac{(1-e^{-\lambda})\mu\nu}{\lambda^2} - |\iota|^2 + \frac{\mu\nu}{\lambda}} e^{\iota^*\alpha - \iota\alpha^*} \\
&= \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, e^{-e^{-\lambda}|\iota|^2 + \left[(1-e^{-\lambda})\frac{\nu}{\lambda} - \alpha^*\right]\iota + \left[\alpha - (1-e^{-\lambda})\frac{\mu}{\lambda}\right]\iota^* + \left[\frac{\mu\nu}{\lambda} - \frac{(1-e^{-\lambda})\mu\nu}{\lambda^2}\right]} \\
&\equiv \frac{1}{\pi^2} e^{|\alpha|^2} \int d^2\iota \, e^{-s|\iota|^2 + t\,\iota + u\,\iota^* + K} \\
&= \frac{1}{\pi^2} e^{|\alpha|^2} e^K \int d^2\iota \, e^{-s|\iota|^2 + t\,\iota + u\,\iota^*} \\
&= \frac{1}{\pi^2} e^{|\alpha|^2} e^K \frac{\pi}{s} e^{\frac{tu}{s}} \\
&= \frac{1}{\pi} e^\lambda e^{|\alpha|^2 + K + e^\lambda tu} \\
&\equiv \frac{1}{\pi} e^\lambda e^{|\alpha|^2 + \left[\frac{\mu\nu}{\lambda} - \frac{(1-e^{-\lambda})\mu\nu}{\lambda^2}\right] + e^\lambda\left[(1-e^{-\lambda})\frac{\nu}{\lambda} - \alpha^*\right]\left[\alpha - (1-e^{-\lambda})\frac{\mu}{\lambda}\right]} \\
&= \frac{1}{\pi} e^\lambda e^{|\alpha|^2 + \left[\frac{\mu\nu}{\lambda} - \frac{(1-e^{-\lambda})\mu\nu}{\lambda^2}\right] + e^\lambda\left[-|\alpha|^2 + \frac{1-e^{-\lambda}}{\lambda}(\nu\alpha + \mu\alpha^*) - \frac{(1-e^{-\lambda})^2}{\lambda^2}\mu\nu)\right]} \\
&= \frac{1}{\pi} e^\lambda e^{\frac{\mu\nu}{\lambda} - \frac{(1-e^{-\lambda})\mu\nu}{\lambda^2} - (e^\lambda - 1)|\alpha|^2 + \frac{e^\lambda - 1}{\lambda}(\nu\alpha + \mu\alpha^*) - \frac{e^\lambda(1-e^{-\lambda})^2}{\lambda^2}\mu\nu} \\
&= \frac{1}{\pi} e^{\lambda + \frac{\mu\nu}{\lambda} - (e^\lambda - 1)|\alpha|^2 + \frac{e^\lambda - 1}{\lambda}(\nu\alpha + \mu\alpha^*) - \frac{e^\lambda - 1}{\lambda^2}\mu\nu} \\
&= \frac{1}{\pi} e^{\lambda + \frac{\mu\nu}{\lambda} - (e^\lambda - 1)\left(\alpha^* - \frac{\nu}{\lambda}\right)\left(\alpha - \frac{\mu}{\lambda}\right)}
\end{aligned} \tag{B19}$$

where we have used the standard complex Gaussian integral on line 7

$$\int d^2z\, e^{-s|z|^2+tz+uz^*} = \frac{\pi}{s} e^{\frac{tu}{s}} \tag{B20}$$

to obtain the desired relation

$$e^{\lambda \hat{a}^\dagger \hat{a}+\mu \hat{a}^\dagger+\nu \hat{a}} = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle e^{\lambda+\frac{\mu\nu}{\lambda}-(e^\lambda-1)\left(\alpha^*-\frac{\nu}{\lambda}\right)\left(\alpha-\frac{\mu}{\lambda}\right)} \langle\alpha| \tag{B21}$$

□

Appendix C

Proof.

Consider

$$\hat{F}(\mu,\tau) = e^{(1-\tau)\hat{A}(\mu)} \frac{\partial}{\partial\mu} e^{\tau\hat{A}(\mu)} \tag{C1}$$

$$\hat{F}(\mu,0) = 0 \tag{C2}$$

$$\hat{F}(\mu,1) = \frac{\partial}{\partial\mu} e^{\hat{A}(\mu)} \tag{C3}$$

$$\begin{aligned}
\frac{\partial\hat{F}(\mu,\tau)}{\partial\tau} &= -\hat{A}(\mu)e^{(1-\tau)\hat{A}(\mu)}\frac{\partial}{\partial\mu}e^{\tau\hat{A}(\mu)} + e^{(1-\tau)\hat{A}(\mu)}\frac{\partial}{\partial\mu}\left(\hat{A}(\mu)e^{\tau\hat{A}(\mu)}\right) \\
&= -\hat{A}(\mu)e^{(1-\tau)\hat{A}(\mu)}\frac{\partial}{\partial\mu}e^{\tau\hat{A}(\mu)} + \hat{A}(\mu)e^{(1-\tau)\hat{A}(\mu)}\frac{\partial}{\partial\mu}e^{\tau\hat{A}(\mu)} + e^{(1-\tau)\hat{A}(\mu)}\frac{\partial\hat{A}(\mu)}{\partial\mu}e^{\tau\hat{A}(\mu)} \\
&= e^{(1-\tau)\hat{A}(\mu)}\frac{\partial\hat{A}(\mu)}{\partial\mu}e^{\tau\hat{A}(\mu)}
\end{aligned} \tag{C4}$$

and

$$\hat{F}(\mu,1) - \hat{F}(\mu,0) = \int_0^1 d\tau\, \frac{\partial\hat{F}(\mu,\tau)}{\partial\tau} \tag{C5}$$

hence

$$\frac{\partial}{\partial\mu} e^{\hat{A}(\mu)} = \int_0^1 d\tau\, e^{(1-\tau)\hat{A}(\mu)}\frac{\partial\hat{A}(\mu)}{\partial\mu}e^{\tau\hat{A}(\mu)} \tag{C6}$$

□