Phase space representation of quantum dynamics. Lecture notes. Boulder Summer School, 2013

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Contents

I. QUICK SUMMARY OF CLASSICAL HAMILTONIAN DYNAMICS IN PHASE-SPACE.

We will generally deal with Hamiltonian systems, which are defined by specifying a set of canonical variables p_j, q_j satisfying canonical relations

$$\{p_i, q_j\} = \delta_{ij}, \tag{1}$$

where $\{\dots\}$ denotes the Poisson bracket.

$$\{A(\vec{p}, \vec{q}), B(\vec{p}, \vec{q})\} = \sum_j \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial B}{\partial p_j}\frac{\partial A}{\partial q_j} = B\Lambda A, \tag{2}$$

where

$$\Lambda = \sum_j \frac{\overleftarrow{\partial}}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\overleftarrow{\partial}}{\partial q_j}\frac{\partial}{\partial p_j}$$

is the sympectic skew symmetric operator. It is easy to check that any orthogonal transformation

$$Q = R(\lambda) q,\ P = R(\lambda) p \tag{3}$$

preserves both the Poisson brackets and the symplectic operator. A general class of transformations which preserve the Poisson brackets are known as canonical transformations and can be expressed trhough the generating functions (1). It is easy to check that infinitesimal canonical transformations can be generated by gauge potentials

$$q_j(\lambda + \delta\lambda) = q_j(\lambda) - \frac{\partial A(\lambda, \vec{p}, \vec{q})}{\partial p_j}\delta\lambda, \tag{4}$$

$$p_j(\lambda + \delta\lambda) = p_j(\lambda) + \frac{\partial A(\lambda, \vec{p}, \vec{q})}{\partial q_j}\delta\lambda, \tag{5}$$

where λ parametrizes the canonical transformation and the gauge potential A is some function of canonical variables and parameters. Then up to the terms of the order of $\delta\lambda^2$ the transformation above preserves the Poisson brackets

$$\{p_i(\lambda + \delta\lambda), q_j(\lambda + \delta\lambda)\} = \delta_{ij} + \delta\lambda\left(\frac{\partial^2 A}{\partial p_j \partial q_i} - \frac{\partial^2 A}{\partial p_j \partial q_i}\right) + O(\delta\lambda^2) = \delta_{ij} + O(\delta\lambda^2). \tag{6}$$

Exercises.

(i) Show that the generator of translations $\vec{q}(X) = \vec{q}_0 - \vec{X}$ is the momentum operator: $\vec{A}_{\vec{X}}(\vec{q}, \vec{p}) = \vec{p}$. You need to treat $\vec{X}$ as a three component parameter $\vec{\lambda}$. Note that the number of particles (and thus phase space dimension) can be much higher than three.

(ii) Show that the generator of the rotations around z-axis:

$$q_x(\theta) = \cos(\theta) q_{x0} - \sin(\theta) q_{y0},\ q_y(\theta) = \cos(\theta) q_{y0} + \sin(\theta) q_{x0},$$

$$p_x(\theta) = \cos(\theta) p_{x0} - \sin(\theta) p_{y0},\ p_y(\theta) = \cos(\theta) p_{y0} + \sin(\theta) p_{x0},$$

is the angular momentum operator: $A_\theta = p_x q_y - p_y q_x$.

(iii) Find the gauge potential A_λ corresponding to the orthogonal transformation (3).

Hamiltonian dynamics is a particular canonical transformation parametrized by time

$$\frac{\partial q_j}{\partial t} = \{H, q_j\} = \frac{\partial H}{\partial p_j},\ \frac{\partial p_j}{\partial t} = \{H, p_j\} = -\frac{\partial H}{\partial q_j} \tag{7}$$

Clearly these Hamiltonian equations are equivalent to Eqs. (5) with the convention $A_t = -H$.

One can extend canonical transformations to the complex variables. Instead of doing this in all generality we will focus on particular phase space variables which are complex wave amplitudes. E.g. for Harmonic oscillators for each normal mode with the Hamiltonian

$$H_k = \frac{p_k^2}{2m} + \frac{m\omega_k^2}{2} q_k^2 \tag{8}$$

we can define new linear combinations

$$p_k = i\sqrt{\frac{m\omega_k}{2}}(a_k^* - a_k),\ q_k = \sqrt{\frac{1}{2m\omega_k}}(a_k + a_k^*) \tag{9}$$

or equivalently

$$a_k^* = \frac{1}{\sqrt{2}}\left(q_k\sqrt{m\omega_k} - \frac{i}{\sqrt{m\omega_k}}p_k\right),\ a_k = \frac{1}{\sqrt{2}}\left(q_k\sqrt{m\omega_k} + \frac{i}{\sqrt{m\omega_k}}p_k\right). \tag{10}$$

Let us now compute the Poisson brackets of the complex wave amplitudes

$$\{a_k, a_k\} = \{a_k^*, a_k^*\} = 0,\ \{a_k, a_k^*\} = i. \tag{11}$$

To avoid dealing with the imaginary Poisson brackets it is convenient to introduce new coherent state Poisson brackets

$$\{A, B\}_c = \sum_k \frac{\partial A}{\partial a_k}\frac{\partial B}{\partial a_k^*} - \frac{\partial B}{\partial a_k}\frac{\partial A}{\partial a_k^*} = A\Lambda_c B, \tag{12}$$

where

$$\Lambda_c = \sum_k \frac{\overleftarrow{\partial}}{\partial a_k}\frac{\partial}{\partial a_k^*} - \frac{\overleftarrow{\partial}}{\partial a_k^*}\frac{\partial}{\partial a_k}. \tag{13}$$

As for the coordinate momentum case, the coherent symplectic operator Λ_c is preserved under the canonical transformations. From this definition it is immediately clear that

$$\{a_k, a_q^*\}_c = \delta_{kq}. \tag{14}$$

Comparing this relation with Eq. (11) we see that standard and coherent Poisson brackets differ by the factor of i:

$$\{\dots\} = i\{\dots\}_c. \tag{15}$$

Exercise. Check that any unitary transformation $\tilde{a}_k = U_{k,k'}a'_k$, where U is a unitary matrix, preserves the coherent state Poisson bracket, i.e. $\{\tilde{a}_k, \tilde{a}_q^*\}_c = \delta_{k,q}$. Verify that the Bogoliubov transformation

$$\gamma_k = \cosh(\theta_k)a_k + \sinh(\theta_k)a_{-k}^*,\ \gamma_k^* = \cosh(\theta_k)a_k^* + \sinh(\theta_k)a_{-k}, \tag{16}$$

with $\theta_k = \theta_{-k}$ also preserves the coherent state Poisson bracket, i.e.

$$\{\gamma_k, \gamma_{-k}\}_c = \{\gamma_k, \gamma_{-k}^*\}_c = 0,\ \{\gamma_k, \gamma_k^*\}_c = \{\gamma_{-k}, \gamma_{-k}^*\}_c = 1. \tag{17}$$

Let us write the Hamiltonian equations of motion for the new coherent variables. Using that

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} - \{A, H\} = \frac{\partial A}{\partial t} - i\{A, H\}_c \tag{18}$$

and using that our variables do not explicitly depend on time (such dependence would amount to going to a moving frame, which we will not consider here) we find

$$i\frac{da_k}{dt} = \{a_k, H\}_c = \frac{\partial H}{\partial a_k^*},\ i\frac{da_k^*}{dt} = \{a_k^*, H\}_c = -\frac{\partial H}{\partial a_k} \tag{19}$$

These equations are also known as Gross-Pitaevskii equations. Note that these equations are arbitrary for arbitrary Hamiltonians and not restricted to Harmonic systems.

And finally let us write down the Liouville equations of motion for the probability distribution $\rho(q, p, t)$ or $\rho(a, a^*, t)$. The latter just express incompressibility of the probability flow, which directly follows conservation of the phase space volume $d\Gamma = dqdp$ or $d\Gamma = dada^*$ for arbitrary canonical transformations including time evolution and from the conservation of the total probability $\rho d\Gamma$:

$$0 = \frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} - \{\rho, H\} = \frac{\partial \rho}{\partial t} - i\{\rho, H\}_c, \tag{20}$$

or equivalently

$$\frac{\partial \rho}{\partial t} = \{\rho, H\},\ i\frac{\partial \rho}{\partial t} = -\{\rho, H\}_c \tag{21}$$

II. QUANTUM SYSTEMS IN FIRST AND SECOND QUANTIZED FORMS. COHERENT STATES.

Now we move to quantum systems. As for the classical systems let us first define the language. We will use two different representations of the operators using either coordinate-momentum (first quantized picture) or creation-annihilation operators (second quantized picture). In the second quantized form we will be only considering bosons because finding semiclassical limit for fermions is still an open question. These phase space variables satisfy canonical commutation relations:

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij},\ [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \tag{22}$$

Throughout these notes we introduce "hat"-notations for the operators to avoid confusion with the phase space variables. From this relations it is clear that in the classical limit the commutator should reduce to the coherent state Poisson bracket. As in the classical systems any Unitary transformation of the canonical variables preserves their commutation relations.

Since we will be always keeping in mind the classical limit we will be predominantly working in the Heisenberg representation where the operators are time dependent and satisfy canonical equations of motion

$$i\hbar\frac{d\hat{q}_i}{dt} = [\hat{q}_i, \hat{H}],\ i\hbar\frac{d\hat{p}_i}{dt} = [\hat{p}_i, \hat{H}], \tag{23}$$

$$i\hbar\frac{d\hat{a}_i}{dt} = [\hat{a}_i, \hat{H}],\ i\hbar\frac{d\hat{a}_i^\dagger}{dt} = [\hat{a}_i^\dagger, \hat{H}]. \tag{24}$$

As in the classical case these equations can be thought of as continuous canonical transformations parametrized by time. Next let us define representation of these operators. For canonical coordinate and momentum the natural representation, which is most often used in literature is coordinate, where

$$\hat{q}_j \to x_j,\ \hat{p}_j = -i\hbar\frac{\partial}{\partial x_j} \tag{25}$$

This representation is realized using coordinate eigenstates $|\vec{x}\rangle = |x_1, x_2, \dots, x_M\rangle$ such that any state $|\psi\rangle$ is written as

$$|\psi\rangle = \int D\vec{x}\, \psi(\vec{x})|\vec{x}\rangle. \tag{26}$$

Here M denotes the total number of independent coordinate components, e.g. in the three-dimensional space M is equal to three times the number of particles.

In a similar fashion the natural representation for creation and annihilation operators is given by coherent states:

$$\hat{a}_j \to \alpha_j,\ \hat{a}_j^\dagger \to -\frac{\partial}{\partial \alpha_j} \tag{27}$$

Clearly in this form the creation and annihilation operators satisfy canonical commutation relations (22). Coherent states can be created from the vacuum state by exponentiating the creation operator:

$$|\alpha_1, \alpha_2, \dots \alpha_M\rangle = \prod_{j=1}^{M} \mathrm{e}^{-|\alpha_j|^2/2}\mathrm{e}^{\alpha_j a_j^\dagger}|0\rangle, \tag{28}$$

where $|0\rangle$ is the global particle vacuum annihilated by all operators $\hat{a}_j$ [1]. One can check that these

[1] Note that there is a sign mismatch between $\hat{a}^\dagger|\alpha_\rangle = \partial_\alpha|\alpha\rangle$ and the representation (27). This is because the derivative operator acting on the basis vector is opposite in sign to the derivative operator acting on the wave function $|\psi\rangle = \int d\alpha\psi(\alpha)|\alpha\rangle$.

coherent states are properly normalized:

$$\int D\alpha D\alpha^* \langle \alpha_1, \alpha_2, \dots \alpha_M | \alpha_1, \alpha_2, \dots \alpha_M \rangle = 1, \tag{29}$$

where we use the integration measure $d\alpha d\alpha^* = d\Re(\alpha) d\Im(\alpha)/\pi$. Unlike the coordinate states they are not orthogonal, which means that the coherent state basis is over-complete.

III. WIGNER-WEYL QUANTIZATION

A. Coordinate-Momentum representation

We are now ready to formulate phase space representation of quantum operators and the density matrix. To simplify notations we suppress component index in phase space variables except when extensions to multiple components is not straightforward. For any Hermitian operator $\hat{\Omega}(\hat{q}, \hat{p})$ we define the Weyl symbol, which depends on the corresponding phase space variables q, p:

$$\Omega_W(q,p) = \int d\xi \left\langle q - \frac{\xi}{2} \right| \hat{\Omega}(\hat{q}, \hat{p}) \left| q + \frac{\xi}{2} \right\rangle \mathrm{e}^{ip\xi/\hbar}. \tag{30}$$

The Weyl symbol is clearly uniquely defined for any operator with off-diagonal elements in the coordinate space decaying to zero. We will consider only such operators. In the classical limit the exponential term $\exp[ip\xi/\hbar]$ very rapidly oscillates unless ξ is very close to zero. Thus we see that the Weyl symbol becomes equal to the classical function $\Omega(q, p)$. Before proceeding let us point that there is some ambiguity in defining quantum classical correspondence in this way. In particular, instead of Eq. (30), one could define a continuous range of functions characterized by some real number ϵ:

$$\Omega_\epsilon(q,p) = \int d\xi \, \langle q - \epsilon\xi | \, \hat{\Omega}(\hat{q}, \hat{p}) \, | q + (1-\epsilon)\xi \rangle \, \mathrm{e}^{ip\xi/\hbar}. \tag{31}$$

This transform is always well defined and one can show that it is possible to build complete and unique phase-space representation of any quantum-mechanical operator for any ϵ. For coherent states such freedom is well understood leading to P and Q (Husimi) representations (see Refs. (2; 3)) for details. Clearly Weyl symbol corresponds to the symmetric choice $\epsilon = 1/2$. In these lectures we will stick only to the Weyl quantization.

Let us now compute the Weyl symbol for some simple operators. First let $\Omega(\hat{q}, \hat{p}) = V(\hat{q})$ depends only on the coordinate. Then obviously

$$V_W(q) = \int d\xi V(q) \delta(\xi) \mathrm{e}^{ip\xi/\hbar} = V(q), \tag{32}$$

i.e. the Weyl symbol amounts to the substitution the operator $\hat{q}$ by the number q. One can check that the same is true for any operator depending only on momentum

$$\Omega_W(p) = \Omega(p) \tag{33}$$

The easiest way to see this is to note that the definition of the Weyl symbol is symmetric with respect to $q \leftrightarrow p$.

Exercise. Write down an explicit expression for the Weyl symbol of a general operator (30) as an integral in the momentum space.

Now let us consider a slightly more complicated operator $\hat{\Omega}(\hat{q},\hat{p}) = \hat{q}\hat{p}$. Then

$$(\hat{q}\hat{p})_W = \int d\xi (q-\xi/2)\langle q-\xi/2|\hat{p}|q+\xi/2\rangle \mathrm{e}^{ip\xi/\hbar} = \int d\xi \int \frac{dk}{2\pi\hbar}(q-\xi/2)k\mathrm{e}^{i(p-k)\xi/\hbar} = pq + \frac{i\hbar}{2} \tag{34}$$

To get the last result we inserted the resolution of identity

$$I = \int \frac{dk}{2\pi\hbar}|k\rangle\langle k|$$

inside the matrix element appearing in the integral. In the same way we can find that

$$(\hat{p}\hat{q})_W = pq - \frac{i\hbar}{2}. \tag{35}$$

Exercise. Complete details of these calculations.

For a general "normal" ordered operator $\hat{\Omega}(\hat{q},\hat{p})$ such that the coordinate operators appear on the left of momentum operators the Weyl symbol (30) can be written as

$$\Omega_W(q,p) = \int \frac{d\xi d\eta}{4\pi\hbar}\,\Omega\left(q-\frac{\xi}{2}, p+\frac{\eta}{2}\right)\mathrm{e}^{-i\xi\eta/2\hbar}. \tag{36}$$

The equivalence of Eqs. (36) and (30) can be established by the same trick of inserting the identity (III.A) into Eq. (30).

Exercise. Consider a fully symmetrized polynomial of $\hat{p}$ and $\hat{q}$ of degree n, which can be represented either as

$$\hat{\Omega}_n(\hat{p},\hat{q}) = \hat{p}\Omega_{n-1}(\hat{p},\hat{q}) + \hat{\Omega}_{n-1}(\hat{p},\hat{q})\hat{p}$$

or as

$$\hat{\Omega}_n(\hat{p},\hat{q}) = \hat{q}\Omega_{n-1}(\hat{p},\hat{q}) + \hat{\Omega}_{n-1}(\hat{p},\hat{q})\hat{q},$$

where $\hat{\Omega}_{n-1}(\hat{p},\hat{q})$ is the symmetrized polynomial of degree $n-1$. Prove that the Weyl symbol of the fully symmetrized polynomial is simply obtained by substituting $\hat{p}\to p$ and $\hat{q}\to q$. For example

$$(\hat{p}\hat{q}+\hat{q}\hat{p})_W = 2pq,\;\; (\hat{p}^2\hat{q}+2\hat{p}\hat{q}\hat{p}+\hat{q}\hat{p}^2)_W = 4p^2q. \tag{37}$$

While the integral expressions for finding the Weyl symbol are very general, it is very useful to introduce the representation of the canonical coordinate and momentum operator, which gives the Weyl symbol right away. This is known as the Bopp representation:

$$\hat{q} = q + \frac{i\hbar}{2}\frac{\partial}{\partial p},\ \hat{p} = p - \frac{i\hbar}{2}\frac{\partial}{\partial q}. \tag{38}$$

This representation clearly respects the canonical commutation relations (22) and is symmetric with respect to coordinate and momentum. Then the Weyl symbol of the arbitrary operator $\hat{\Omega}(\hat{q},\hat{p})$ is given by

$$\Omega_W(q,p) = \hat{\Omega}(q + i\hbar/2\,\partial_p, p - i\hbar/2\,\partial_q)1, \tag{39}$$

We wrote unity on the right of this expression showing that derivatives acting on unity give zero. For example

$$(\hat{q}\hat{p})_W = \left(q + \frac{i\hbar}{2}\partial_p\right)\left(p - \frac{i\hbar}{2}\partial_q\right)1 = \left(q + \frac{i\hbar}{2}\partial_p\right)p = pq + \frac{i\hbar}{2}, \tag{40}$$

which is the correct result. Similarly

$$(\hat{q}^2\hat{p}^2)_W = \left(q + \frac{i\hbar}{2}\partial_p\right)^2 p^2 = q^2p^2 + 2q\frac{i\hbar}{2}\partial_p\, p^2 - \frac{\hbar^2}{4}\partial_p^2\, p^2 = p^2q^2 + 2i\hbar qp - \frac{\hbar^2}{2}. \tag{41}$$

One can check that this is also the correct result by e.g. explicitly performing integration in Eq. (36).

Let us prove Eq. (39). First note that if we prove this statement for a normal ordered operator $\hat{\Omega}_{mn}\hat{x}^m\hat{p}^n$ then we will automatically prove this statement for any operator, which is analytic in $\hat{q}$ and $\hat{p}$. Indeed obviously any analytic function can be represented as a sum of normal ordered polynomials of $\hat{q}$ and $\hat{p}$. Thus if we prove the statement for $\hat{\Omega}_{mn}$ we prove it for any operator. Since the latter is normal ordered we can use Eq. (36)

$$(\hat{q}^m\hat{p}^n)_W = \int\!\!\int \frac{d\xi d\eta}{4\pi\hbar}\left(q - \frac{\xi}{2}\right)^m \left(p + \frac{\eta}{2}\right)^n \mathrm{e}^{-i\xi\eta/(2\hbar)} = \int\!\!\int \frac{d\xi d\eta}{4\pi\hbar}\left(p + \frac{\eta}{2}\right)^n (q - i\hbar\partial_\eta)^m\, \mathrm{e}^{-i\xi\eta/(2\hbar)}$$
$$= \int d\eta \left(p + \frac{\eta}{2}\right)^n (q - i\hbar\partial_\eta)^m\,\delta(\eta) = (q + i\hbar\partial_\eta)^m \left(p + \frac{\eta}{2}\right)^n |_{\eta=0} = \left(q + \frac{i\hbar}{2}\partial_p\right)^m p^n \tag{42}$$

Thus we proved that the representation of $\hat{q}$ is indeed given by the Bopp operator. Bopp representation of $\hat{p}$ e.g. immediately follows from the commutation relation. Alternatively it follows from the symmetry of the definition of the Weyl operator with respect to the change $p \leftrightarrow q$, $\xi \leftrightarrow -\eta$.

Let us note that there is an alternative Bopp representation expressed through the left derivatives:

$$\hat{q} = q - \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial p},\ \hat{p} = p + \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial q}, \tag{43}$$

where the left derivative now acts on the operator on the left. While for now left and right representations are equivalent as we will see later causality uniquely defines the correct representation when we consider non-equal time correlation functions.

Exercise. Considering polynomial functions or otherwise prove the equivalence of two Bopp representations (38) and (43).

As a next ingredient of the Weyl quantization we will establish rules for addition and multiplication of operators. The former are trivial

$$(\hat{\Omega}_1 + \hat{\Omega}_2)_W = \Omega_{1W} + \Omega_{2W}, \tag{44}$$

The Weyl symbol of the product of two operators is much less trivial; it is given by the Moyal product:

$$(\Omega_1\Omega_2)_W(q,p) = \Omega_{1,W}(q,p)\exp\left[-\frac{i\hbar}{2}\Lambda\right]\Omega_{2,W}(q,p), \tag{45}$$

where Λ is the symplectic operator introduced earlier (I). As earlier, before proving this relation let us first check that it agrees with simple results

$$(\hat{q}\hat{p})_W = q\exp\left[-\frac{i\hbar}{2}\Lambda\right]p = qp - q\frac{i\hbar}{2}\left[\frac{\overleftarrow{\partial}}{\partial p}\frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\partial}{\partial p}\right]p + 0 = pq + \frac{i\hbar}{2}, \tag{46}$$

where we used that all higher order terms in the expansion of the exponent give zero because they contain higher order derivatives with respect to q and p. Clearly we got the correct result. Similarly

$$(\hat{q}^2\hat{p}^2)_W = q^2\exp\left[-\frac{i\hbar}{2}\Lambda\right]p^2 = qp - q^2\frac{i\hbar}{2}\left[\frac{\overleftarrow{\partial}}{\partial p}\frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\partial}{\partial p}\right]p^2 - q^2\frac{\hbar^2}{8}\left[\frac{\overleftarrow{\partial}}{\partial p}\frac{\partial}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\partial}{\partial p}\right]p^2$$
$$= p^2q^2 + 2i\hbar pq - \frac{\hbar^2}{2}, \tag{47}$$

which is again the correct result (cf. Eq. (41)). The proof of the Moyal product relation is straightforward, but somewhat lengthy. It can be found e.g. in Ref. (4). Another way to prove this relation is to consider the Bopp representation and check manually that

$$(\hat{q}^n\hat{p}^m)_W\exp\left[-\frac{i\hbar}{2}\Lambda\right]\Omega_{2,W}(q,p) = \left(q + \frac{i\hbar}{2}\partial_p\right)^n\left(p - \frac{i\hbar}{2}\partial_q\right)^m\Omega_2(\hat{q},\hat{p}). \tag{48}$$

Exercise. Optional. Prove the relation above starting from $m = 0$ and arbitrary n and then generalizing the proof to arbitrary m.

The Moyal product obviously satisfies the following relation

$$\Omega_{1,W} \exp\left[-\frac{i\hbar}{2}\Lambda\right]\Omega_{2,W} = \Omega_{2,W} \exp\left[+\frac{i\hbar}{2}\Lambda\right]\Omega_{1,W}. \tag{49}$$

From this relation we immediately derive the Weyl symbol of the commutator

$$[\hat{\Omega}_1, \hat{\Omega}_2]_W = -2i\Omega_{1,W} \sin\left(\frac{\hbar}{2}\Lambda\right)\Omega_{2W} = -i\hbar \left\{\Omega_{1,W}, \Omega_{2,W}\right\}_{MB}, \tag{50}$$

where "MB" stands for the Moyal bracket:

$$\{A, B\}_{MB} = \frac{2}{\hbar} A \sin\left(\frac{\hbar}{2}\Lambda\right) B.$$

Obviously in the classical limit $\hbar \to 0$ the Moyal bracket reduces to the Poisson bracket (cf. Eq. (2)).

Weyl symbol of the density matrix $\hat{\rho}$ is known as the Wigner function:

$$W(q,p) = \int d\xi \langle q - \xi/2|\hat{\rho}|q + \xi/2\rangle \mathrm{e}^{ip\xi/\hbar} = \int d\xi \rho(q - \xi/2, q + \xi/2)\mathrm{e}^{ip\xi/\hbar}. \tag{51}$$

In particular, if the density matrix represents a pure state: $\hat{\rho} = |\psi\rangle\langle\psi|$ then

$$W(q,p) = \int d\xi \psi^*(q + \xi/2)\psi(q - \xi/2)\mathrm{e}^{ip\xi/\hbar}. \tag{52}$$

The Wigner function is normalized and in this sense it is similar to the classical probability distribution

$$\int \frac{dqdp}{2\pi\hbar} W(q,p) = \int dqd\xi \rho(q - \xi/2, q + \xi/2)\delta(\xi) = \mathrm{Tr}[\hat{\rho}] = 1. \tag{53}$$

Unlike probability distribution, the Wigner function is not necessarily positive (as we see later considering explicit examples). Therefore it is often referred to as the quasi-probability distribution.

Now let us prove that the expectation value of any operator is given by the average of the corresponding Weyl symbol over the Wigner function:

$$\langle\hat{\Omega}(\hat{q},\hat{p})\rangle \equiv \mathrm{Tr}[\hat{\rho}\hat{\Omega}(\hat{q},\hat{p})] = \int \frac{dqdp}{2\pi\hbar} W(q,p)\Omega_W(q,p) \tag{54}$$

This statement proves that the Wigner-Weyl quantization, i.e. representation of quantum systems through the Weyl symbols and the Wigner function, is complete. The proof of this statement is straightforward:

$$\int \frac{dqdp}{2\pi\hbar} W(q,p)\Omega_W(q,p) = \int \frac{dqdp}{2\pi\hbar} \int d\xi \int d\xi' \langle q-\xi/2|\hat{\rho}|q+\xi/2\rangle\langle q-\xi'/2|\hat{\Omega}|q+\xi'/2\rangle \exp[ip(\xi+\xi')/\hbar]$$
$$= \int dq \int d\xi \langle q - \xi/2|\hat{\rho}|q + \xi/2\rangle\langle q + \xi/2|\hat{\Omega}|q - \xi/2\rangle = \int dq \langle q|\hat{\rho}\hat{\Omega}|q\rangle = \mathrm{Tr}[\hat{\rho}\hat{\Omega}]. \tag{55}$$

Let us consider an example of a harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2. \tag{56}$$

First consider the zero temperature density matrix corresponding to the ground state wave function

$$|\psi_0\rangle = \frac{1}{(2\pi a_0^2)^{1/4}} \mathrm{e}^{-q^2/(4a_0^2)}, \ a_0 = \sqrt{\frac{\hbar}{2m\omega}}. \tag{57}$$

Then the Wigner function

$$W(q,p) = \int d\xi \frac{1}{\sqrt{2\pi a_0^2}} \exp\left[-\frac{(q+\xi/2)^2}{4a_0^2} - \frac{(q-\xi/2)^2}{4a_0^2}\right] \mathrm{e}^{ip\xi/\hbar} = 2\exp\left[-\frac{q^2}{2a_0^2} - \frac{p^2}{2p_0^2}\right], \ p_0 = \frac{\hbar}{2a_0}. \tag{58}$$

Thus the Wigner function is positive Gaussian function for the Harmonic oscillators in the ground state. It is easy to realize that this is true for any harmonic system in the ground state since the latter can be always represented as a product of the ground state for each normal mode. This simple Gaussian structure persists to finite temperature states. In particular for a thermal density matrix

$$\hat{\rho} = \frac{1}{Z} \sum_n \mathrm{e}^{-\beta\hbar\omega(n+1/2)} |n\rangle\langle n| \tag{59}$$

the Wigner function reads:

$$W(q,p) = 2\tanh(\hbar\omega/2T) \exp\left[-\frac{q^2}{2a_0^2\coth(\hbar\omega/2T)} - \frac{p^2}{2p_0^2\coth(\hbar\omega/2T)}\right] \tag{60}$$

This result clearly reduces to Eq. (58) in the zero temperature limit. In the high temperature regime $\hbar\omega \ll T$ we can approximate $\coth(\hbar\omega/2T)$ by $2T/\hbar\omega$ and thus

$$W(q,p) \approx \frac{\hbar\omega}{T} \exp\left[-\frac{p^2/2m + m\omega^2 q^2/2}{T}\right], \tag{61}$$

which is exactly the classical Boltzmann's distribution of the Harmonic oscillator up to the factor of $\hbar$, which is due to the integration measure $dqdp/(2\pi\hbar)$.

Exercise. Prove Eq. (60). Hint. One possibility is to expand both the Wigner function and the final result in powers of $\exp[-\beta\hbar\omega]$. *Another possibility is to use coherent state representation of the Wigner function discussed below, where all calculations are much simpler since they do not require using Hermite polynomials.*

B. Coherent state representation.

All results in the momentum representation immediately translate to the coherent state representation. Since the proofs are almost identical we will simply list the main results and show several examples.

First let us define the Weyl symbol of an arbitrary operator written in the second quantized form $\hat{\Omega}(\hat{a}, \hat{a}^\dagger)$. As earlier we suppress the single-particle state index in the operators $\hat{a}$ and $\hat{a}^\dagger$ to simplify notations.

$$\Omega_W(a, a^*) = \int\int d\eta^* d\eta \left\langle a - \frac{\eta}{2} \middle| \hat{\Omega}(\hat{a}, \hat{a}^\dagger) \middle| a + \frac{\eta}{2} \right\rangle \mathrm{e}^{\frac{1}{2}(\eta^* a - \eta a^*)}. \tag{62}$$

Here $|\alpha\rangle$ denote coherent states. As in the coordinate momentum representation the Weyl symbol of a symmetrically ordered operator can be obtained by simple substitution $\hat{a} \to a$ and $\hat{a}^\dagger \to a^*$.

Exercise. Using the definition of the Weyl symbol above prove that $(\hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger)_W = 2aa^*$.

For normally ordered operators, where all $\hat{a}^\dagger$ terms appear on the left of $\hat{a}$ terms, Eq. (62) implies

$$\Omega_W(a, a^*) = \int\int d\eta d\eta^* \Omega\left(a^* - \eta^*/2, a + \eta/2\right) \mathrm{e}^{-|\eta|^2/2}. \tag{63}$$

As in the coordinate representation Weyl quantization is naturally associated with the coherent state Bopp representation

$$\hat{a}^\dagger = a^* - \frac{1}{2}\frac{\partial}{\partial a} = a^\star + \frac{1}{2}\frac{\overleftarrow{\partial}}{\partial a}, \tag{64}$$

$$\hat{a} = a + \frac{1}{2}\frac{\partial}{\partial a^*} = a - \frac{1}{2}\frac{\overleftarrow{\partial}}{\partial a^*}. \tag{65}$$

The complex derivatives here are understood in the standard way through the derivatives with respect to real and imaginary parts of a:

$$\frac{\partial}{\partial a} = \frac{1}{2}\frac{\partial}{\partial \Re a} - \frac{i}{2}\frac{\partial}{\partial \Im a},\ \frac{\partial}{\partial a^*} = \frac{1}{2}\frac{\partial}{\partial \Re a} + \frac{i}{2}\frac{\partial}{\partial \Im a}. \tag{66}$$

The choice of the representation with the conventional (right) derivatives and the one with left derivatives is arbitrary. However, as we discuss below, for time dependent problems it is dictated by causality. This representation of creation and annihilation operators is clearly symmetric and preserves the correct commutation relations. It also automatically reproduces the Weyl symbol of any operator. Let us illustrate this representation with a couple of simple examples. First consider the number operator $\hat{n} = \hat{a}^\dagger \hat{a}$ and its normal ordered square: $: n^2 := a^\dagger a^\dagger a a$. First we evaluate the Weyl symbol using Eq. (73):

$$n_W = \int d\eta d\eta^* (a^* - \eta^*/2)(a + \eta/2) \exp[-|\eta|^2/2] = a^* a - \frac{1}{2},$$

$$(: \hat{n}^2 :)_W = \int d\eta d\eta^* (a^* - \eta^*/2)^2 (a + \eta/2)^2 \exp[-|\eta|^2/2] = |a|^4 - 2|a|^2 + \frac{1}{2}. \tag{67}$$

Next we do the same calculation using the Bopp representation

$$
\begin{aligned}
n_w &= \left(a^* - \frac{1}{2}\partial_a\right) a = a^* a - \frac{1}{2},\\
(:\hat{n}^2:)_W &= \left(a^* - \frac{1}{2}\partial_a\right)^2 a^2 = |a|^4 - a^*\partial_a a^2 + \frac{1}{4}\partial_a^2 a^2 = |a|^4 - 2|a|^2 + \frac{1}{2}.
\end{aligned} \tag{68}
$$

For simple polynomial operators Bopp representation gives the simplest way to evaluate the Weyl symbols of the operators.

Again by a close analogy to the coordinate-momentum representation it is straightforward to show that the Weyl symbol of the product of two operators is given by the Moyal product (cf. Eq. (45)):

$$
(\hat{\Omega}_1\hat{\Omega}_2)_W = \Omega_{1,W} \exp\left[\frac{\Lambda_c}{2}\right] \Omega_{2,W}, \tag{69}
$$

where the symplectic coherent state operator Λ_c is defined in Eq. (13). From this result we immediately derive that the Weyl symbol of the commutator of the two operators is

$$
[\hat{\Omega}_1, \hat{\Omega}_2] = 2\Omega_{1,W} \sinh\left[\frac{\Lambda_c}{2}\right] \Omega_{2,W}, \tag{70}
$$

which can be termed as the coherent state Moyal bracket.

Let us check that in this way we can reproduce the Weyl symbol of the operators considered before

$$
\begin{aligned}
(\hat{a}^\dagger\hat{a})_W &= a^* \exp[\Lambda_c/2] a = a^* a + \frac{1}{2} a^* \Lambda_c a + 0 = a^* a - \frac{1}{2},\\
(\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a})_W &= (a^*)^2 [1 + \Lambda_c/2 + \Lambda_c^2/8 + 0] a^2 = |a|^4 - 2|a|^2 + \frac{1}{2},
\end{aligned} \tag{71}
$$

which are identical to Eq. (68).

The Wigner function is again defined as the Weyl symbol of the density matrix:

$$
W(a, a^*) = \int\int d\eta^* d\eta \left\langle a - \frac{\eta}{2} \right| \hat{\rho} \left| a + \frac{\eta}{2} \right\rangle \mathrm{e}^{\frac{1}{2}(\eta^* a - \eta a^*)}. \tag{72}
$$

The expectation value of any operator is given by averaging the corresponding Weyl symbol weighted with the Wigner function:

$$
\langle \hat{\Omega}(\hat{a}, \hat{a}^\dagger) \rangle = \int\int da da^* \, W(a, a^*) \Omega_W a, a^*). \tag{73}
$$

So the Wigner function again plays the role of the quasi-probability distribution of the complex amplitudes.

Let us consider few simple examples of Wigner functions. We start from the vacuum state: $\hat\rho = |0\rangle\langle 0|$. Note that the overlap of the ground state and the coherent state is

$$\langle 0|a\rangle = \exp[-|a|^2/2]. \tag{74}$$

Thus

$$W_0(a^*,a) = \int\int d\eta^* d\eta \exp[-|a|^2 - |\eta|^2/4] \mathrm{e}^{\frac{1}{2}(\eta^* a - \eta a^*)} = 2\exp[-2|a|^2] \tag{75}$$

Exercise. Prove the result above by completing the square.

Similarly the Wigner function of any coherent state is a shifted Gaussian. If $\hat\rho = |\alpha\rangle\langle\alpha|$ then

$$W_\alpha(a^*,a) = 2\exp[-2|a-\alpha|^2] \tag{76}$$

The proof of this result is essentially the same using that:

$$\langle\alpha|a\rangle = \exp[-|a|^2/2 - |\alpha|^2/2 + \alpha^* a]. \tag{77}$$

Exercise. Prove that for finite temperature density matrix of the non-interacting system $H = \hbar\omega a^\dagger a$ the Wigner function is a Gaussian:

$$W_T(a^*,a) = 2\coth\left(\frac{\hbar\omega}{2T}\right)\exp\left[-2|a^2|\tanh\left(\frac{\hbar\omega}{2T}\right)\right]. \tag{78}$$

Another important example is the Wigner function of the Fock state

$$|N\rangle = \frac{(a^\dagger)^N}{\sqrt{N!}}|0\rangle \tag{79}$$

The overlap of the Fock state and coherent state is obviously

$$\langle N|a\rangle = \frac{a^N\exp[-|a|^2/2]}{\sqrt{N!}} \tag{80}$$

Therefore

$$W_N(a^*,a) = \frac{1}{N!}\int\int d\eta d\eta^* \left(a^* - \frac{\eta^*}{2}\right)^N \left(a + \frac{\eta}{2}\right)^N \mathrm{e}^{-|a|^2 - |\eta|^2/4}\mathrm{e}^{\frac{1}{2}(\eta^* a - \eta a^*)}$$
$$= \frac{4}{N!}\int\int d\tilde\eta d\tilde\eta^* (2a^* - \tilde\eta^*)^N (2a+\tilde\eta)^N \mathrm{e}^{-2|a|^2 - |\tilde\eta|^2} = 4\mathrm{e}^{-2|a|^2}\sum_{m=0}^N (-1)^{N-m}|2a|^{2m}\frac{N!}{(m!)^2((N-m)!)^2}$$
$$\int\int d\tilde\eta d\tilde\eta^* |\tilde\eta|^{2(N-m)}\mathrm{e}^{-|\tilde\eta|^2} = 4(-1)^N \mathrm{e}^{-2|a|^2}\sum_{m=0}^N (-1)^m |2a|^{2m}\frac{N!}{(m!)^2(N-m)!} = 2\mathrm{e}^{-2|a|^2}L_N(4|a|^2), \tag{81}$$

where $L_N(x)$ is the Laguerre polynomial:

$$L_N(x) = (-1)^N \sum_{m=0}^{N} (-1)^m \frac{N!}{(m!)^2(N-m)!} x^m.$$

Exercise. Complete calculations to prove Eq. (81). Visualize this distribution for various N.

Unlike previous examples involving coherent states, the Wigner function for the Fock state is very non-local, especially at large N. It highly oscillates at $|a|^2 < N$ and then rapidly decays at $|a|^2 > N$. Due to these oscillations it is e.g. very hard to use this Wigner function for Monte-Carlo sampling so one can try to find approximate Wigner functions which correctly reproduce the lowest moments of the true distribution. The simplest example of an approximate Wigner function would be a Gaussian $Wg(n)$, where $n = a^* a$:

$$Wg(n) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-\frac{(n-n_0)^2}{2\sigma^2}}. \tag{82}$$

Because we will be interested in large N we can extend the range of n to the full real axis. Unphysical negative values of n will occur with vanishingly small probability. We will require that this function correctly reproduces the first two moments of the number operator:

$$N = \langle \hat{n} \rangle = \int_{-\infty}^{\infty} dn n_w Wg(n) = \overline{n} - \frac{1}{2} = n_0 - \frac{1}{2} \tag{83}$$

and

$$N^2 = \langle \hat{n}^2 \rangle = \langle : \hat{n}^2 : + \hat{n} \rangle = \overline{n^2 - 2n + 1/2 + n - 1/2} = n_0^2 + \sigma^2 - n_0, \tag{84}$$

where the over-line implies averaging with respect to the approximate Wigner function $Wg(n)$. The first equation implies $n_0 = N + 1/2$ and the second gives

$$N^2 = N^2 + N + \frac{1}{4} - N - \frac{1}{2} + \sigma^2 \;\Rightarrow\; \sigma = \frac{1}{2}. \tag{85}$$

Thus the best Gaussian approximation to the Wigner function for the Fock state is

$$Wg(n) = \frac{2}{\sqrt{2\pi}} \mathrm{e}^{-2\left(n - N - \frac{1}{2}\right)^2}. \tag{86}$$

C. Coordinate-momentum versus coherent state representations.

To summarize the discussion above we will contrast the two phase-space pictures in Table I. This table highlights close analogy between particle and wave pictures. While the two representations are formally equivalent one can build different approximation schemes using these representations as starting points, e.g. expanding around different classical limits one representing classical particles evolving according to the Newton's laws and another classical waves evolvong according to Gross-Pitaevskii (or Ginzburg-Landau) equations.

TABLE I Coherent state versus coordinate momentum phase space

Representation	coordinate-momentum	coherent
Phase space variables	$\mathbf{q}, \mathbf{p}$	$\boldsymbol{a}, \boldsymbol{a}^*$
Quantum operators	$\hat{\mathbf{q}}, \hat{\mathbf{p}}$	$\hat{\boldsymbol{a}}, \hat{\boldsymbol{a}}^\dagger$
Standard representation	$\hat{\mathbf{q}} \to \mathbf{q},\ \hat{\mathbf{p}} \to -i\hbar\partial_{\mathbf{q}}$ (coordinate basis)	$\hat{\boldsymbol{a}} \to \boldsymbol{a},\ \hat{\boldsymbol{a}}^\dagger \to -\partial_{\boldsymbol{a}}$ (coherent state basis)
Canonical commutation relations	$[\hat{q}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha,\beta}$ (α, β refer to different particles)	$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$ (i, j refer to single-particle states)
Quantum-classical correspondence	$\hat{\mathbf{q}} \to \mathbf{q},\ \hat{\mathbf{p}} \to \mathbf{p},\ [\hat{A}, \hat{B}] \to -i\hbar\{A, B\}$ $\{A, B\} = \sum_\alpha \frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha} - \frac{\partial A}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha}$	$\hat{\boldsymbol{a}} \to \boldsymbol{a},\ \hat{\boldsymbol{a}}^\dagger \to \boldsymbol{a}^*,\ [\hat{A}, \hat{B}] \to \{A, B\}_c$ $\{A, B\}_c = \sum_j \frac{\partial A}{\partial a_j}\frac{\partial B}{\partial a_j^*} - \frac{\partial A}{\partial a_j^*}\frac{\partial B}{\partial a_j}$
Wigner function	$W(\mathbf{q}, \mathbf{p}) = \int d\boldsymbol{\xi} \left\langle \mathbf{q} - \frac{\boldsymbol{\xi}}{2} \right\| \hat{\rho} \left\| \mathbf{q} + \frac{\boldsymbol{\xi}}{2} \right\rangle e^{i\mathbf{p}\boldsymbol{\xi}/\hbar}$	$W(\boldsymbol{a}, \boldsymbol{a}^*) = \int\int d\boldsymbol{\eta}^\star d\boldsymbol{\eta} \left\langle \boldsymbol{a} - \frac{\boldsymbol{\eta}}{2} \right\| \hat{\rho} \left\| \boldsymbol{a} + \frac{\boldsymbol{\eta}}{2} \right\rangle \times e^{\frac{1}{2}(\boldsymbol{\eta}^* \boldsymbol{a} - \boldsymbol{\eta}\boldsymbol{a}^*)}$
Weyl symbol	$\Omega_W(\mathbf{q}, \mathbf{p}) = \int d\boldsymbol{\xi} \left\langle \mathbf{q} - \frac{\boldsymbol{\xi}}{2} \right\| \hat{\Omega} \left\| \mathbf{q} + \frac{\boldsymbol{\xi}}{2} \right\rangle e^{i\mathbf{p}\boldsymbol{\xi}/\hbar}$	$\Omega_W(\boldsymbol{a}, \boldsymbol{a}^*) = \int\int d\boldsymbol{\eta}^\star d\boldsymbol{\eta} \left\langle \boldsymbol{a} - \frac{\boldsymbol{\eta}}{2} \right\| \hat{\Omega} \left\| \boldsymbol{a} + \frac{\boldsymbol{\eta}}{2} \right\rangle \times e^{\frac{1}{2}(\boldsymbol{\eta}^* \boldsymbol{a} - \boldsymbol{\eta}\boldsymbol{a}^*)}$
Moyal product	$(\Omega_1\Omega_2)_W = \Omega_{1,W} \exp\left[-\frac{i\hbar}{2}\Lambda\right] \Omega_{2,W},$ $\Lambda = \sum_\alpha \frac{\overleftarrow{\partial}}{\partial p_\alpha}\frac{\overrightarrow{\partial}}{\partial q_\alpha} - \frac{\overleftarrow{\partial}}{\partial q_\alpha}\frac{\overrightarrow{\partial}}{\partial p_\alpha}$	$(\Omega_1\Omega_2)_W = \Omega_{1,W} \exp\left[\frac{\Lambda_c}{2}\right] \Omega_{2,W},$ $\Lambda_c = \sum_j \frac{\overleftarrow{\partial}}{\partial a_j}\frac{\overrightarrow{\partial}}{\partial a_j^*} - \frac{\overleftarrow{\partial}}{\partial a_j^*}\frac{\overrightarrow{\partial}}{\partial a_j}$
Moyal bracket	$\{\Omega_1, \Omega_2\}_{MB} = \frac{2}{\hbar}\Omega_1 \sin\left[\frac{\hbar}{2}\Lambda\right] \Omega_2$	$\{\Omega_1, \Omega_2\}_{MBC} = 2\Omega_1 \sinh\left[\frac{1}{2}\Lambda_c\right] \Omega_2$
Bopp operators	$\hat{\mathbf{q}} = \mathbf{q} + \frac{i\hbar}{2}\frac{\partial}{\partial \mathbf{p}} = \mathbf{q} - \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial \mathbf{p}},$ $\hat{\mathbf{p}} = \mathbf{p} - \frac{i\hbar}{2}\frac{\partial}{\partial \mathbf{q}} = \mathbf{p} + \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial \mathbf{q}}$	$\hat{\boldsymbol{a}}^\dagger = \boldsymbol{a}^* - \frac{1}{2}\frac{\partial}{\partial \boldsymbol{a}} = \boldsymbol{a}^* + \frac{1}{2}\frac{\overleftarrow{\partial}}{\partial \boldsymbol{a}},$ $\hat{\boldsymbol{a}} = \boldsymbol{a} + \frac{1}{2}\frac{\partial}{\partial \boldsymbol{a}^*}, = \boldsymbol{a} - \frac{1}{2}\frac{\overleftarrow{\partial}}{\partial \boldsymbol{a}^*}$

D. Spin systems.

The machinery developed above allows one to extend the Weyl quantization to spin systems. The spin operators satisfy the canonical commutation relations:

$$[\hat{s}_a, \hat{s}_b] = i\epsilon_{abc}\hat{s}_c, \tag{87}$$

where ϵ_{abc} is the fully antisymmetric tensor. The classical limit corresponds to the spin quantum number $S \gg 1$ so we expect that quantum-classical correspondence will be exact in the large S-limit. Formally spin systems can be mapped to boson systems using the Schwinger representation:

$$\hat{s}^z = \frac{\hat{\alpha}^\dagger\hat{\alpha} - \hat{\beta}^\dagger\hat{\beta}}{2},\ \hat{s}^+ = \hat{\alpha}^\dagger\hat{\beta},\ \hat{s}^- = \hat{\beta}^\dagger\hat{\alpha}. \tag{88}$$

This representation allows us to apply results from the previous section directly to the spin systems without need to introduce spin-coherent states. The bosonic fields α and β in Eq. (88) should satisfy an additional constraint $\hat{n} = \hat{\alpha}^\dagger\hat{\alpha} + \hat{\beta}^\dagger\hat{\beta} = 2S$. Note that any spin-spin interactions commute with this constraint for each spin, therefore if the constraint is satisfied by the initial state, spin dynamics is equivalent to the dynamics of bosons.

Using Eqs. (64) and (65) we can find an analogue of the Bopp operators for the spin systems:

$$\hat{s}_z = \frac{\alpha^\star\alpha - \beta^\star\beta}{2} - \frac{1}{8}\left(\frac{\partial^2}{\partial\alpha^\star\partial\alpha} - \frac{\partial^2}{\partial\beta^\star\partial\beta}\right) - \frac{1}{4}\left(\alpha^\star\frac{\partial}{\partial\alpha^\star} - \alpha\frac{\partial}{\partial\alpha} - \beta^\star\frac{\partial}{\partial\beta^\star} + \beta\frac{\partial}{\partial\beta}\right), \quad (89)$$

$$\hat{s}_+ = \alpha^\star\beta + \frac{1}{2}\left(\alpha^\star\frac{\partial}{\partial\beta^\star} - \beta\frac{\partial}{\partial\alpha}\right) - \frac{1}{4}\frac{\partial^2}{\partial\alpha\partial\beta^\star}, \quad (90)$$

$$\hat{s}_- = \alpha\beta^\star + \frac{1}{2}\left(\alpha\frac{\partial}{\partial\beta} - \beta^\star\frac{\partial}{\partial\alpha^\star}\right) - \frac{1}{4}\frac{\partial^2}{\partial\alpha^\star\partial\beta}. \quad (91)$$

These equations can be also written using compact notations:

$$\hat{\mathbf{s}} = \mathbf{s} - \frac{i}{2}\left[\mathbf{s}\times\vec{\nabla}\right] - \frac{1}{8}\left[\vec{\nabla} + (\mathbf{s}\cdot\vec{\nabla})\vec{\nabla} - \frac{1}{2}\mathbf{s}\nabla^2\right], \quad (92)$$

or equivalently

$$\hat{s}_z = s_z - \frac{i}{2}\left(s_x\frac{\partial}{\partial s_y} - s_y\frac{\partial}{\partial s_x}\right) - \frac{1}{8}\frac{\partial}{\partial s_z} - \frac{s_z}{16}\left(\frac{\partial^2}{\partial s_z^2} - \frac{\partial^2}{\partial s_x^2} - \frac{\partial^2}{\partial s_y^2}\right) - \frac{s_x}{8}\frac{\partial^2}{\partial s_x\partial s_z} - \frac{s_y}{8}\frac{\partial^2}{\partial s_y\partial s_z}. \quad (93)$$

and similarly for other components. Here $\vec{\nabla} = \partial/\partial\mathbf{s}$ and

$$s_z = \frac{\alpha^*\alpha - \beta^*\beta}{2},\ s_x = \frac{\alpha^*\beta + \beta^*\alpha}{2},\ s_y = \frac{\alpha^*\beta - \beta^*\alpha}{2i} \quad (94)$$

are the Schwinger representation of the classical spins. One can check that these momentum variables satisfy standard angular momentum relations:

$$\{s_\alpha, s_\beta\} = \epsilon_{\alpha,\beta,\gamma}s_\gamma. \quad (95)$$

These expressions can be used in constructing Weyl symbols for various spin operators. Let us give a few specific examples:

$$(\hat{s}_z)_W = s_z,\ (\hat{s}_z^2)_W = s_z^2 - \frac{1}{8},\ (\hat{s}_z\hat{s}_x)_W = s_z s_x + \frac{i}{2}s_y. \quad (96)$$

Exercise. Verify the equations above.

In principle, the mapping (88) is sufficient to express the Wigner function of any initial state in terms of the bosonic fields α and β. General expressions can be quite cumbersome, however, one can use a simple trick to find a Wigner transform of any pure single spin state and the generalize it to any given density matrix. Assume that a spin is pointing along the z-axis. This can always be achieved by a proper choice of a coordinate system. Then in terms of bosons $\hat{\alpha}$ and $\hat{\beta}$ the initial state is just $|2S, 0\rangle$. In other words the wave function is a product of two Fock states one having $2S$ particles and one 0 particles. The corresponding Wigner function is then (see Eq. (81):

$$W(\alpha, \alpha^\star, \beta, \beta^\star) = 4\mathrm{e}^{-2|\alpha|^2 - 2|\beta|^2} L_{2S}(4|\alpha|^2). \quad (97)$$

At large S the Laguerre polynomial is a rapidly oscillating function and very inconvenient to deal with. So instead of the exact expression to a very good accuracy (up to $1/S^2$) we can use a Gaussian approximation (cf. Eq. (86) one can use

$$W(\alpha,\beta) \approx 2\sqrt{2}\mathrm{e}^{-2|\beta|^2}\mathrm{e}^{-2(|\alpha|^2-2S-1/2)^2}. \tag{98}$$

Then the best Gaussian approximation for the Wigner function reads

$$W(s_z,\vec{s}_\perp) \approx \frac{2}{\pi\sqrt{\pi}S}\mathrm{e}^{-s_\perp^2/S}\mathrm{e}^{-4(s_z-S)^2}. \tag{99}$$

The Wigner function is properly normalized using the integration measure $ds_x ds_y ds_z = 2\pi s_\perp ds_\perp ds_z$. This Wigner function has a transparent interpretation. If the quantum spin points along the z direction, because of the uncertainty principle, the transverse spin components still fluctuate due to zero-point motion so that

$$\langle s_x^2\rangle = \langle s_y^2\rangle = \frac{S}{2}. \tag{100}$$

This is indeed the correct quantum-mechanical result. It also correctly reproduces the second moment of s_z:

$$\langle s_z^2\rangle = \overline{s_z^2 - 1/8} = S^2 + \frac{1}{8} - \frac{1}{8} = S^2, \tag{101}$$

where we used Eq. (96) for the Weyl symbol for s_z^2. Clearly from Eq. (97) one can derive the Wigner function for a spin with an arbitrary orientation by the appropriate rotation of the coordinate axes.

IV. QUANTUM DYNAMICS IN PHASE SPACE.

Next we move to time-dependent systems. In this section we will focus on coherent state phase space since it found more applications to interacting systems. All results immediately translate to the coordinate-momentum picture using Table I. We will explicitly quote only final expressions where necessary.

A. von Neumann's equation in phase space representation. Truncated Wigner approximation

Time evolution of the density matrix for an arbitrary Hamiltonian system is given by the von Neumann equation:

$$i\hbar\dot{\hat{\rho}} = [\hat{\mathcal{H}},\hat{\rho}]. \tag{102}$$

Taking the Weyl transform of both sides of the equation and using Eq. (70) for the coherent state Moyal bracket we find:

$$i\hbar\dot{W} = 2H_W \sin\left[\frac{1}{2}\Lambda_c\right] W.. \tag{103}$$

This equation in the coordinate-momentum representation reads

$$\dot{W} = \frac{2}{\hbar} W \sin\left(\frac{\hbar}{2}\Lambda\right) H_W \tag{104}$$

If we expand the Moyal bracket in the powers of the symplectic operator Λ_c (or Λ) and stop at the leading order then clearly the von Neumann's equations (103) and (104) will reduce to the classical Liouville

$\hbar$ and stop in the leading order then the Moyal bracket reduces to the Poisson bracket and the von Neumann's equation (21) reduces to the classical Liouville equations (21) with the Wigner function replacing the classical probability distribution. It is interesting that in the coordinate-momentum picture the classical limit is formally recovered as $\hbar \to 0$ as expected. In the coherent state picture the classical limit is found when the occupation number of relevant modes becomes large $N = a^* a \to \infty$. The Planck's constant merely sets the time units and can be completely rescaled. Of course the mode occupation number in e.g. harmonic equilibrium systems is given by the ratio T and $\hbar\omega$ and diverges as $\hbar \to 0$ so there is no inconsistency.

This leading order approximation where the Wigner function satisfies the classical Liouville equations is known in literature as the truncated Wigner approximation (TWA). Formally it is obtained by truncating the expansion of the von Neumann's equation

$$i\dot{W} = 2H_W \sin\left[\frac{1}{2}\Lambda_c\right] W = H_W \Lambda_c W + \frac{1}{4} H_W \Lambda_c^3 W + \dots \approx H_W \Lambda_c W \tag{105}$$

at the leading order in $1/N$ ($\hbar$). Let us make a few comments about TWA. First we observe that it is exact for non-interacting systems which involve particles in a harmonic potential, non-interacting particles in arbitrary time-dependent potential, arbitrary non-interacting spin systems in time-dependent magnetic fields and others. This observation immediately follows from noticing that for such systems all terms involving third and higher order derivatives of the Hamiltonian identically vanish. Second we observe that the Liouville equation can be solved by characteristics, i.e. the probability distribution is conserved along the classical trajectories. Thus classical trajectories have the same interpretation within TWA: they conserve the Wigner function. This implies that within TWA the expectation value of an arbitrary observable can be written as

$$\langle \hat{O}(t) \rangle = \int da da^* W_0(a_0, a_0^*) O_W(a(t), a^*(t), t), \tag{106}$$

where $W_0(a_0, a_0^*)$ is the initial Wigner function and $a(t)$ and $a^*(t)$ are solutions of the classical Gross-Pitaevski (Netwon's in the corpuscular case) equations satisfying the initial conditions $a(t) = a_0,\ a^*(t) = a_0^*$. Finally let us point that TWA is asymptotically exact at short times. We will present the formal proof in the next section when we discuss the structure of quantum corrections. But heuristically this statement relies on noting that formally $\hbar$, divided by an energy scale, sets the time unit and thus the classical limit $\hbar \to 0$ is equivalent to looking into very short times.

In many-particle systems one rarely considers interactions higher than two body, i.e. involving more than four creation and annihilation operators. This means that the expansion of the Moyal bracket always stops at the third order and the exact evolution equation for the Wigner function is

$$i\dot{W} = \sum_j \frac{\partial H_W}{\partial a_j}\frac{\partial W}{\partial a_j^*} - \frac{\partial H_W}{\partial a_j^*}\frac{\partial W}{\partial a_j} + \frac{1}{8}\sum_{i,j,k} \frac{\partial^3 \mathcal{H}_W}{\partial a_i \partial a_j^* \partial a_k^*}\frac{\partial^3 W}{\partial a_i^* \partial a_j \partial a_k} - \frac{\partial^3 \mathcal{H}_W}{\partial a_i^* \partial a_j \partial a_k}\frac{\partial^3 W}{\partial a_i \partial a_j^* \partial a_k^*}, \quad (107)$$

where for completeness we inserted all single-particle indices. This third order Fokker-Planck equation is relatively simple looking. However, there are no available methods to solve it for complex systems. In particular, it can not be solved by the methods of characteristics, i.e. there is no well defined notion of trajectories. In the next section we will show how one can solve this equation perturbatively using the notion of quantum jumps.

Quantum jumps also appear in the context of finding non-equal time correlation functions. Intuitively such jumps are expected from basic uncertainty principle. E.g. measuring the position of a particle at time t necessarily induces uncertainty in its momentum and affects the outcome of the second measurement at a later time. It turns out that the Bopp representation is most suitable to analyze the non-equal time correlation function. We simply understand derivatives appearing in Eqs. (38), (43), (64), (65) as a response to an infinitesimal jumps in phase space variable, which can be calculated either instantaneously for equal time-correlation functions or at a later time for non-equal time correlation functions. E.g. for $t_1 < t_2$

$$\langle \hat{a}^\dagger(t_1)\hat{a}(t_2)\rangle = \int\int da_0 da_0^* W(a_0, a_0^*)\left(a^*(t_1)a(t_2) - \frac{1}{2}\frac{\partial a(t_2)}{\partial a(t_1)}\right) \quad (108)$$

The last term is understood as a linear response of the function $a(t_2)$ to infinitesimal jump in a at the moment t_1: $a(t_1) \to a(t_1) + \delta a$. This representation is valid even if $t_1 > t_2$ but then it becomes not casual because the response of $a(t_2)$ is evaluated to the jump, which will occur in the future. Here it is much more convenient to restore causality by using the left Bopp representation (43). Then e.g. again assuming that $t_1 < t_2$

$$\langle \hat{a}(t_2)a^\dagger(t_1)\rangle = \int\int da_0 da_0^* W(a_0, a_0^*)\left(a(t_2)a^*(t_1) + \frac{1}{2}\frac{\partial a(t_2)}{\partial a(t_1)}\right) \quad (109)$$

In the classical limit the two expressions clearly coincide but in general the two responses are different. In particular, the non-equal time commutator, which is up to a factor is the retarder Green's function appearing in standard Kubo linear response theory, is given purely by the response to the jump:

$$\langle [\hat{a}^\dagger(t_1), \hat{a}(t_2)] \rangle = -\int\int da_0 da_0^* W(a_0, a_0^*) \frac{\partial a(t_2)}{\partial a(t_1)} \tag{110}$$

Clearly as $t_2 \to t_1 + 0$ we recover standard bosonic commutation relations. Conversely the symmetric correlation function, which appears e.g. in dissipative response of the systems, does not contain quantum jumps:

$$\langle [\hat{a}^\dagger(t_1), \hat{a}(t_2)]_+ \rangle = 2 \int\int da_0 da_0^* W(a_0, a_0^*) a^*(t_1) a(t_2). \tag{111}$$

While this representation of the non-equal time correlation functions is completely general, it is most useful within TWA, where response at a later time can be easily computed as a difference between two classical trajectories: the original one and the one infinitesimally shifted at time t_1.

TWA is a very powerful tool for analyzing quantum dynamics in the semiclassical limit, where quantum fluctuations are responsible for initial seed triggering the dynamics but the consequent evolution is nearly classical. There are many applications to quantum optics, physics of ultracold gases, simulation of kinetics of chemical reactions, evolution of early universe and others. In these lectures we will only consider simple applications to simple systems. Further more complicated examples can be found e.g. in Refs. (5; 6).

1. Single particle in a harmonic potential.

As a first illustration of the phase space methods for studying quantum dynamics let us consider a particle moving in a harmonic potential. Here all the calculations can be done analytically without any approximations. The Hamiltonian of a single harmonic oscillator is

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2 = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2), \tag{112}$$

where the coordinate and momentum operators $\hat{q}$ and $\hat{p}$ are related to creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$ in a standard way:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right). \tag{113}$$

Now suppose that the particle is prepared in the ground state and we are suddenly applying a linear potential $V(q) = -\lambda q$. So that the Hamiltonian becomes

$$\hat{H} = \hat{H}_0 - \lambda \hat{q} \tag{114}$$

Next we compute various observables as a function of time.

Coordinate-momentum representation. First we will solve this problem using the coordinate-momentum representation. The corresponding Wigner function is a Gaussian computed earlier (58). Next we need to solve the classical equations of motion:

$$\frac{dp}{dt} = -m\omega^2 q + \lambda, \quad \frac{dq}{dt} = \frac{p}{m} \tag{115}$$

satisfying the initial conditions $q(0) = q_0$, $p(0) = p_0$. Clearly the solution is

$$q(t) = q_{\rm cl}(t) + q_0 \cos(\omega t) + \frac{p_0}{m\omega}\sin(\omega t), \tag{116}$$

where $q_{\rm cl}(t) = \lambda/m\omega^2(1 - \cos(\omega t))$ is the classical trajectory describing the motion of the particle, which is initially set to rest. Then we need to substitute this solution to the observable corresponding to the quantum operator of interest and find the average over the initial conditions.

For the expectation value of the position we trivially find $\langle \hat q(t)\rangle = q_{cl}(t)$, which is just a particular case of the Ehrenfest's principle. Similarly we find

$$\langle \hat q^2\rangle = \overline{q^2(t)} = q_{\rm cl}^2(t) + a_0^2. \tag{117}$$

This is of course also the correct result, which can be easily obtained from the solution of the Schrödinger equation.

Next let us show how to compute a non-equal time correlation function. In particular, $\langle \hat q(t)\hat q(t')\rangle$ with $t < t'$. For this we will use the time-dependent Bopp representation (38)

$$\hat q(t) = q(t) + \frac{i\hbar}{2}\frac{\partial}{\partial p(t)} \tag{118}$$

and interpret this derivative as a response to the infinitesimal jump in momentum at time t. Then

$$\begin{aligned}\langle \hat q(t)\hat q(t')\rangle = &\overline{\left(q_{cl}(t) + q_0\cos(\omega t) + \frac{p_0}{m\omega}\sin(\omega t) + \frac{i\hbar}{2}\frac{\partial}{\partial \delta p}\right)} \\ &\overline{\times\left(q_{cl}(t') + q_0\cos(\omega t') + \frac{p_0}{m\omega}\sin(\omega t') + \frac{\delta p}{m\omega}\sin(\omega(t'-t)\right)} \\ &= q_{\rm cl}(t)q_{\rm cl}(t') + a_0^2\cos(\omega(t-t')) + i a_0^2 \sin(\omega(t'-t)).\end{aligned} \tag{119}$$

Note that this correlation function is complex because it does not correspond to the expectation value of a Hermitian operator. Similarly for the correlation function with the opposite ordering of t and t' we find

$$\langle \hat q(t')\hat q(t)\rangle = q_{\rm cl}(t)q_{\rm cl}(t') + a_0^2\cos(\omega(t-t')) - i a_0^2 \sin(\omega(t'-t)) \tag{120}$$

Therefore the symmetric part of the correlation function is simply given by

$$\left\langle \frac{\hat{q}(t')\hat{q}(t) + \hat{q}(t)\hat{q}(t')}{2} \right\rangle = q_{\rm cl}(t) q_{\rm cl}(t') + a_0^2 \cos(\omega(t - t')) \tag{121}$$

and the expectation value for the commutator is

$$\langle \hat{q}(t)\hat{q}(t') - \hat{q}(t')\hat{q}(t) \rangle = 2ia_0^2 \sin(\omega(t' - t)). \tag{122}$$

This commutator vanishes at $t \to t'$ and rapidly oscillates if $\omega(t' - t) \gg 1$.

Coherent state representation. For illustration purposes we repeat this calculation in the coherent state representation. In the second quantized form the Hamiltonian of the system reads

$$\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2) - \lambda a_0(\hat{a} + \hat{a}^\dagger). \tag{123}$$

The classical (Gross-Pitaevski) equation for the oscillator reads:

$$i\hbar \frac{\partial \alpha}{\partial t} = \hbar\omega\alpha - \lambda a_0. \tag{124}$$

We use $\alpha(t)$ and $\alpha^*(t)$ do denote phase space variables to avoid confusion with the notation a_0 for the oscillator length. This equation has the following solution

$$\alpha(t) = \frac{\lambda a_0}{\hbar\omega}\left(1 - \mathrm{e}^{-i\omega t}\right) + \alpha_0 \mathrm{e}^{-i\omega t}. \tag{125}$$

Using the explicit form of the Wigner function of the vacuum state (75) we immediately find

$$\langle \hat{q}(t) \rangle = a_0 \overline{(\alpha(t) + \alpha^*(t))} = \frac{2a_0^2\lambda}{\hbar\omega}(1 - \cos(\omega t)) = q_{\rm cl}(t). \tag{126}$$

Similarly

$$\langle \hat{q}^2(t) \rangle = a_0^2 \overline{(\alpha^2(t) + (\alpha^\star(t))^2 + 2\alpha(t)\alpha^\star(t))} = q_{\rm cl}^2(t) + a_0^2. \tag{127}$$

We obviously got the same answers as before. Similarly one can verify the result for the non-equal time correlation function. Of course it is not surprising that both methods give identical exact results for harmonic systems. However, it is important to realize that once we deal with more complicated interacting models the correct choice of the phase space can significantly simplify the problem. Moreover the expansions around the two possible classical limits are very different. Thus for a system of noninteracting particles moving in some external potential TWA in the coordinate-momentum representation is only approximate unless the potential is harmonic. At the same time TWA in the coherent state representation is exact.

2. Collapse (and revival) of a coherent state

Next consider a slightly more complicated case of an initial single-mode coherent state evolving according to the quartic interacting Hamiltonian

$$\hat{H} = \frac{U}{2}\hat{a}^\dagger\hat{a}(\hat{a}^\dagger\hat{a} - 1). \tag{128}$$

Clearly the eigenstates of this Hamiltonian are the Fock states $|n\langle$ with eigen energies

$$\epsilon_n = \frac{U}{2}n(n-1).$$

This problem is closely related the collapse-revival experiment by M. Greiner et. al. (7). Because the problem does not have kinetic term it can be easily solved analytically. In particular, the expectation value of the annihilation operator can be found by expanding the coherent state in the Fock basis and propagating it in time

$$|\psi(t)\rangle = \mathrm{e}^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle \mathrm{e}^{-i\epsilon_n t}. \tag{129}$$

Then we find

$$\langle\psi(t)|\hat{a}|\psi(t)\rangle = \mathrm{e}^{-|\alpha|^2}\sum_{n,m}\frac{(\alpha^*)^n(\alpha^m)}{\sqrt{n!m!}}\mathrm{e}^{i(\epsilon_n-\epsilon_m)t}\langle n|a|m\rangle = \mathrm{e}^{-|\alpha|^2}\sum_n \frac{(\alpha^*)^n\alpha^{n+1}}{\sqrt{n!(n+1)!}}\sqrt{n+1}\,\mathrm{e}^{i(\epsilon_n-\epsilon_{n+1})t}$$
$$= \alpha\mathrm{e}^{-|\alpha|^2}\sum_n \frac{|\alpha^2|^n}{n!}\mathrm{e}^{-iUn} = \alpha\exp\left[|\alpha|^2\left(\mathrm{e}^{-iUt}-1\right)\right]. \tag{130}$$

Qualitatively at larger $N = |\alpha|^2$ this solution gives first rapid decay of the coherence, where $\langle\hat{a}(t)\rangle$ decays to an exponentially small number at a characteristic time $\tau = UN$ and then at a much later time $t_0 = 2\pi/U$ there is a complete revival of the state. The classical limit here corresponds to $N\to\infty$, $U\to 0$ and $UN = \lambda$ fixed. Clearly in the classical limit there is still collapse of the state by no revival since $t_0 \sim 2\pi N/\lambda \to \infty$.

Next we solve the problem using TWA. For doing this we first compute the Weyl symbol of the Hamiltonian (128):

$$H_W(a^*, a) = \frac{U}{2}|a|^2(|a|^2 - 2) + \frac{U}{4}. \tag{131}$$

Note that there is an extra -1 in the first term Hamiltonian as compared to the naive substitution $\hat{a}\to a$ due to the Weyl ordering. Using this Hamiltonian we find classical Gross-Pitaveski equations of motion for the complex amplitudes:

$$i\frac{\partial a(t)}{\partial t} = U(|a|^2 - 1)a(t). \tag{132}$$

This equation can be trivially solved using that $|a(t)|^2 = |a_0|^2$ is the integral of motion:

$$a(t) = a_0 \mathrm{e}^{-iU(|a_0|^2-1)t} \tag{133}$$

The solution should be supplemented by random initial conditions distributed according to the Wigner function:

$$W(a_0, a_0^*) = 2\exp[-2|a_0 - \alpha|^2]. \tag{134}$$

Using the explicit analytic solution of Eq. (132) and the Wigner function above we can calculate the expectation value of the coherence $\langle \hat{a}(t)\rangle$ within TWA by Gaussian integration

$$a(t) \approx \alpha \exp\left[-\frac{iU|\alpha|^2 t}{1+iUt/2}\right] \exp[iUt]\frac{1}{(1+iUt/2)^2}, \tag{135}$$

This expression is more complicated than the simple exact quantum results. Let us discuss its qualitative features. First of all we an see that at a characteristic time $\tau = 1/(UN)$ there is a collapse of the coherence as in the quantum case. One can check that for times much shorter than the revival time the TWA solution very closely matches the exact solution. However the TWA result completely misses revivals, which are thus intrinsically quantum related to discreteness of the Fock basis.

Exercise. Using Mathematica or other software plot dependence $\langle \hat{a}(t)\rangle$ both using the exact result and TWA approximation. Choose N of the order of 10 and fix U at one (this can be always done by choosing appropriate time units). Check that TWA very accurately reproduces collapse already for $N \sim 4, 5$. Check that if you use naive classical Hamiltonian as opposed to the Weyl symbol $H = \frac{U}{2}|a|^2(|a|^2-1)$ the agreement even at short times will be much worse.

This example highlights important potential issue with TWA: it can miss long time behavior. One can imagine that if there is some small dephasing in the system e.g. due to decoherence such that revivals are destroyed then TWA solution will be accurate at all times.

Let us make a remark concerning Weyl ordering in simulations of bosonic systems using TWA. Most commonly one deals with two-body density-density interactions so typical Hamiltonian is

$$H(\hat{a}_j, \hat{a}_j^\dagger) = \sum_{ij}\left[V_{ij}\hat{a}_i^\dagger \hat{a}_j + U_{ij}\hat{a}_i^\dagger \hat{;} a_j^\dagger \hat{a}_j \hat{a}_i\right]. \tag{136}$$

where V_{ij} includes both kinetic part and the single particle potential and i and j can be either descrete or continuous indexes. Using the Bopp representation we find that the Weyl symbol for the Hamiltonian is

$$H_W(a_j^*, a_j) = \sum_{ij}\left[V_{ij}\alpha_i^*\alpha_j + U_{ij}|\alpha_i|^2|\alpha_j|^2\right] - \frac{1}{2}\sum_i V_{ii} - \sum_{ij}|\alpha_i|^2 U_{ij} - \sum_i |\alpha_i|^2 U_{ii} + \frac{1}{2}\sum_i U_{ii} \tag{137}$$

The constant terms are clearly non-important since they only give an energy shift. The only two important terms, which distinguish between Weyl symbol and naive classical Hamiltonian are

$$-\sum_{ij}|\alpha_i|^2(U_{ij}+\delta_{ij}U_{ii}).$$

In general these terms can be very important for accurate description of dynamics using TWA. But in the most common case of translationally invariant interactions $U_{ij}=U_{|i-j|}$ it is clear that this contribution is simply proportional to the number of particles and thus has no effect on dynamics in isolated systems since the latter is conserved. If we aer dealing with e.g. two different species of bosons like a two-component system then this correction can become very important.

3. Spin dynamics in a linearly changing magnetic field: multi-level Landau-Zener problem.

As a final simple illustrative example we consider another situation where TWA is exact. In particular, we will analyze dynamics of an arbitrary spin S in a linearly changing magnetic field:

$$\hat{H}=2h_z(t)\hat{s}^z+2g\hat{s}^x, \tag{138}$$

where $h_z(t)=\delta t$. We assume that the system is initially prepared in some way at $t=-t_0$ and will be interested in finding expectation values of various observables at $t=t_0$, where t_0 is large so that $h_z(t_0)\gg g$.

As we discussed in Sec. III.D one can map the time evolution of noninteracting spins to the evolution of noninteracting bosons using the Schwinger representation. Therefore TWA is exact in this case. Using Eqs. (88) the Hamiltonian (138) becomes:

$$\hat{H}=h_z(t)(\hat{\alpha}^\dagger\hat{\alpha}-\hat{\beta}^\dagger\hat{\beta})+g(\hat{\alpha}^\dagger\hat{\beta}+\hat{\beta}^\dagger\hat{\alpha}). \tag{139}$$

The Weyl symbol of this Hamiltonian is obtained by simply replacing quantum operators $\hat{\alpha},\hat{\beta},\hat{\alpha}^\dagger,\hat{\beta}^\dagger$ by complex amplitudes $\alpha,\beta,\alpha^*,\beta^*$. Then the corresponding equations of motion are

$$i\frac{d\alpha}{dt}=\delta t\alpha+g\beta, \tag{140}$$

$$i\frac{d\beta}{dt}=g\alpha-\delta t\beta. \tag{141}$$

These equations should be supplemented by the initial conditions distributed according to the Wigner transform of the initial density matrix.

Note that Eqs. (140) and (141) map exactly to the equations describing the conventional Landau-Zener problem. Then the evolution can be described by a unitary 2×2 matrix:

$$\alpha_\infty=T\alpha_0+Re^{i\phi}\beta_0,\quad \beta_\infty=-Re^{-i\phi}\alpha_0+T\beta_0, \tag{142}$$

where (see e.g. Ref. (8))

$$T = \mathrm{e}^{-\pi\gamma},\ R = \sqrt{1-T^2},\ \phi = \gamma\,[\ln(\gamma) - 1] - 2\gamma\ln(\sqrt{2\delta}T), \tag{143}$$

and $\gamma = g^2/(2\delta)$ is the Landau-Zener parameter.

Using this result we can re-express different spin components at $t \to \infty$ through the initial values:

$$\begin{aligned} s^z_\infty &= (T^2 - R^2)\frac{\alpha_0^\star\alpha_0 - \beta_0^\star\beta_0}{2} + \alpha_0^\star\beta_0 RT\mathrm{e}^{i\phi} + \alpha_0\beta_0^\star RT\mathrm{e}^{-i\phi} \\ &= (T^2 - R^2)s^z_0 + 2RT\cos(\phi)s^x_0 - 2RT\sin(\phi)s^y_0, \\ s^x_\infty &= -2RT\cos(\phi)s^z_0 + (T^2 - R^2\cos(2\phi))s^x_0 + R^2\sin(2\phi)s^y_0, \\ s^y_\infty &= 2RT\sin(\phi)s^z_0 + R^2\sin(2\phi)s^x_0 + (T^2 + R^2\cos(2\phi))s^y_0. \end{aligned} \tag{144}$$

Now using these expressions and the Weyl symbols of spin operators and their bilinears derived in Sec. III.D we can compute expectation values of various operators. This can be done for any initial state but for concreteness we choose initial stationary state polarized along the z-direction. In the language of Schwinger bosons this is a Fock state $|S-n, n\rangle$, where a particular value of n corresponds to the initial polarization $s^z_0 = S - n$.

$$\begin{aligned} &\langle \hat{s}^z_\infty\rangle = (T^2 - R^2)s^z_0 \\ &\langle (\hat{s}^z_\infty)^2\rangle = \left[T^4 + R^4 - 4T^2R^2\right](s^z_0)^2 + 2T^2R^2 s(s+1), \\ &\langle \hat{s}^z_\infty\hat{s}^x_\infty + \hat{s}^z_\infty\hat{s}^x_\infty\rangle = 2RT(T^2 - R^2)\cos(\phi)\left[s(s+1) - 3\langle(\hat{s}^z_0)^2\rangle\right]. \end{aligned} \tag{145}$$

Note that for the conventional Landau-Zener problem corresponding to the spin $s = 1/2$ the last two equations become trivial: $\langle(\hat{s}^z_\infty)^2\rangle = 1$ and $\langle \hat{s}^z_\infty\hat{s}^x_\infty + \hat{s}^z_\infty\hat{s}^x_\infty\rangle = 0$. But for larger values of spin these correlation functions are nontrivial with e.g. $\langle \hat{s}^z_\infty\hat{s}^x_\infty + \hat{s}^x_\infty\hat{s}^z_\infty\rangle$ being an oscillating function of the rate δ and the Landau-Zener parameter γ.

V. PATH INTEGRAL DERIVATION.

In the final section of these notes we will see how all the concepts introduced earlier: Wigner function, Weyl symbol, Bopp operators etc. naturally emerge from the Feynmann's path integral representation of the evolution operator. Using this approach it is also possible to understand structure of the quantum corrections beyond TWA and understand potential extension of this formalism to other setups: open systems, quantum tunneling problems (as possible non-classical saddle points). The derivations shown in this section will closely follow the discussion in Ref. (6) with additional exercises and details of derivations. The derivation itself is very similar to the formalism used in the Keldysh approach to dynamics of quantum systems (9). The main difference is that we will be focusing on expansion of dynamics in the effective Planck's constant, while in the Keldysh technique the expansion parameter is usually the interaction strength. So the two approaches are rather complimentary to each other despite many similarities. As in the previous section we will concentrate on the coherent state representation and only quote final results in the coordinate-momentum space.

Our starting point will be expectation value pf some operator $\hat{\Omega}(\hat{a}, \hat{a}^\dagger, t)$. We assume that this operator is written in the normal ordered form. To shorten notations we will skip the single-particle indices in the bosonic fields and reinsert them only when needed.

$$\Omega(t) \equiv \langle \hat{\Omega}(\hat{a}, \hat{a}^\dagger, t)\rangle = \mathrm{Tr}\left[\rho\, T_\tau\, \mathrm{e}^{i\int_0^t \hat{H}(\tau)d\tau} \hat{\Omega}(\hat{a}, \hat{a}^\dagger, t) e^{-i\int_0^t \hat{H}(\tau)d\tau}\right], \tag{146}$$

Because in the coherent state picture the Planck's constant plays the mere role of conversion between time and energy units we set $\hbar = 1$ throughout this section to simplify notations. Here time ordering symbol T_τ implies that in both exponents later times appear closer to the middle, i.e. closer to the $\hat{\Omega}$. Next we split the exponent of the time ordered integral over time into a product:

$$T_\tau \mathrm{e}^{i\int_0^t \hat{H}(\tau)d\tau} = \prod_{j=1}^{M} \mathrm{e}^{i\Delta\tau \hat{H}(\tau_j)} \approx \prod_{j=1}^{M} (1 + i\Delta\tau \hat{H}(\tau_j)),\ T_\tau \mathrm{e}^{-i\int_0^t \hat{H}(\tau)d\tau} = \prod_{j=M}^{1} \mathrm{e}^{-i\Delta\tau \hat{H}(\tau_j)},$$

where $\tau_j = j\Delta\tau$ is the discretized time (we assume that initial time is zero), $\Delta\tau = t/M$ and M is a large number. We will eventually take the limit $M \to \infty$. Next we insert the resolution of identity

$$I = \int d\alpha_j d\alpha_j^* |\alpha_j\rangle\langle\alpha_j|$$

between each of the terms in the product. Because we have two exponents on the left and on the right of the operator $\hat{\Omega}$ we need to distinguish two different α fields. The one, which corresponds to the positive exponent we term forward field $\alpha_{f\mathrm{J}}$ and the one which corresponds to the negative exponent backward field $\alpha_{b\,j}$. This notation is conventional in Keldysh technique and comes from the ordering in the Schwinger-Keldysh contour. Loosely speaking as we move from left to right we first increase time from 0 to t and then decrease it backward to zero. Then we find

$$\Omega(t) = \int \dots \int D\alpha_f D\alpha_f^* D\alpha_b D\alpha_b^* \,\langle \alpha_{b\,0}|\hat{\rho}|\alpha_{f\,0}\rangle\, \mathrm{e}^{-\alpha_{f0}^*\alpha_{f0}/2 + \alpha_{f\,0}^*\alpha_{f\,1} + iH(\alpha_{f\,0}, \alpha_{f\,1}^*)\Delta\tau} \dots$$
$$\mathrm{e}^{-\alpha_{f\,M}^* a_{f\,M}} \Omega(\alpha_{f\,M}^*, \alpha_{b\,M}, t) \mathrm{e}^{\alpha_{f\,M}^* a_{b\,M}} \mathrm{e}^{-\alpha_{b\,M}^* a_{b\,M} + a_{b\,M}^* a_{b\,M-1} - iH(a_{b\,M}, a_{b\,M-1}^*)\Delta\tau} \dots \mathrm{e}^{-\alpha_{b\,0}^*\alpha_{b\,0}/2}. \tag{147}$$

Next let us change the variables:

$$\alpha_j = \frac{\alpha_{f\,j} + \alpha_{b\,j}}{2},\ \eta_j = \alpha_{f\,j} - \alpha_{b\,j},\ \Leftrightarrow\ \alpha_{f\,j} = \alpha_j + \frac{\eta_j}{2},\ \alpha_{b\,j} = \alpha_j - \frac{\eta_j}{2}.$$

As we will see below this choice of variables automatically leads to the Weyl quantization. Other choices e.g. $\alpha_b = \alpha,\ \alpha_f = \alpha + \eta$ will naturally lead to other representations. Physically the symmetric field α corresponds to the classical field and η is a quantum field. It is intuitively clear that in the classical limit there is a unique classical trajectory satisfying fixed initial conditions and thus the forward and backward fields should be essentially the same. Performing this change of variables and taking the continuum $M \to \infty$ limit we find

$$\Omega(t) = \int D\eta D\eta^* D\alpha D\alpha^* \left\langle \alpha_0 - \frac{\eta_0}{2} \middle| \hat{\rho} \middle| \alpha_0 + \frac{\eta_0}{2} \right\rangle \Omega\left[\alpha^*(t) + \frac{\eta^*(t)}{2}, \alpha(t) - \frac{\eta(t)}{2}\right] \mathrm{e}^{-\frac{1}{2}|\eta(t)|^2} \mathrm{e}^{\frac{1}{2}(\eta_0^*\alpha_0 - \eta_0\alpha_0^*)}$$
$$\exp\left\{\int_0^t d\tau \left[\eta^*(\tau)\frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau)\frac{\partial \alpha^*(\tau)}{\partial \tau}\right.\right.$$
$$\left.\left. + iH_W\left(\alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau\right) - iH_W\left(\alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau\right)\right]\right\}, \quad (148)$$

One can recognize that the integrals over boundary quantum fields η_0 and η_t automatically give the Wigner function and the Weyl symbol of the operator $\hat{\Omega}$ so that the expression above becomes

$$\Omega(t) = \int D\eta D\eta^* D\alpha D\alpha^* W(\alpha_0, \alpha_0^*) \exp\left\{\int_0^t d\tau \left[\eta^*(\tau)\frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau)\frac{\partial \alpha^*(\tau)}{\partial \tau}\right.\right.$$
$$\left.\left. + iH_W\left(\alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau\right) - iH_W\left(\alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau\right)\right]\right\} \Omega_W(\alpha(t), \alpha^*(t), t), \quad (149)$$

Before deriving TWA from this expression let us give a few comments on details of the derivation of Eq. (148), which is quite subtle.

First we analyze all the terms appearing in the path integral, which do not involve Hamiltonian:

$$S_1 = \alpha_{f0}^*\alpha_{f0}/2 + \alpha_{b0}^*\alpha_{b0}/2 + \sum_{i=1}^{M-1}\left[\alpha_{fi}^*(\alpha_{f\,i+1} - \alpha_{fi}) - \alpha_{bi}^*(\alpha_{bi} - a_{b\,i-1})\right]$$
$$+ \alpha_{f0}^*(\alpha_{f1} - \alpha_{f0}) - \alpha_{bM}^*(\alpha_{bM} - \alpha_{b\,M-1}) - \alpha_{b0}^*\alpha_{b0} + \alpha_{fM}^*(\alpha_{bM} - \alpha_{fM}). \quad (150)$$

The first sum in the continuum limit becomes an integral:

$$\sum_{i=1}^{M-1} \alpha_{fi}^*(\alpha_{f\,i+1} - \alpha_{fi}) - \alpha_{bi}^*\alpha_{bi} - \alpha_{b\,i-1}) \to \int_0^t d\tau \left(\alpha_f^*(\tau)\frac{\partial \alpha_f(\tau)}{\partial \tau} - \alpha_b^*(\tau)\frac{\partial \alpha_b(\tau)}{\partial \tau}\right), \quad (151)$$

which under the substitutions $\alpha_f \to \alpha + \eta/2$, $\alpha_b \to \alpha - \eta/2$ and after integrating by parts becomes:

$$\int_0^t d\tau \left(\eta^*(\tau)\frac{\partial \alpha(\tau)}{\partial \tau} - \eta(\tau)\frac{\partial \alpha^*(\tau)}{\partial \tau}\right) + \alpha^*(t)\eta(t) - \alpha_0^*\eta_0. \tag{152}$$

In the continuum limit the first and the second terms after the sum in (150) clearly go to zero and the last two read:

$$\alpha_{fM}^*(\alpha_{bM} - \alpha_{fM}) - \alpha_{b\,0}^*\alpha_{b\,0} = -|\alpha_0|^2 - |\eta_0|^2/4 + \frac{1}{2}(\alpha_0^*\eta_0 + \eta_0^*\alpha_0) - \alpha^*(t)\eta(t) - |\eta(t)|^2/2. \tag{153}$$

Combining Eqs. (150) - (153) we derive:

$$S_1 = \int_0^t d\tau \left(\eta^*(\tau)\frac{\partial \psi(\tau)}{\partial \tau} - \eta(\tau)\frac{\partial \psi^*(\tau)}{\partial \tau}\right) - \frac{|\eta(t)|^2}{2} + \frac{1}{2}(\eta_0^*\alpha_0 - \alpha_0^*\eta_0). \tag{154}$$

This immediately leads to the correct Hamiltonian independent part in Eq. (148). The part involving the Hamiltonian in that equation is very straightforward, essentially this is just the difference of Hamiltonians evaluated on forward and backward trajectory. A more subtle result is the emergence of the Weyl ordering. Formally it appears because the fields α and α^* appear at slightly different times. As we will see below quantum field η plays the role of the derivative with respect to the classical field α. Thus the normal ordered Hamiltonian is actually evaluated at Bopp operators giving the Weyl symbol H_W.

Exercise. Repeat derivation of Eq. (148). Complete missing calculations.

In the leading order in quantum fluctuations we expand the integrand in Eq. (162) up to the linear terms in η. Then the functional integral over $\eta(t)$ enforces the δ-function Gross-Pitaevskii constraint on the classical field $\alpha(t)$:

$$i\partial_t \alpha = \frac{\partial H_W(\alpha(t), \alpha^*(t), t)}{\partial \alpha^*(t)} \equiv \{\alpha(t), H_W(\alpha(t), \alpha^\star(t), t)\}_c \tag{155}$$

and we recover TWA (106).

Next let us move to discussion of non-equal time correlation functions. The simplest one will be

$$\langle \hat{a}^\dagger(t_1)\hat{a}(t_2)\rangle. \tag{156}$$

First we assume $t_1 < t_2$. We proceed in the same way as in the equal-time case by writing this expression in the path integral form inserting forward and backward coherent states. The only new ingredient is an extra term we encounter on the forward path

$$a_f^*(t) = a^*(t) + \frac{\eta^*(t)}{2} \tag{157}$$

Note that in the path integral η^* couples to $d\alpha = \alpha(t+\Delta t) - \alpha(t)$. This implies that

$$\frac{\eta^*(t_1)}{2} = -\frac{i}{2}\frac{\partial}{\partial \delta\alpha} \mathrm{e}^{i[\alpha(t_1+\Delta t)+\delta\alpha-\alpha(t_1)]\eta^*} = -\frac{i}{2}\frac{\partial}{\partial \delta\alpha} \mathrm{e}^{i[\alpha(t_1+\Delta t)+\delta\alpha-\alpha(t_1)]\eta^*},$$

where we understand the partial derivative as infinitesimal response to the jump in α at the moment t_1. Thus we recover that in order to measure the non-equal time correlation functions we simply need to make the substitution

$$\hat{a}^\dagger(t) = \alpha^*(t) - \frac{i\hbar}{2}\frac{\partial}{\partial \alpha(t)} \tag{158}$$

In the same way we can see that

$$\hat{a}(t) = \alpha(t) + \frac{i\hbar}{2}\frac{\partial}{\partial \alpha^*(t)} \tag{159}$$

This is nothing but the Bopp representation of the creation and annihilation operators. As we already know for equal time correlation functions they automatically generate the Weyl symbol of the observable. But for non-equal time correlation function the Bopp operators give very nice interpretation of the response which occurs at a later time. It is remarkable that like the Wigner function and the Weyl symbol the Bopp operators automatically appear in the path integral formalism.

For the opposite ordering $t_1 > t_2$ we hit earlier time on the backward contour so the same analysis as above holds except that we change $a_f \to a_b$. But this results in change in sign in η and thus in change in sign in derivatives. So we immediately recover the left Bopp representation with the same interpretation for non-equal time correlation functions

$$\hat{a}^\dagger(t) = \alpha^*(t) + \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial \alpha(t)}\; \hat{a}(t) = \alpha(t) - \frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial \alpha^*(t)} \tag{160}$$

While as we discussed earlier for equal time correlation functions both representations are equivalent and give the Weyl symbol, for non-equal time correlation functions there is an important difference. Namely the correct representation is dictated by causality so that we always evaluate the response to a jump, which occurred at an earlier time.

Interpretation of Bopp operators as a response to quantum jumps is particularly simple within TWA. Then the time evolution is essentially classical before and after the jump. Thus the response of a Weyl symbol $\Omega_2(t_2)$ to say a jump in α at moment t_1 is literary a difference of Ω_2 evaluated on two trajectories with and without jump divided over this jump:

$$\frac{\partial \Omega_2(\alpha(t_2), \alpha^*(t_2), t_2)}{\partial a(t_1)} = \frac{\Omega(\alpha'(t_2), \alpha'^*(t_2), t_2) - \Omega(\alpha(t_2), \alpha^*(t_2), t_2)}{\delta\alpha},$$

where $\alpha'(t_2)$ is the classical trajectory corresponding to an infinitesimal jump in $\alpha(t_1)$: $\alpha(t_1) = \alpha(t_1) + \delta\alpha$ and $\alpha(t_2)$ is the same trajectory without this jump. From the Bopp representation it is clear that for fully symmetric operators (equal or non-equal time) the quantum jump contributions drop and we can evaluate them by substituting operators $\hat{a}$ by phase space variables α. Conversely for commutators the only surviving contribution is the one containing at least one quantum jump.

While we focused our discussion on two-point correlation functions, derivation of the Bopp representation was completely general and extends to arbitrary number of creation and annihilation operators e.g. to three-point functions like

$$\langle \hat{a}^\dagger(t_1)\hat{a}(t_2)\hat{a}(t_3)\rangle \tag{161}$$

Note, however, there is an important subtlety when we have three or more times involved. Namely not all correlation functions have causal representation. In particular, if $t_2 < t_1, t_3$ there is no casual representation of the three-point function above. This implies that these functions are not physical and can not appear in any response. In functions, which have casual representation later times should always occur closer to the middle.

Another advantage in the path formulation of the evolution is that it allows us to go beyond the TWA and represent quantum corrections to dynamics as stochastic quantum jumps. We will be quite sketchy here, further details of derivation can be found in Ref. (6). In our previous discussion leading to TWA we neglected third order terms in quantum fluctuations coming from the difference

$$iH_W\left(\alpha(\tau) + \frac{\eta(\tau)}{2}, \alpha^*(\tau) + \frac{\eta^*(\tau)}{2}, \tau\right) - iH_W\left(\alpha(\tau) - \frac{\eta(\tau)}{2}, \alpha^*(\tau) - \frac{\eta^*(\tau)}{2}, \tau\right)$$

in Eq. (162). To stay more focused consider the Hubbard model where (up to unimportant quadratic in α and α^* terms

$$H_W(\alpha, \alpha^*) = \sum_j \frac{U}{2}|\alpha_j|^4.$$

Thus the difference above becomes

$$i\sum_j\left(\eta_j^*(\tau)\frac{\partial H_w(\tau)}{\partial \alpha_j^*(\tau)} + \eta_j(\tau)\frac{\partial H_w(\tau)}{\alpha_j(\tau)}\right) + \frac{i}{4}U\sum_j |\eta_j(\tau)|^2[\eta_j(\tau)\alpha_j^*(\tau) + \eta_j^*(\tau)\alpha_j(\tau)].$$

So the exact path integral representation of the evolution gevine by Eq. 162 becomes

$$\Omega(t) = \int D\eta D\eta^* D\alpha D\alpha^* W(\alpha_0, \alpha_0^*) \exp\Bigg\{\int_0^t d\tau \sum_j \Bigg[\eta_j^*(\tau)\left(\frac{\partial \alpha_j(\tau)}{\partial \tau} + i\frac{\partial H_w(\tau)}{\partial \alpha_j^*(\tau)}\right)$$
$$- \eta_j(\tau)\left(\frac{\partial \alpha_j^*(\tau)}{\partial \tau} - i\frac{\partial H_w(\tau)}{\alpha_j(\tau)}\right)\Bigg] + i\frac{U}{4}|\eta_j(\tau)|^2(\eta_j^*(\tau)\alpha_j(\tau) + \eta_j(\tau)\alpha_j^*(\tau))\Bigg\}\Omega_W(\alpha_j(t), \alpha_j^*(t), t), \tag{162}$$

Before we were ignoring these cubic in η terms so that functional integration over the quantum field $\eta(\tau)$ becomes trivial essentially enforcing the constraint of the classical Gross-Pitaevski equations of motion for the classical field α. This was the TWA. With the cubic term we can no longer evaluate this path integral. Let us treat this cubic term perturbatively by expanding the exponent:

$$\mathrm{e}^{i\sum_j \int_0^t d\tau \frac{U}{4}|\eta_j(\tau)|^2[\eta_j(\tau)\alpha_j^*(\tau)+\eta_j^*(\tau)\alpha_j(\tau)]} = 1 + i\frac{U}{4}\sum_j \int_0^t d\tau \frac{U}{4}|\eta_j(\tau)|^2[\eta_j(\tau)\alpha_j^*(\tau) + \eta_j^*(\tau)\alpha_j(\tau)]$$
$$-\frac{U^2}{16}\int\int_{0<\tau_1<\tau_2<t} |\eta_j(\tau_1)|^2[\eta_j(\tau_1)\alpha_j^*(\tau_1)+\eta_j^*(\tau_1)\alpha_j(\tau_1)]|\eta_j(\tau_2)|^2[\eta_j(\tau_2)\alpha_j^*(\tau_2)+\eta_j^*(\tau_2)\alpha_j(\tau_2)]+\dots \tag{163}$$

Now let us recall that when we discussed non-equal time correlation functions we realized that

$$\eta_j^*(\tau) = -i\frac{\partial}{\partial\alpha_j(\tau)},\ \eta_j^*(\tau) = i\frac{\partial}{\partial\alpha_j^*(\tau)}$$

with the interpretation of derivatives as a response. Thus the expression for the expectation value including the first quantum correction reads:

$$\langle\hat{\Omega}(\hat{\alpha},\hat{\alpha^\dagger},t)\rangle \approx \int\int d\alpha_0 d\alpha_0^* W_0(\alpha_0,\alpha_0^*)$$
$$\left(1 - i\frac{U}{4}\int_0^t d\tau \sum_j \left[\alpha_j^*(\tau)\frac{\partial^3}{\partial\alpha_j(\tau)\partial\alpha_j^*(\tau)\partial\alpha_j^*(\tau)} - c.c.\right]\right)\Omega_W(\alpha(t),\alpha^*(t),t). \tag{164}$$

The interpretation of this expression is very straightforward. The first quantum correction to TWA represents a third order response of our observable to an infinitesimal jump in the classical field during the evolution $\alpha(\tau)\to\alpha(\tau)+\delta\alpha$, $\alpha^*(\tau)\to\alpha^*(\tau)+\delta\alpha^*$. This jump can occur at any time during the evolution and at any space location and we need to sum over these jumps. Further corrections appear as multiple quantum jumps. It is clear that each quantum correction carries extra factor of $1/N^2$ ($\hbar^2$ in the coordinate momentum representation) thus we have a well defined expansion parameter.

It is interesting to note that this nonlinear response can be expressed through stochastic quantum jumps with non-positive probability distribution:

$$\langle\hat{\Omega}(\hat{a},\hat{a^\dagger},t)\rangle \approx \int\int d\alpha_0 d\alpha_0^* W_0(a_0,a_0^\star)$$
$$\left[1 - i\frac{U}{4}\sum_n\sum_j\int d\xi_j d\xi_j^*\left(\alpha_j^*(\tau_n)F(\xi_j,\xi_j^*) - \alpha_j(\tau_n)F^\star(\xi_j,\xi_j^*)\right)\Big|_{\delta\alpha_j(\tau_n)=\xi_j\sqrt[3]{\Delta\tau}}\Omega_W(\alpha'(t),\alpha'^\star(t),t)\right], \tag{165}$$

Here we discretized time and introduced stochastic variable ξ_j. At time τ_n we randomly choose ξ_j according to the (quasi)probability distribution $F(\xi,\xi^a st)$ and shift the classical fields α_j: and α_j^* by the amounts $\delta\alpha_j = \xi_j \sqrt[3]{\Delta}\tau$ and $\delta\alpha_j^* = \xi_j^* \sqrt[3]{\Delta\tau}$ (e.g. $\alpha_j' = \alpha_j + \delta\alpha_j$). This procedure is very similar to the mapping of ordinary Fokker-Planck equation describing diffusion to the Langevin dynamics with two important differences: (i) In the Langevin dynamics the jumps are proportional to $\sqrt{\Delta\tau}$ while here to $\sqrt[3]{\Delta(\tau)}$. (ii) In Langevin dynamics the function F can be chosen as a Gaussian with the second moment given by the diffusion constant. Here the (quasi)probability distribution can not be chosen as a positive function. Indeed in order for Eq. (165) to be equivalent to (164) we need to ensure that the first two moments of ξ_j and ξ_j^* vanish and the third moment gives non-vanishing contribution

$$\int\int d\xi_j d\xi_j^* \; \xi_j^2 \xi_j^* F(\xi_j, \xi_j^*) = 2 \tag{166}$$

One can see this equivalence by expanding Ω_W in terms of $\delta\alpha$ (for simplicity we suppress spatial indexes):

$$\begin{aligned}\Omega_W(\alpha'(t), \alpha^*(t), t) = \Omega_W(\alpha(t), \alpha^*(t), t) + \frac{\partial\Omega_W}{\partial\delta\alpha}\delta\alpha + \frac{\partial\Omega_W}{\partial\delta\alpha^*}\delta\alpha^* \\ + \frac{1}{2}\left(\frac{\partial^2\Omega_W}{\partial\delta\alpha\partial\delta\alpha}\delta\alpha^2 + \frac{\partial^2\Omega_W}{\partial\delta\alpha^*\partial\delta\alpha^*}(\delta\alpha^*)^2 + 2\frac{\partial^2\Omega_W}{\partial\delta\alpha\partial\delta\alpha^*}\delta\alpha\delta\alpha^*\right) \\ + \frac{1}{8}\left(\frac{\partial^3\Omega_W}{\partial(\delta\alpha)^3}\delta\alpha^3 + 4\frac{\partial^3\Omega_W}{\partial\delta\alpha^*(\delta\alpha)^2}\delta\alpha^*(\delta\alpha)^2 + 4\frac{\partial^3\Omega_W}{\partial(\delta\alpha^*)^2\delta\alpha}(\delta\alpha^*)^2\delta\alpha + \frac{\partial^3\Omega_W}{\partial(\delta\alpha^*)^3}(\delta\alpha^*)^3\right) + \dots\end{aligned} \tag{167}$$

Now if we use that $\delta\alpha = \xi\sqrt[3]{\Delta\tau}$ and integrate over ξ we see that the first two terms in the expansion vanish because F is chosen such that ξ has vanishing first and second moments and the requirement (166) gives non-zero third order response, which is precisely equivalent to Eq. (164). All higher order derivative terms clearly vanish in the limit $\Delta\tau \to 0$. Let us give an example of such a function, which all the requirements:

$$F(\xi_j, \xi_j^*) = \xi_j^* \left(|\xi_j|^2 - 2\right) \mathrm{e}^{-|\xi_j|^2}. \tag{168}$$

Thus we get equivalent representation of the quantum corrections either in the form of the nonlinear response or in the form of stochastic quantum jumps. Note that because these jumps have non-positive probability distribution full simulation of stochastic dynamics results in a severe sign problem. However, if one is interested in leading order quantum corrections one needs to take into account only a few jumps and the sign problem is not very severe. But at the moment there are no known optimization schemes to simulate the dynamics even with few jumps.

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