JOURNEYS TO AND IN QUANTUM PHASE SPACE: Extended Quantum Phase-Space Formulations of Quantum Many-Body Theory and Quantum Information Theory

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OUTLINE

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• 1. Brief Motivation

– several starting points, but let me mention just one:

→ there appears to be a basic asymmetry in our usual description of QM (as follows:)

→ we start with a classical Hamiltonian $H(x,p)$ which treats (x,p) coordinates on a completely equal footing (i.e., 'symmetrically')

→ we then quantize to $\hat{H}(\hat{x},\hat{p})$, which still retains this 'symmetry'

→ but: when we now use $\hat{H}(\hat{x},\hat{p})$ in the Schrödinger equation we usually choose to go into either the x-representation or the p-representation, and hence break the 'symmetry'

⇒ QUESTION: Can we avoid this and use a description with a joint (x,p) representation?

ANSWER: Our first thought is: "No, we can't", because of QM uncertainty relations, etc. But, this isn't true, because the use of e.g., the Wigner function $W(x,p)$ and other phase-space distribution functions, or holomorphic wavefunctions, etc. clearly somehow disproves this. However, it's all rather opaque! So, instead:

⇒ Let's go right back to classical mechanics, and see if we can somehow reformulate it, since the only real (safe) way we know how to formulate QM is to canonically quantize a classical counterpart!!

⇒

• 2. Classical Mechanics Revisited: Generalized (or Extended) Lagrangians and Hamiltonians

- $L_x = L_x(x, \dot{x})$ is a classical Lagrangian, where $x \equiv \{x_i\}$ is a set of generalized coordinates
- The Euler-Lagrange equations $\frac{d}{dt}\frac{\partial L_x}{\partial \dot{x}_i} - \frac{\partial L_x}{\partial x_i} = 0$ (1) specify the trajectory $x = x(t)$ in x-space
- The canonically conjugate momentum, p_i, to coordinate x_i is

$$p_i \equiv \frac{\partial L_x}{\partial \dot{x}_i} \qquad (2)$$

- The Hamiltonian is: $H = H(x,p) \equiv p_i \dot{x}_i - L_x(x, \dot{x})$ (3)

  (Note: The canonical momentum p_i is defined only along the actual classical path, and not along any other "virtual paths")

- Key point!: Although it's (highly) unusual to do so, (query: has anyone here ever seen it done?) there is nothing in principle to stop us from formulating the Lagrangian formalism with the roles of $x \rightleftharpoons p$ interchanged.

  → suppose $L_p = L_p(p, \dot{p})$ is the classical Lagrangian for the same system "in the p-representation"

  ⇒

- The trajectory $p = p(t)$ in p-space is again obtained from the Euler-Lagrange equations $\frac{d}{dt}\frac{\partial L_p}{\partial \dot{p}_i} - \frac{\partial L_p}{\partial p_i} = 0$ (4)

  → one can now fairly easily show that

- The canonically conjugate coordinate, x_i, to momentum p_i is

$$x_i \equiv \frac{\partial L_p}{\partial \dot{p}_i} \qquad (5)$$

  (Note: again, x_i is defined only along the classical p-trajectories)

⟹

- Key point #2! : The same Hamiltonian can fairly readily be shown to be given as

$$H = H(x,p) = -x_i \dot{p}_i + L_p(p,\dot{p}) \qquad (6)$$

- We now come to a central point and key motivation:
  → so as not to lose the "symmetry" between x_i and p_i in H on quantization → $\hat{H}$ + choice of representation, let us try to preserve it by defining a generalized Lagrangian (or extended Lagrangian) in the joint (x,p) classical phase-space representation, as follows:

$$L(x,p,\dot{x},\dot{p}) \equiv -\dot{x}_i p_i - x_i \dot{p}_i + L_x(x,\dot{x}) + L_p(p,\dot{p}) \qquad (7)$$

(Note: It's important to realize that $L(x,p,\dot{x},\dot{p}) = 0$ along classical paths, i.e., when (x_i, p_i) are canonically conjugate pairs, since then it's just the difference between Eqs. (3) and (6)

but: outside the space of the actual classical paths (x_i, p_i) can be considered as independent variables, → just the usual classical phase space.)

⇒

- With (x_i, p_i) considered as independent variables, the equations of motion are now obtained from the pairs of extended Euler-Lagrange equations:

$$(8) \begin{cases} \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{x}_i} - \dfrac{\partial L}{\partial x_i} = 0 \Rightarrow \dfrac{d}{dt}\dfrac{\partial L_x}{\partial \dot{x}_i} - \dfrac{\partial L_x}{\partial x_i} = 0 \\ \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{p}_i} - \dfrac{\partial L}{\partial p_i} = 0 \Rightarrow \dfrac{d}{dt}\dfrac{\partial L_p}{\partial \dot{p}_i} - \dfrac{\partial L_p}{\partial p_i} = 0 \end{cases}$$

— which simply reproduce Eqs. (1) and (4)

— so, has anything been gained? Let's see!

→

- <u>Note</u>: Equation (7) for L contains a total derivative, $-\dot{x}_i p_i - x_i \dot{p}_i = \frac{d}{dt}(-x_i p_i)$, which has zero effect in classical mechanics, BUT which in QM will introduce a phase factor in wave functions which cannot be ignored $\Rightarrow$ ¡ BE PREPARED !
- In Eqs. (7) and (8) we have now achieved our goal of having a Lagrangian formalism in which (x_i, p_i) are treated on an equal footing. The interest now finally comes in going over to a Hamiltonian formalism in which (x_i, p_i) are considered completely independent (i.e., so that only on classical paths are they conjugate variables) $\Rightarrow$
- <u>Canonically conjugate variables</u> (X_i, P_i) are now defined via $L(x, p, \dot{x}, \dot{p})$ as usual:

$$P_i \equiv \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial L_x}{\partial \dot{x}_i} - p_i \qquad (9a)$$

$$X_i \equiv \frac{\partial L}{\partial \dot{p}_i} = \frac{\partial L_p}{\partial \dot{p}_i} - x_i \qquad (9b)$$

(<u>Note</u>: On classical paths, $X_i = 0 = P_i$, from Eqs. (2) & (5))
$\Rightarrow$

- <u>The extended Hamiltonian</u>, G is now defined as usual via an (extended) Legendre transformation on L:

$$G = G(x, p, X, P) \equiv P_i \dot{x}_i + X_i \dot{p}_i - L(x, p, \dot{x}, \dot{p}) \qquad (10)$$

  - use of Eq. (7) $\Rightarrow$

$$G = (p_i + P_i)\dot{x}_i + (x_i + X_i)\dot{p}_i - L_x(x, \dot{x}) - L_p(p, \dot{p}) \qquad (11)$$

  - now eliminate $\dot{x}_i$ and $\dot{p}_i$ in favour of X_i and P_i:

Eqs. (2), (3) $\Rightarrow$ $L_x(x, \dot{x}) = -H\left(x_i, \frac{\partial L_x}{\partial \dot{x}_i}\right) + \dot{x}_i \frac{\partial L_x}{\partial \dot{x}_i}$ (12a)

and Eqs. (5)/(6) $\Rightarrow$ $L_p(p, \dot{p}) = H\left(\frac{\partial L_p}{\partial \dot{p}_i}, p_i\right) + \dot{p}_i \frac{\partial L_p}{\partial \dot{p}_i}$ (12b)

  - insert Eqs. (12a, b) into Eq. (11) $\Rightarrow$

$$G(x,p,X,P) = \left(p_i + P_i - \frac{\partial L_x}{\partial \dot{x}_i}\right)\dot{x}_i + \left(x_i + X_i - \frac{\partial L_p}{\partial \dot{p}_i}\right)\dot{p}_i + H\left(x_i, \frac{\partial L_x}{\partial \dot{x}_i}\right) - H\left(\frac{\partial L_p}{\partial \dot{p}_i}, p_i\right) \tag{13}$$

– finally, insert Eqs. (9a, b) into Eq. (13) ⇒

$$\boxed{\begin{aligned} G(x,p,X,P) &= H(x, p+P) - H(x+X, p) && (14a) \\ &= \sum_{n=1}^{\infty} \frac{1}{n!}\left[\frac{\partial^n H}{\partial p_i^n} P_i^n - \frac{\partial^n H}{\partial x_i^n} X_i^n\right] && (14b) \end{aligned}}$$

↳ VERY INTERESTING RESULT!

(Note particularly that G is the difference of 2 Hamiltonians → c.f., thermofield dynamics, which actually provided a second a priori motivation for this work)

- Note: On classical paths, $G \equiv 0$, since $X = 0 = P$
- Finally (for any doubters among you!), we can easily check that G does indeed correctly reproduce classical dynamics →

  – since (x_i, p_i) are treated here as "generalized coordinates" and (X_i, P_i) as the corresponding "generalized momenta", the Hamiltonian equations of motion are:

$$\dot{p}_i = \frac{\partial G}{\partial X_i} \; ; \; \dot{x}_i = \frac{\partial G}{\partial P_i} \; ; \; \dot{P}_i = -\frac{\partial G}{\partial x_i} \; ; \; \dot{X}_i = -\frac{\partial G}{\partial p_i} \tag{15}$$

  – now use Eq. (14a) ⇒

$$\dot{p}_i = -\left.\frac{\partial H}{\partial x_i}\right|_{x+X,\,p} \; ; \; \dot{x}_i = +\left.\frac{\partial H}{\partial p_i}\right|_{x,\,p+P} \tag{16a}$$

$$\dot{P}_i = -\left.\frac{\partial H}{\partial x_i}\right|_{x,\,p+P} + \left.\frac{\partial H}{\partial x_i}\right|_{x+X,\,p} \; ; \; \dot{X}_i = -\left.\frac{\partial H}{\partial p_i}\right|_{x,\,p+P} + \left.\frac{\partial H}{\partial p_i}\right|_{x+X,\,p} \tag{16b}$$

  – clearly Eqs. (16b) have the (correct) solution $P_i = 0 = X_i$, and thence Eqs. (16a) simply become the usual canonical Hamiltonian equations of motion:

$$\dot{p}_i = -\frac{\partial H(x_i, p_i)}{\partial x_i} \; ; \; \dot{x}_i = +\frac{\partial H(x_i, p_i)}{\partial p_i}$$

→ So far, so good! ⇒ let's quantize:

• 3. Quantization in the Extended (x-p-X-P) Phase Space

■ Postulates to quantize the extended classical phase space theory

▲ **Postulate #1**: The classical c-numbers $\{x_i, p_i, X_i, P_i\}$

→ operators: $x \to \hat{x}$, $p \to \hat{p}$, $X \to \hat{X}$, $P \to \hat{P}$

with the following canonical commutation relations:

$$[\hat{P}_i, \hat{x}_j] = -i\hbar\delta_{ij} \; ; \; [\hat{X}_i, \hat{p}_j] = -i\hbar\delta_{ij} \tag{17a}$$

Note sign! (and see below*)

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = [\hat{x}_i, \hat{p}_j] = 0 \tag{17b}$$

$$[\hat{X}_i, \hat{X}_j] = [\hat{P}_i, \hat{P}_j] = [\hat{X}_i, \hat{P}_j] = 0 \tag{17c}$$

$$[\hat{X}_i, \hat{x}_j] = [\hat{P}_i, \hat{p}_j] = 0 \tag{17d}$$

– The operators $\{\hat{x}, \hat{p}, \hat{X}, \hat{P}, \hat{\mathbb{1}}\}$ thus form a representation of the Heisenberg-Weyl group, $W(2,\mathbb{R})$ or, more generally, $\{\hat{x}_i, \hat{p}_i, \hat{X}_i, \hat{P}_i, \hat{\mathbb{1}}\} \to W(2n, \mathbb{R})$ with $i = 1, 2, \cdots, n$

* NOTE: One may compare the commutation relations (17a-d) with the more usual $[\hat{x}_i, \hat{p}_j] = +i\hbar\delta_{ij}$ in the usual Hilbert space. We note particularly the "wrong sign" (in the usual convention) in the second of Eqs. (17a) because we now treat $\hat{x}_i, \hat{p}_i$ on an equal footing as generalized (phase-space) coordinates, with $\hat{P}_i, \hat{X}_i$ as the corresponding conjugate generalized momenta. However, if we wish to do so later, we can easily regain complete equivalence with the more usual $[\hat{x}_i, \hat{p}_i] = +i\hbar\delta_{ij}$ by making a parity transformation,

$$\hat{X}_i \to \hat{X}_i' = -\hat{X}_i$$

▲ Postulate # 2:

– The Wigner quantum phase space $\mathcal{P}$ is the function space of all (square-)integrable complex functions $\omega(x,p)$ of the 2 real variables (x,p), viz:

$$\mathcal{P} \equiv \left\{ \omega(x,p) \,\middle|\, \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \, |\omega(x,p)|^2 < \infty \right\} \tag{18}$$

– A realization of the algebra (I) in $\mathcal{P}$ is thus

$$\hat{x}_i \to x_i \,, \quad \hat{p}_i \to p_i \,, \quad \hat{X}_i \to -i\hbar \frac{\partial}{\partial p_i} \,, \quad \hat{P}_i \to -i\hbar \frac{\partial}{\partial x_i} \tag{19}$$

(Note: once again, beware this sign (& see previous note*).)

– The Weyl quantum phase space $\tilde{\mathcal{P}}$ is, similarly

$$\tilde{\mathcal{P}} \equiv \left\{ \tilde{\omega}(X,P) \,\middle|\, \int_{-\infty}^{\infty} dX \int_{-\infty}^{\infty} dP \, |\tilde{\omega}(X,P)|^2 < \infty \right\} \tag{20}$$

where, for the moment, we leave open any mappings $\omega(x,p) \leftrightarrow \tilde{\omega}(X,P)$

– A realization of the commutation algebra (I) in $\tilde{\mathcal{P}}$ is thus

$$\hat{x}_i \to +i\hbar \frac{\partial}{\partial P_i} \,, \quad \hat{p}_i \to +i\hbar \frac{\partial}{\partial X_i} \,, \quad \hat{X}_i \to X_i \,, \quad \hat{P}_i \to P_i \tag{21}$$

(Note: in $\tilde{\mathcal{P}}$: $\hat{x}_i$ has the "correct" sign, but now $\hat{p}_i$ has the "wrong" sign, again because of the same "wrong" sign for $\hat{X}_i$, as before.)

– Inner Products are defined as expected in $\mathcal{P}$ and $\tilde{\mathcal{P}}$:

$$(\omega_1|\omega_2) \equiv \iint \frac{dx\,dp}{2\pi\hbar} \, \omega_1^*(x,p)\,\omega_2(x,p) \;; \quad \omega_1, \omega_2 \in \mathcal{P} \tag{22a}$$

$$(\tilde{\omega}_1|\tilde{\omega}_2) \equiv \iint \frac{dX\,dP}{2\pi\hbar} \, \tilde{\omega}_1^*(X,P)\,\tilde{\omega}_2(X,P) \;; \quad \tilde{\omega}_1, \tilde{\omega}_2 \in \tilde{\mathcal{P}} \tag{22b}$$

▲ Postulate # 3: The extended Schrödinger equation in $\mathcal{P}$

We postulate that the quantum phase-space function, $\rho \in \mathcal{P}$, satisfies the extended Schrödinger equation:

$$\hat{G}\rho = i\hbar\frac{\partial\rho}{\partial t} \quad ; \quad \rho = \rho(x,p,t) \in \mathcal{P} \tag{23a}$$

— now, use of Eqs. (14a), (19) $\Rightarrow$

$$\boxed{\left[H\left(x_i, p_i - i\hbar\frac{\partial}{\partial x_i}\right) - H\left(x_i - i\hbar\frac{\partial}{\partial p_i}, p_i\right)\right]\rho(x_i,p_i,t) = i\hbar\frac{\partial\rho(x_i,p_i,t)}{\partial t}} \tag{23b}$$

Note: Ordering Ambiguity

With the operator arguments in the Hamiltonians in Eq. (23b) we have the usual ambiguity about the orderings of products of factors in the expansion of $H(x_i,p_i)$ — although the problem disappears if $\hat{H} \to \frac{\hat{p}^2}{2m} + V(\hat{x})$, as usual. In the more general case, let's take however as a working hypothesis that each H is ordered so that the derivatives do not act internally, but rather act purely to the right, i.e., directly on ρ itself. In that case we may expand Eq. (23b) to give:

$$\boxed{\sum_{n=1}^{\infty}\frac{(-i\hbar)^n}{n!}\left[\frac{\partial^n H}{\partial p_i^n}\frac{\partial^n\rho}{\partial x_i^n} - \frac{\partial^n H}{\partial x_i^n}\frac{\partial^n\rho}{\partial p_i^n}\right] = i\hbar\frac{\partial\rho}{\partial t}} \tag{23c}$$

Note: Physically admissible solutions

We also defer till later the necessary imposition of conditions that solutions of the extended Schrödinger equation (23) need to fulfill in order to be physically admissible (i.e., not all solutions of Eq. (23) will necessarily be physically admissible)

▲ **Postulate #4: Expectation values**

In $\mathcal{P}$ operators $f(\hat{x},\hat{p})$ are simply c-numbers $f(x,p)$. We postulate that their expectation values are:

$$\boxed{\langle f\rangle = \iint\frac{dx\,dp}{2\pi\hbar}f(x,p)\rho(x,p,t)} \tag{24}$$

– putting $f=1$ $\Rightarrow$

normalization condition
$$\boxed{\iint \frac{dx\,dp}{2\pi\hbar}\,\rho(x,p,t)=1} \qquad (25)$$

Note: Once again we have an ordering ambiguity which will need to be resolved later, i.e., the definition of $f(\hat{x},\hat{p})$ is ambiguous in cases where, for example, $\hat{x}\to x$, $\hat{p}\to -i\hbar\frac{d}{dx}$ as in the x-representation of ordinary Q.M.

Solution of the extended Schrödinger equation (23)

Clue: The presence in Eq. (7) for the extended classical Lagrangian of the total derivative $-\frac{d}{dt}(x_i p_i)$ strongly suggests the appearance of a phase factor $\exp(-ix_ip_i/\hbar)$ in the solution for $\rho(x,p,t)$
$\Rightarrow$ let's try a solution of the form:

$$\rho(x_i,p_i,t)=f(x_i,p_i,t)\,e^{-i\vec{x}\cdot\vec{p}/\hbar} \qquad (26)$$

– we now easily see that

(1) $\left(p_i-i\hbar\frac{\partial}{\partial x_i}\right)\rho(x_i,p_i,t)=\left[\cancel{p_if}-i\hbar\frac{\partial f}{\partial x_i}\cancel{-i\hbar f\left(\frac{-ip_i}{\hbar}\right)}\right]e^{\frac{-ix_ip_i}{\hbar}}$

$$\Rightarrow\quad \left(p_i-i\hbar\frac{\partial}{\partial x_i}\right)\rho=-i\hbar e^{-ix_ip_i/\hbar}\frac{\partial f}{\partial x_i} \qquad (27a)$$

(2) and similarly:

$$\left(x_i-i\hbar\frac{\partial}{\partial p_i}\right)\rho=-i\hbar e^{-ix_ip_i/\hbar}\frac{\partial f}{\partial p_i} \qquad (27b)$$

– Equations (27a, b) $\Rightarrow$

$$H\left(x_i,p_i-i\hbar\frac{\partial}{\partial x_i}\right)\rho=e^{-ix_ip_i/\hbar}H\left(x_i,-i\hbar\frac{\partial}{\partial x_i}\right)f \qquad (28a)$$

$$H\left(x_i-i\hbar\frac{\partial}{\partial p_i},p_i\right)\rho=e^{-ix_ip_i/\hbar}H\left(-i\hbar\frac{\partial}{\partial p_i},p_i\right)f \qquad (28b)$$

where we have made the same assumptions as before about the ordering of operators inside the Hamiltonians

– now insert Eqs. (28a, b) into Eq. (23)

$\Longrightarrow$

$$\left[H\left(x_i, -i\hbar\frac{\partial}{\partial x_i}\right) - H\left(-i\hbar\frac{\partial}{\partial p_i}, p_i\right)\right] f(x_i, p_i; t) = i\hbar \frac{\partial f(x_i, p_i, t)}{\partial t} \qquad (29)$$

– Clearly, by inspection, Eq. (29) has separable solutions

$$f(x_i, p_i; t) = \psi_\alpha(x_i, t)\,\eta_\beta(p_i, t) \qquad (30)$$

where ψ_α and η_β satisfy:

$$H\left(x_i, -i\hbar\frac{\partial}{\partial x_i}\right)\psi_\alpha(x, t) = i\hbar\frac{\partial \psi_\alpha(x_i, t)}{\partial t} \qquad (31a)$$

$$H\left(-i\hbar\frac{\partial}{\partial p_i}, p_i\right)\eta_\beta(p_i, t) = -i\hbar\frac{\partial \eta_\beta(p_i, t)}{\partial t} \qquad (31b)$$

– Note 1: Eq. (31a) is simply the usual Schrödinger equation for the ket state: $\hat{H}|\alpha\rangle = i\hbar\frac{\partial}{\partial t}|\alpha\rangle$ (32a)
in the x-representation where

$$\langle x_i|\alpha\rangle \equiv \psi_\alpha(x_i, t) \qquad (33a)$$

and with $\hat{p}_i = -i\hbar\frac{\partial}{\partial x_i}, \hat{x}_i \to x_i \Rightarrow [\hat{x}_i, \hat{p}_j] = +i\hbar\delta_{ij}$ (34a)

– Note 2: By taking the complex conjugate of Eq. (31b) and using the Hermiticity of $\hat{H}$ $\Rightarrow$

$$H\left(i\hbar\frac{\partial}{\partial p_i}, p_i\right)\eta^*_\beta(p_i, t) = +i\hbar\frac{\partial \eta^*_\beta(p_i, t)}{\partial t}$$

which is simply the usual Schrödinger equation for the ket state $\hat{H}|\beta\rangle = i\hbar\frac{\partial}{\partial t}|\beta\rangle$ (32b)
in the p-representation where

$$\langle p_i|\beta\rangle \equiv \tilde{\psi}_\beta(p_i, t) \qquad (33b)$$

and with $\hat{x}_i = +i\hbar\frac{\partial}{\partial p_i}, \hat{p}_i \to p_i \Rightarrow [\hat{x}_i, \hat{p}_j] = +i\hbar\delta_{ij}$ (34b)

$$\Rightarrow \eta_\beta(p_i, t) = \tilde{\psi}^*_\beta(p_i, t) \qquad (35)$$

– Note 3: momentum eigenstates (plane waves)
– be careful with signs of phases (important!)

$$\hat{p}_i|p_i\rangle = p_i|p_i\rangle \qquad (36)$$

$$\Rightarrow \langle x_i|\hat{p}_i|p\rangle = p_i\langle x_i|p_i\rangle \Rightarrow -i\hbar\frac{\partial}{\partial x_i}\langle x_i|p_i\rangle = p_i\langle x_i|p_i\rangle$$

$$\Rightarrow \boxed{\langle x_i|p_i\rangle = \text{const.} \times e^{+ix_ip_i/\hbar}} \tag{37}$$

$\Rightarrow$ our convention: const. = 1

- Fourier transforms

$$\tilde{\psi}_\beta(p_i) \equiv \langle p_i|\beta\rangle = \int_{-\infty}^{\infty} dx_i \langle p_i|x_i\rangle\langle x_i|\beta\rangle$$

$$\Rightarrow \tilde{\psi}_\beta(p_i) = \int_{-\infty}^{\infty} dx_i\, e^{-ip_ix_i/\hbar}\,\psi_\beta(x_i) \tag{38a}$$

$$\Leftrightarrow \psi_\beta(x_i) = \int_{-\infty}^{\infty} \frac{dp_i}{2\pi\hbar}\, e^{+ip_ix_i/\hbar}\,\tilde{\psi}_\beta(p_i) \tag{38b}$$

- Finally, Eqs. (26), (30) and (35) $\Rightarrow$

the extended Schrödinger equation (23) has solutions:

$$\boxed{\rho(x_i,p_i,t) = \psi_\alpha(x_i,t)\tilde{\psi}_\beta^*(p_i,t)e^{-ip_ix_i/\hbar}} \tag{39}$$

- General solution

Since the extended Schrödinger equation (23) is linear, we have the general solution:

$$\boxed{\rho(x_i,p_i,t) = r_{\alpha\beta}\,\psi_\alpha(x_i,t)\,\tilde{\psi}_\beta(p_i,t)e^{-ip_ix_i/\hbar}} \tag{40}$$

summation convention implied

Note: We still need later to put conditions on the matrix $r_{\alpha\beta}$ for $\rho(x_i,p_i,t)$ to be physically admissible.

- Normalization: insert Eq. (40) into Eq. (25) $\rightarrow$

$$r_{\alpha\beta}\int_{-\infty}^{\infty} dx\,\psi_\alpha(x,t)\underbrace{\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\tilde{\psi}_\beta^*(p,t)e^{-ipx/\hbar}}_{=\psi_\beta^*(x,t) \text{ from Eq. (38b)}} = 1$$

$$\Rightarrow r_{\alpha\beta}\int_{-\infty}^{\infty} dx\,\psi_\alpha(x,t)\psi_\beta^*(x,t) = 1$$

Assume the set $\{\psi_\alpha\}$ is orthonormalized $\Rightarrow$

$$\Leftrightarrow \boxed{\begin{aligned} &\int_{-\infty}^{\infty} dx\, \psi_\alpha(x,t)\psi_\beta^*(x,t) = \delta_{\alpha\beta} \\ &\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \tilde{\psi}_\alpha(p,t)\tilde{\psi}_\beta^*(p,t) = \delta_{\alpha\beta} \end{aligned}} \tag{41}$$

$\Rightarrow$ normalization of $\rho(x,p,t)$ $\Rightarrow$ $\boxed{r_{\alpha\alpha} \equiv \mathrm{tr}\, r = 1}$ (42)

- Some notations and definitions

(1) x-space projector:

$$\Rightarrow \boxed{\begin{aligned} &\hat{P}_x \equiv |x\rangle\langle x| \\ &\int_{-\infty}^{\infty} dx\, \hat{P}(x) = \hat{\mathbb{1}} \end{aligned}} \tag{43}$$

(2) p-space projector

$$\Rightarrow \boxed{\begin{aligned} &\hat{P}_p \equiv |p\rangle\langle p| \\ &\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \hat{P}(p) = \hat{\mathbb{1}} \end{aligned}} \tag{44}$$

(3) density operator

$$\boxed{\hat{\rho} = \hat{\rho}(t) \equiv r_{\alpha\beta}\, |\alpha,t\rangle\langle\beta,t|} \tag{45}$$

Equations (43)–(45) $\Rightarrow$

$$\begin{aligned} \mathrm{Tr}\left(\hat{P}_x \hat{\rho} \hat{P}_p\right) &= \mathrm{Tr}\left(|x\rangle\langle x|\, r_{\alpha\beta}\, |\alpha\rangle\langle\beta|p\rangle\langle p|\right) \\ &= r_{\alpha\beta}\, \langle x|\alpha\rangle\langle\beta|p\rangle\langle p|x\rangle \\ &= r_{\alpha\beta}\, \psi_\alpha(x,t)\tilde{\psi}_\beta^*(p,t)\, e^{-ipx/\hbar} = \rho(x,p,t) \end{aligned}$$

$$\Rightarrow \boxed{\begin{aligned} \rho(x,p,t) &= \mathrm{Tr}\left(\hat{P}_x \hat{\rho} \hat{P}_p\right) \\ &= \langle x|\hat{\rho}|p\rangle\langle p|x\rangle \end{aligned}} \tag{46}$$

Note: normalization, Eqs. (25), (42) $\Rightarrow$

$$\boxed{\mathrm{Tr}\, \hat{\rho} = \mathrm{tr}\, r = 1} \tag{47}$$

(4) energy eigenfunctions

Equations (31a, b) have energy eigenfunction solutions →

$$\psi_\alpha(x,t) = \psi_\alpha(x)\, e^{-iE_\alpha t/\hbar} \;:\; H(x_i, -i\hbar \tfrac{\partial}{\partial x_i})\psi_\alpha(x_i) = E_\alpha \psi_\alpha(x_i)$$

$$\eta_\beta(p,t) = \tilde{\psi}^*_\beta(p)\, e^{+iE_\beta t/\hbar} \;:\; H(-i\hbar \tfrac{\partial}{\partial p_i}, p_i)\tilde{\psi}^*_\beta(p_i) = E_\beta \tilde{\psi}^*_\beta(p_i)$$

Hence, in terms of energy eigenfunctions:

$$\rho(x,p,t) = \rho_{\alpha\beta}(t)\,\psi_\alpha(x)\,\tilde{\psi}^*_\beta(p)\, e^{-ixp/\hbar} \qquad (48)$$

$$\rho_{\alpha\beta}(t) \equiv r_{\alpha\beta}\, e^{-i(E_\alpha - E_\beta)t/\hbar} \qquad (49)$$

and Eq. (47) ⇒

normalization $\quad \boxed{\mathrm{Tr}\,\hat{\rho}(t) = \rho_{\alpha\alpha} = \mathrm{tr}\,\rho(t) = 1} \qquad (50)$

— Before proceeding further with the formalism, let's look at 3 different "correspondence principles" in order to shed more light on where we now stand →

▪ (1) Classical correspondence

— In the limit $\hbar \to 0$, the extended Schrödinger eqn. (23c) →

$$\boxed{\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0} \qquad (51)$$

where $\{A,B\} \equiv \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}$ is usual Poisson bracket

— Eq. (51) is the usual Liouville equation of (equilibrium or non-equilibrium) classical statistical mechanics

— Note: Eq. (51) may have complex or real non-positive solutions, but the physically admissible solutions are interpreted as classical probability densities ⇒ we permit only the real positive solutions

– Note: The classical limit is obtained very transparently.

– Note: IMPORTANT! Quite unlike the usual classical derivation where one considers a system of many degrees of freedom or an ensemble, our derivation has nowhere introduced any such concepts. In the usual classical stat. mech. the notion of probability is by choice (i.e., we choose not to solve the entire system exactly, but instead assign probabilities to circumvent a complete solution). By contrast, in our above derivation, although we take the $\hbar \to 0$ limit, the quantum mechanics (with its inherent and inescapable ideas of uncertainties, probabilities, etc.) has not disappeared altogether in this limit. Thus, the statistical aspect of classical statistical mechanics has not arisen by choice (via ensemble theory, etc.), but has arisen intrinsically due to the "remaining inescapable shadow of Q.M." (c.f., the Cheshire Cat's grin!) even in the $\hbar \to 0$ limit.

(2) Pure state quantum mechanics correspondence

– When we set $\rho_{\alpha\beta} \to \delta_{\alpha\beta}$; i.e., $\rho \to |\alpha\rangle\langle\alpha|$, we expect to regain all the usual results of (pure state) Q.M $\leftrightarrow$ nothing lost and nothing gained?

– In fact, not quite so, as we'll see $\to$ since we do gain a better understanding of what $f(x,p)$ means, for example, with regard to the ordering ambiguity in Eq. (24), as we now show $\to$

– Equations (24) and (46) $\Rightarrow$

$$\langle f\rangle = \iint \frac{dx\,dp}{2\pi\hbar}\, \rho(x,p,t)\, f(x,p)$$

$$= \iint \frac{dx\,dp}{2\pi\hbar} \langle x|\hat{\rho}|p\rangle\langle p|x\rangle f(x,p)$$

Now, let us write $f(x,p) \to f_s(x,p)$ where

$$\boxed{\langle p|f_s(\hat{x},\hat{p})|x\rangle \equiv f_s(x,p)\langle p|x\rangle} \qquad (52a)$$

$$\Rightarrow \langle f_s \rangle = \iint \frac{dx\,dp}{2\pi\hbar} \langle x|\hat{\rho}|p\rangle\langle p|f_s(\hat{x},\hat{p})|x\rangle$$

$$\Rightarrow \boxed{\langle f_s \rangle = \mathrm{Tr}(\hat{\rho}\hat{f}_s)} \quad \text{as expected!} \qquad (52b)$$

– Clearly, Eqs. (52a,b) are consistent iff $f_s(\hat{x},\hat{p}) = :f_s(\hat{x},\hat{p}):$ where the standard ordering operation $: \;:$ means (by definition) that all operators $\hat{p}$ stand to the left of all operators $\hat{x}$ in every term.

– We can now easily show that, with this identification of the ordering, we regain the usual pure-state QM in <u>either</u> the x-space representation <u>or</u> the p-space representation.

Thus, put $\rho_{\alpha\beta} = \delta_{\alpha\beta}$

$$\Rightarrow \langle f_s \rangle = \iint \frac{dx\,dp}{2\pi\hbar} \psi_\alpha(x)\tilde{\psi}^*_\alpha(p) e^{-ipx/\hbar} f_s(x,p)$$

With no loss of generality, put $f_s(\hat{x},\hat{p}) = P(\hat{p})Q(\hat{x})$

$$\Rightarrow \langle P(\hat{p})Q(\hat{x})\rangle = \iint \frac{dx\,dp}{2\pi\hbar} \psi_\alpha(x)\tilde{\psi}^*_\alpha(p) e^{-ipx/\hbar} P(p)Q(x) \qquad (53)$$

– So, first, in the x-space representation, Eq (53) $\Rightarrow$

$$\langle P(\hat{p})Q(\hat{x})\rangle = \iint \frac{dx\,dp}{2\pi\hbar} \psi_\alpha(x)\tilde{\psi}^*_\alpha(p) Q(x) P\left(+i\hbar\frac{\partial}{\partial x}\right) e^{-ipx/\hbar}$$

simply by letting $+i\hbar\frac{\partial}{\partial x}$ act to right

$$= \int_{-\infty}^{\infty} dx\, \psi_\alpha(x) Q(x) P\left(+i\hbar\frac{\partial}{\partial x}\right) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \tilde{\psi}^*_\alpha(p) e^{-ipx/\hbar}$$

use Eq. (38b)

$$= \int_{-\infty}^{\infty} dx\, \psi_\alpha(x) Q(x) P\left(+i\hbar\frac{\partial}{\partial x}\right) \psi^*_\alpha(x)$$

integrate by parts as usual ($\leftrightarrow$ Hermiticity of $i\hbar\frac{\partial}{\partial x}$)

$$\Rightarrow \langle P(\hat{p})Q(\hat{x})\rangle = \int_{-\infty}^{\infty} dx\, \psi^*_\alpha(x) P\left(-i\hbar\frac{\partial}{\partial x}\right) Q(x)\psi_\alpha(x) \qquad (54a)$$

and Eq. (54a) is exactly the usual pure-state QM average in the x-space representation

$\Rightarrow$ our ordering procedure, $f \rightarrow f_s$, is justified

– Secondly, just to be sure(!), let's repeat in the p-space representation, where Eq. (53) →

$$\langle P(\hat{p})Q(\hat{x})\rangle = \iint \frac{dx\,dp}{2\pi\hbar}\,\psi_\alpha(x)\tilde{\psi}_\alpha^*(p)\,e^{-ipx/\hbar}\,P(p)Q(x)$$

$$= \iint \frac{dx\,dp}{2\pi\hbar}\,\psi_\alpha(x)\tilde{\psi}_\alpha^*(p)P(p)Q\left(+i\hbar\frac{\partial}{\partial p}\right)e^{-ipx/\hbar}$$

simply by letting $i\hbar\frac{\partial}{\partial p}$ act to the right

$$= \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\tilde{\psi}_\alpha^*(p)P(p)Q\left(+i\hbar\frac{\partial}{\partial p}\right)\int_{-\infty}^{\infty}dx\,\psi_\alpha(x)\,e^{-ipx/\hbar}$$

use Eq. (38a)

$$\Rightarrow \quad \langle P(\hat{p})Q(\hat{x})\rangle = \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\tilde{\psi}_\alpha^*(p)P(p)Q\left(+i\hbar\frac{\partial}{\partial p}\right)\tilde{\psi}_\alpha(p) \qquad (54b)$$

and Eq. (54b) is again the usual pure-state Q.M. average, but now in the p-space representation

—//—

Note: The pure-state $\rho(x,p,t) = \psi_\alpha(x)\tilde{\psi}_\alpha^*(p)\,e^{-ipx/\hbar}$ satisfies the suggestive relations:

$$(1)\quad \int_{-\infty}^{\infty}dx\,\rho(x,p,t) = |\tilde{\psi}_\alpha(p,t)|^2 \qquad (55a)$$

$$(2)\quad \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\rho(x,p,t) = |\psi_\alpha(x,t)|^2 \qquad (55b)$$

for pure state only

—//—

(3) Quantum statistical mechanics correspondence

– We have, from Eq. (48), $\rho(x,p,t) = \rho_{\alpha\beta}(t)\psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,e^{-ipx/\hbar}$

$$\Rightarrow \quad i\hbar\frac{\partial\rho}{\partial t} = i\hbar\dot{\rho}_{\alpha\beta}\,\psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,e^{-ipx/\hbar}$$

and, use of Eq. (23b) ⇒

$$i\hbar\dot{\rho}_{\alpha\beta}\,\psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,e^{-ipx/\hbar} = \rho_{\alpha\beta}\left[H\left(x,\,p-i\hbar\frac{\partial}{\partial x}\right) - H\left(x-i\hbar\frac{\partial}{\partial p},\,p\right)\right] \times \psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,e^{-ipx/\hbar}$$

and, use of Eqs. (27a, b) ⇒

$$i\hbar\dot{\rho}_{\alpha\beta}\,\psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,\cancel{e^{-ipx/\hbar}} = \rho_{\alpha\beta}\left[H\left(x,-i\hbar\frac{\partial}{\partial x}\right) - H\left(-i\hbar\frac{\partial}{\partial p},\,p\right)\right] \times \psi_\alpha(x)\tilde{\psi}_\beta^*(p)\,\cancel{e^{-ipx/\hbar}}$$

$\Rightarrow$

$$i\hbar \dot{\rho}_{\alpha\beta} \psi_\alpha(x) \tilde{\psi}^*_\beta(p) = \rho_{\alpha\beta}\left[H(x, -i\hbar \tfrac{\partial}{\partial x}) \psi_\alpha(x)\right] \tilde{\psi}^*_\beta(p)$$
$$- \rho_{\alpha\beta} \psi_\alpha(x) \left[H(-i\hbar \tfrac{\partial}{\partial p}, p) \psi^*_\beta(p)\right]$$

— now take $\iint \frac{dx\,dp}{2\pi\hbar} \psi^*_\kappa(x) \psi_\lambda(p) \times$ (above equation) $\Rightarrow$

$$i\hbar \dot{\rho}_{\kappa\lambda} = \rho_{\alpha\beta} \langle \kappa | \hat{H} | \alpha \rangle \delta_{\beta\lambda} - \rho_{\alpha\beta} \delta_{\alpha\kappa} \langle \beta | H | \lambda \rangle$$
$$= \rho_{\alpha\lambda} \langle \kappa | \hat{H} | \alpha \rangle - \rho_{\kappa\beta} \langle \beta | \hat{H} | \lambda \rangle$$

$\Rightarrow$
$$\boxed{i\hbar \dot{\rho}_{\kappa\lambda} = H_{\kappa\alpha} \rho_{\alpha\lambda} - \rho_{\kappa\beta} H_{\beta\lambda}} \qquad (56a)$$

or, equivalently, in the usual QM operator matrix notation,

$\Leftrightarrow$
$$\boxed{i\hbar \dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]} \qquad (56b)$$

— Equations (56a, b) are just the usual von Neumann equation for the density matrix of quantum stat. mech.

— Once again, just as for its classical analogue of Eq. (51), we need to restrict the solutions of Eq. (56) to those which are physically admissible. In particular, we require that:

(1) if $f(x,p)$ is an observable with corresponding Hermitian matrix in terms of matrix elements $\langle \alpha | f_s(x, -i\hbar \frac{\partial}{\partial x}) | \beta \rangle \equiv f_{\alpha\beta}$ (i.e., with $f_{\alpha\beta} = f^*_{\beta\alpha}$) $\Rightarrow$ the expectation value $\langle f_s \rangle$ should be real; and

(2) if $f(x,p)$ is a positive-definite observable (i.e., with $f_{\alpha\alpha} > 0,\ \forall \alpha$) $\Rightarrow$ its expectation value $\langle f_s \rangle$ should be positive definite.

— <u>Note again</u>: <u>IMPORTANT!</u> In the usual von Neumann density matrix an ensemble average is introduced; <u>cf.</u>, our derivation has involved no such averaging — the <u>only</u> averaging has involved the QM expectation value in the extended sense.

Canonical Transformations

- In the extended x-p-X-P quantum phase space we have the 4 operators $\hat{x}, \hat{p}, \hat{X}, \hat{P}$ (or, more generally, $4n$ operators $\hat{x}_i, \hat{p}_i, \hat{X}_i, \hat{P}_i$; $i = 1, 2, \cdots, n$) which obey the Heisenberg-Weyl algebra $W(2,\mathbb{R})$ (or $W(2n,\mathbb{R})$) of Eqs. (17a-d). For simplicity, let's stay with $n=1$
- Now, the 10 bilinear products $\hat{X}\hat{P}, \hat{x}\hat{p}, \hat{X}^2, \hat{P}^2, \hat{x}^2, \hat{p}^2, \hat{x}\hat{P}, \hat{p}\hat{X}, \hat{x}\hat{X}, \hat{p}\hat{P}$ form the closed algebra $Sp(4,\mathbb{R})$ under commutation. They generate canonical transformations on the basic $W(2,\mathbb{R})$ commutation relations.

  [Note: Actually these are nothing more than the most general two-mode squeezing operations]

▲ example (1): the $\hat{X}\hat{P}$ generator

- Consider the unitary operator: $\hat{U}_1 \equiv e^{i\lambda\hat{P}\hat{X}/\hbar}$; $\lambda \in \mathbb{R}$ (57)

  and consider its mode of action on $\hat{x}, \hat{p}, \hat{X}, \hat{P}$

  i.e., ask for $\hat{U}_1 \hat{\Theta} \hat{U}_1^\dagger$ for $\hat{\Theta} \to \hat{x}, \hat{p}, \hat{X}, \hat{P}$

  → use $e^A B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \cdots$ (58)

  and Eqs. (17a-d) $\Rightarrow$

$$\boxed{\begin{aligned} \hat{x}' &\equiv \hat{U}_1 \hat{x} \hat{U}_1^\dagger = \hat{x} + \lambda \hat{X} \\ \hat{p}' &\equiv \hat{U}_1 \hat{p} \hat{U}_1^\dagger = \hat{p} + \lambda \hat{P} \\ \hat{X}' &\equiv \hat{U}_1 \hat{X} \hat{U}_1^\dagger = \hat{X} \\ \hat{P}' &\equiv \hat{U}_1 \hat{P} \hat{U}_1^\dagger = \hat{P} \end{aligned}} \tag{59}$$

- We easily check that the above transformations are canonical, i.e., $\hat{x}', \hat{p}', \hat{X}', \hat{P}'$ obey the same $W(2,\mathbb{R})$ commutation relations as $\hat{x}, \hat{p}, \hat{X}, \hat{P}$ from Eq. (17)
- Under this transformation the extended Schrödinger equation for $\rho = \rho(x,p,t)$ in $\mathcal{P}$ of Eq. (23), viz.

  $\hat{G}\rho = i\hbar \frac{\partial \rho}{\partial t}$ becomes

$$(\hat{U}_1 \hat{G} \hat{U}_1^\dagger)(\hat{U}_1 \rho) = i\hbar \frac{\partial}{\partial t}(\hat{U}_1 \rho)$$

with $\hat{G} = H(\hat{x}, \hat{p}+\hat{P}) - H(\hat{x}+\hat{X}, \hat{P})$

$$\Rightarrow \hat{U}_1 \hat{G} \hat{U}_1^\dagger = H(\hat{x}+\lambda\hat{X}, \hat{p}+(\lambda+1)\hat{P}) - H(\hat{x}+(\lambda+1)\hat{X}, \hat{p}+\lambda\hat{P}) \quad (60a)$$

Thus, in the Wigner quantum phase space $\mathcal{P}$

$$\hat{U}_1 \hat{G} \hat{U}_1^\dagger = H\left(x - i\hbar\lambda\frac{\partial}{\partial p}, p - i\hbar(\lambda+1)\frac{\partial}{\partial x}\right) - H\left(x - i\hbar(\lambda+1)\frac{\partial}{\partial p}, p - i\hbar\lambda\frac{\partial}{\partial x}\right) \quad (60b)$$

and in the space $\mathcal{P}$ we put

$$\boxed{\begin{aligned} &\hat{U}_1 \rho(x,p,t) \equiv W_\lambda(x,p,t) && (61a) \\ \Rightarrow\ &W_\lambda(x,p,t) = \exp\left(-i\hbar\lambda\frac{\partial^2}{\partial x \partial p}\right)\rho(x,p,t) && (61b) \end{aligned}}$$

– let's just evaluate Eq. (61b) $\Rightarrow$

$$W_\lambda(x,p,t) = \rho_{\alpha\beta}(t) \exp\left(-i\hbar\lambda\frac{\partial^2}{\partial x\partial p}\right)\left(\psi_\alpha(x)\tilde{\psi}_\beta^*(p) e^{-ipx/\hbar}\right)$$

↙ use Eq. (38a)

$$= \rho_{\alpha\beta}\int_{-\infty}^{\infty} dx' \psi_\beta^*(x') \exp\left(-i\hbar\lambda\frac{\partial^2}{\partial x \partial p}\right)\left(\psi_\alpha(x) e^{ip(x'-x)/\hbar}\right)$$

$$= \rho_{\alpha\beta}\int_{-\infty}^{\infty} dx' \psi_\beta^*(x')\left[1 + \lambda(x'-x)\frac{\partial}{\partial x} + \frac{\lambda^2}{2!}(x'-x)^2\frac{\partial^2}{\partial x^2} + \dots\right] \times \left(\psi_\alpha(x) e^{ip(x'-x)/\hbar}\right)$$

→ change integration variables: $x' = x - y$

$$= \rho_{\alpha\beta}\int_{-\infty}^{\infty} dy\, e^{-ipy/\hbar}\left[1 - \lambda y\frac{\partial}{\partial x} + \frac{\lambda^2 y^2}{2!}\frac{\partial^2}{\partial x^2} + \dots\right]\left(\psi_\alpha(x)\psi_\beta^*(x-y)\right)$$

$\Rightarrow$

$$\boxed{W_\lambda(x,p,t) = \rho_{\alpha\beta}(t)\int_{-\infty}^{\infty} dy\, e^{-ipy/\hbar}\psi_\alpha(x-\lambda y)\psi_\beta^*(x-(\lambda+1)y)} \quad (62)$$

$$\Rightarrow [W_\lambda(x,p,t)]^* = \rho_{\alpha\beta}^*\int_{-\infty}^{\infty} dy\, e^{ipy/\hbar}\psi_\alpha^*(x-\lambda y)\psi_\beta(x-(\lambda+1)y)$$

Use Eq. (45) and $\hat{\rho} = \hat{\rho}^\dagger \Rightarrow \rho_{\alpha\beta}^* = \rho_{\beta\alpha}$ (Hermitian)

$$\Rightarrow [W_\lambda(x,p,t)]^* = \rho_{\beta\alpha}\int_{-\infty}^{\infty} dy\, e^{ipy/\hbar}\psi_\beta(x-(\lambda+1)y)\psi_\alpha^*(x-\lambda y)$$

– now put $\alpha \rightleftarrows \beta$; $y \to -y$

$$\Rightarrow [W_\lambda(x,p,t)]^* = \rho_{\alpha\beta} \int_{-\infty}^{\infty} dy\, e^{-ipy/\hbar}\, \psi_\alpha(x+(\lambda+1)y)\psi_\beta^*(x+\lambda y)$$

– compare with Eq. (62) $\Rightarrow$

$$\boxed{[W_\lambda(x,p,t)]^* = W_{-\lambda-1}(x,p,t)} \qquad (63)$$

– special case (1) : $\lambda = -1$

put $\lambda = 0$ in Eq. (63) $\Rightarrow$

$$W_{-1}(x,p,t) = [W_0(x,p,t)]^* = [\rho(x,p,t)]^* \qquad (64a)$$

– special case (2) : $\lambda = -\frac{1}{2}$

Eq. (62) $\Rightarrow$

$$\boxed{W_{-\frac{1}{2}}(x,p,t) \equiv W(x,p,t) = \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} dX\, e^{-ipX/\hbar}\, \psi_\alpha(x+\tfrac{1}{2}X)\psi_\beta^*(x-\tfrac{1}{2}X)} \qquad (64b)$$

– which is just the usual Wigner function associated with the density operator $\hat{\rho}$ → how wonderful! Excellent!

– Wigner and Weyl functions

– From the class of unitarily equivalent solutions $\{W_\lambda(x,p,t) \mid \lambda \in \mathbb{R}\}$, the Wigner function (with $\lambda = -\frac{1}{2}$) is unique in being real (c.f., Eq. (63)). Indeed, this is precisely why Wigner chose it originally, since it satisfies the same marginal relations (55a, b) as $\rho(x,p,t)$ for the pure-state case (viz., $\rho_{\alpha\beta} \to \delta_{\alpha\beta}$)

$$\left.\begin{array}{l} (1) \displaystyle\int_{-\infty}^{\infty} dx\, W(x,p,t) = |\tilde{\chi}_\alpha(p)|^2 \\[2ex] (2) \displaystyle\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, W(x,p,t) = |\psi_\alpha(x)|^2 \end{array}\right\} \text{for pure state only}$$

and thus acts as a quasiprobability distribution in x-p phase space, although it turns out $W(x,p)$ can be negative. In fact, we can show →

$$\boxed{-2 \leq W(x,p,t) \leq 2} \qquad \forall\, \rho(x,p,t) \tag{65}$$

– The Wigner function of Eq. (64b) can be written in either of the forms:

$$\boxed{\begin{aligned} W(x,p,t) &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} d\underline{X}\, e^{-ip\underline{X}/\hbar}\, \psi_\alpha(x+\tfrac{1}{2}\underline{X})\, \psi^*_\beta(x-\tfrac{1}{2}\underline{X}) \\ &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} \frac{d\underline{P}}{2\pi\hbar}\, e^{+ix\underline{P}/\hbar}\, \tilde{\psi}_\alpha(p+\tfrac{1}{2}\underline{P})\, \tilde{\psi}^*_\beta(p-\tfrac{1}{2}\underline{P}) \end{aligned}} \tag{66}$$

– The Fourier transform of the Wigner function is defined to be the Weyl function:

$$\boxed{\tilde{W}(\underline{X},\underline{P},t) \equiv \iint_{-\infty}^{\infty} \frac{dx\,dp}{2\pi\hbar}\, e^{-i(\underline{P}x+\underline{X}p)/\hbar}\, W(x,p,t)} \tag{67}$$

Using Eq. (66) it is easy to show the explicit forms:

$$\boxed{\begin{aligned} \tilde{W}(\underline{X},\underline{P},t) &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} dx\, e^{-i\underline{P}x/\hbar}\, \psi_\alpha(x-\tfrac{1}{2}\underline{X})\, \psi^*_\beta(x+\tfrac{1}{2}\underline{X}) \\ &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{-i\underline{X}p/\hbar}\, \tilde{\psi}_\alpha(p+\tfrac{1}{2}\underline{P})\, \tilde{\psi}^*_\beta(p-\tfrac{1}{2}\underline{P}) \end{aligned}} \tag{68a}$$

– which may be made even more 'symmetric' with respect to Eq. (66) by letting $\underline{X} \to -\underline{X}$ (and recall our earlier discussion on p. 6 about the coordinates $\underline{X}_i$ having a "wrong" sign!) $\Rightarrow$

$$\boxed{\begin{aligned} \tilde{W}(-\underline{X},\underline{P},t) &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} dx\, e^{-i\underline{P}x/\hbar}\, \psi_\alpha(x+\tfrac{1}{2}\underline{X})\, \psi^*_\beta(x-\tfrac{1}{2}\underline{X}) \\ &= \rho_{\alpha\beta}(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{+i\underline{X}p/\hbar}\, \tilde{\psi}_\alpha(p+\tfrac{1}{2}\underline{P})\, \tilde{\psi}^*_\beta(p-\tfrac{1}{2}\underline{P}) \end{aligned}} \tag{68b}$$

Note: for this reason many authors call $\tilde{W}(-\underline{X},\underline{P})$ the Weyl transform

– More generally, since $\hat{\rho} \equiv \rho_{\alpha\beta}(t)\,|\alpha\rangle\langle\beta|$, we may write Eq. (66) as

$$W(x,p,t) \equiv W(\hat{\rho}(t);x,p) \tag{69}$$

where we extend the definition to give the Wigner representation of an arbitrary operator $\hat{\Theta}$ as:

$$\boxed{\begin{aligned} W(\hat{\Theta};x,p) &\equiv \int_{-\infty}^{\infty} dX\, e^{-ipX/\hbar}\, {}_x\langle x+\tfrac{1}{2}X|\hat{\Theta}|x-\tfrac{1}{2}X\rangle_x \\ &= \int_{-\infty}^{\infty} \frac{dP}{2\pi\hbar}\, e^{+ixP/\hbar}\, {}_p\langle p+\tfrac{1}{2}P|\hat{\Theta}|p-\tfrac{1}{2}P\rangle_p \end{aligned}} \tag{70}$$

with their 2D Fourier transforms defining the corresponding Weyl representations:

$$\boxed{\tilde{W}(\hat{\Theta};X,P) \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dx\,dp}{2\pi\hbar}\, e^{-i(Px+Xp)/\hbar}\, W(\hat{\Theta};x,p)} \tag{71}$$

$\Rightarrow$

$$\boxed{\begin{aligned} \tilde{W}(\hat{\Theta};-X,P) &= \int_{-\infty}^{\infty} dx\, e^{-iPx/\hbar}\, {}_x\langle x+\tfrac{1}{2}X|\hat{\Theta}|x-\tfrac{1}{2}X\rangle_x \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{+iXp/\hbar}\, {}_p\langle p+\tfrac{1}{2}P|\hat{\Theta}|p-\tfrac{1}{2}P\rangle_p \end{aligned}} \tag{72}$$

– We can also show that expectation values of operators can equivalently be written as:

$$\boxed{\begin{aligned} \langle\hat{\Theta}\rangle &\equiv \mathrm{Tr}(\hat{\rho}\,\hat{\Theta}) \\ &= \iint \frac{dx\,dp}{2\pi\hbar}\, \rho(x,p,t)\,\Theta_s(x,p) \\ &= \iint \frac{dx\,dp}{2\pi\hbar}\, \underbrace{W(x,p,t)}_{\equiv\, W(\hat{\rho}(t);x,p)}\, W(\hat{\Theta};x,p) \end{aligned}} \tag{73}$$

– We can easily derive the properties:

$$\boxed{\begin{aligned}\int_{-\infty}^{\infty} dx\, W(\hat{\theta};x,p) &= \langle p|\hat{\theta}|p\rangle \\ \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} W(\hat{\theta};x,p) &= \langle x|\hat{\theta}|x\rangle \\ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dx\,dp}{2\pi\hbar} W(\hat{\theta};x,p) &= \mathrm{Tr}(\hat{\theta})\end{aligned}} \quad (74a)$$

$$\boxed{\begin{aligned}\int_{-\infty}^{\infty} d\underline{X}\, \tilde{W}(\hat{\theta};\underline{X},\underline{P}) &= \langle \tfrac{1}{2}\underline{P}|\hat{\theta}|-\tfrac{1}{2}\underline{P}\rangle \\ \int_{-\infty}^{\infty} \frac{d\underline{P}}{2\pi\hbar} \tilde{W}(\hat{\theta};\underline{X},\underline{P}) &= \langle -\tfrac{1}{2}\underline{X}|\hat{\theta}|\tfrac{1}{2}\underline{X}\rangle \\ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{d\underline{X}\,d\underline{P}}{2\pi\hbar} \tilde{W}(\hat{\theta};\underline{X},\underline{P}) &= W(0,0)\end{aligned}} \quad (74b)$$

$$\boxed{\begin{aligned}&[W(\hat{\theta};x,p)]^* = W(\hat{\theta};x,p) \Rightarrow \\ &W(\hat{\theta};x,p) \in \mathbb{R} \text{ if } \hat{\theta} = \hat{\theta}^\dagger\end{aligned}} \quad (75a)$$

$$\boxed{[\tilde{W}(\hat{\theta};-\underline{X},-\underline{P})]^* = \tilde{W}(\hat{\theta}^\dagger;\underline{X},\underline{P})} \quad (75b)$$

– Let's now return to our extended Schrödinger equation (23) but now work instead in the Weyl quantum phase space $\tilde{\mathcal{P}}$ rather than the Wigner quantum phase space $\mathcal{P}$ we've looked at so far →

$$\hat{G}\tilde{\rho} = i\hbar \frac{\partial \tilde{\rho}}{\partial t} \; ; \; \tilde{\rho} = \tilde{\rho}(\underline{X},\underline{P},t) \in \tilde{\mathcal{P}} \quad (76a)$$

$\Rightarrow$

$$\left[H\left(i\hbar\frac{\partial}{\partial P_i}, i\hbar\frac{\partial}{\partial X_i} + P_i\right) - H\left(i\hbar\frac{\partial}{\partial P_i} + X_i, i\hbar\frac{\partial}{\partial X_i}\right)\right]\tilde{\rho}(X_i,P_i,t) = i\hbar\frac{\partial\tilde{\rho}(X_i,P_i,t)}{\partial t} \quad (76b)$$

which is difficult to solve directly; but →

Clearly $\tilde{\rho}(X_i, P_i, t)$ is the 2D Fourier transform of $\rho(x_i, p_i, t)$ as expected

$$\boxed{\tilde{\rho}(X,P,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dx\,dp}{2\pi\hbar}\, \rho(x,p,t)\, e^{-i(Px+Xp)/\hbar}} \qquad (77)$$

By inserting the solution (48) into Eq. (77) we find the explicit solution:

$$\boxed{\tilde{\rho}(X,P,t) = e^{\frac{i}{2\hbar}PX}\, \tilde{W}(X,P,t)} \qquad (78)$$

in terms of the Weyl function of Eq. (68a)

[Note: Eq. (78) also follows directly from Eq. (61) with $\lambda = -1/2$, viz.

$$\rho(x,p,t) = e^{\frac{i}{2\hbar}\hat{P}\hat{X}}\, W(x,p,t)$$
]

— We can now proceed to explore also the other 9 canonical transformations generated by the 9 remaining $Sp(4,\mathbb{R})$ generators

→ also very interesting! (but not now!)

— Note: Eq. (77) easily yields:

$$\int_{-\infty}^{\infty} \frac{dP}{2\pi\hbar}\, \tilde{\rho}(X,P,t) = {}_x\langle 0|\hat{\rho}|X\rangle_x \qquad (79a)$$

$$\int_{-\infty}^{\infty} dX\, \tilde{\rho}(X,P,t) = {}_p\langle P|\hat{\rho}|0\rangle_p \qquad (79b)$$

c.f.

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \rho(x,p,t) = {}_x\langle x|\hat{\rho}|x\rangle_x \qquad (79c)$$

$$\int_{-\infty}^{\infty} dx\, \rho(x,p,t) = {}_p\langle p|\hat{\rho}|p\rangle_p \qquad (79d)$$

• 4. Further Extensions

■ 1. We now have an extended (x-p-X-P) quantum phase space, and we can ask the comparable question again as at our start, viz; Can we find a second-extended Hamiltonian in which these 4 variables are treated as "coordinates" and introduce a further 4 conjugate "momenta", such that in this 8-dimensional phase space we can find a wave function $\rho_2 = \rho_2(x,p,X,P,t)$, say in the extended Wigner space?

– Our formalism makes it trivial to perform:

(1) We treat (x,p) as generalized coordinates $\vec{x} = (x,p)$ and their conjugate generalized momenta $\vec{p} = (P,X)$

(2) All our previous results go through with

$$x \to \vec{x},\ p \to \vec{p} \qquad : \text{ doubled}$$

– In particular, by comparison with Eq. (48):

$$\boxed{\begin{aligned}\rho_2(\vec{x},\vec{p},t) &= \rho_1(\vec{x},t)\,\tilde{\rho}^*(\vec{p},t)\,e^{-i\vec{x}\cdot\vec{p}/\hbar}\\ &= \rho(x,p,t)\,\tilde{\rho}^*(X,P,t)\,e^{-i(xP+pX)/\hbar}\end{aligned}} \qquad (80)$$

– Similarly, the extended Wigner function is, by comparison with Eq. (61b), with $\lambda = -1/2$:

$$\left.\begin{aligned}W_2(\vec{x},\vec{p},t) &= e^{i\frac{\hbar}{2}\vec{\nabla}_{\vec{x}}\cdot\vec{\nabla}_{\vec{p}}}\,\rho_2(\vec{x},\vec{p},t)\\ \text{c.f. Eq. (66a)}\quad &= \iint \frac{d\vec{x}'}{2\pi\hbar}\,e^{-i\vec{p}\cdot\vec{x}'/\hbar}\,\rho_1(\vec{x}+\tfrac{1}{2}\vec{x}',t)\,\rho_1^*(\vec{x}-\tfrac{1}{2}\vec{x}',t)\\ \text{c.f. Eq. (66b)}\quad &= \iint \frac{d\vec{p}'}{2\pi\hbar}\,e^{i\vec{x}\cdot\vec{p}'/\hbar}\,\tilde{\rho}_1(\vec{p}+\tfrac{1}{2}\vec{p}',t)\,\tilde{\rho}_1^*(\vec{p}-\tfrac{1}{2}\vec{p}',t)\end{aligned}\right\} \quad (81a)$$

$\Rightarrow$

$$\boxed{\begin{aligned} W_2(x,p,X,P,t) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dx'dp'}{2\pi\hbar}\, e^{-i(Px'+Xp')/\hbar}\, \rho(x+\tfrac{1}{2}x', p+\tfrac{1}{2}p', t) \\ &\qquad \times\ \rho^*(x-\tfrac{1}{2}x', p-\tfrac{1}{2}p', t) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dX'dP'}{2\pi\hbar}\, e^{+i(pX'+xP')/\hbar}\, \tilde{\rho}(X+\tfrac{1}{2}X', P+\tfrac{1}{2}P', t) \\ &\qquad \times\ \tilde{\rho}^*(X-\tfrac{1}{2}X', P-\tfrac{1}{2}P', t) \end{aligned}} \qquad (81b)$$

from which we readily prove:

$$\boxed{W_2(x,p,X,P,t) \text{ is real}} \qquad (82)$$

[NOTE: The above W_2 is very similar to (but not the same as) that introduced by Chountasis and Vourdas (1999) who essentially had a definition of $W_2(x,p,X,P)$ as in Eq. (81) except everywhere on RHS $\rho(x,p)$ and $\tilde{\rho}(X,P)$ are replaced by $W(x,p)$ and $\tilde{W}(X,P)$! Because we actually have wavefunctions $\rho(x,p)$ and $\tilde{\rho}(X,P)$ our scheme seems much more natural]

– We may readily prove analagous relations to Eqs. (79a–d):

$$\boxed{\begin{aligned} &\iint \frac{d\vec{x}}{2\pi\hbar}\, \varrho_2(\vec{x},\vec{p},t) = |\tilde{\rho}(\vec{p},t)|^2 \\ &\iint \frac{d\vec{p}}{2\pi\hbar}\, \varrho_2(\vec{x},\vec{p},t) = |\rho(\vec{x},t)|^2 \\ &\iint \frac{d\vec{x}}{2\pi\hbar} \iint \frac{d\vec{p}}{2\pi\hbar}\, \varrho_2(\vec{x},\vec{p},t) = \mathrm{Tr}(\hat{\rho}^2) = \mathrm{tr}(\rho^2) \leq 1 \\ &\iint \frac{d\vec{x}'}{2\pi\hbar}\, \tilde{\varrho}_2(\vec{x}',\vec{p}',t) = \tilde{\rho}(\vec{p}',t)\tilde{\rho}^*(0,t) \\ &\iint \frac{d\vec{p}'}{2\pi\hbar}\, \tilde{\varrho}_2(\vec{x}',\vec{p}',t) = \rho(0,t)\rho^*(x',t) \end{aligned}} \qquad (83)$$

– and many similar relations also for

$\varrho_2(\vec{x},\vec{p},t) \rightarrow W_2(\vec{x},\vec{p},t)$; $\tilde{\varrho}_2(\vec{x}',\vec{p}',t) \rightarrow \tilde{W}_2(\vec{x}',\vec{p}',t)$

■ 2. Entropy measures : No statistical mechanics is complete without an underlying thermodynamics. The theory so far is an initial value problem for $\rho(x,p,t)$. For a system of many degrees of freedom $i=1,2,\cdots N$ with $N \gg 1$, it is not practical to use $\rho(x_i, p_i, t) \Rightarrow$ usual practice is then to introduce a maximum entropy principle
→ clearly one way to proceed anew!

■ 3. Entanglement measures : many exist on the market, but does anything now emerge naturally? (and see below)

■ 4. Further phase space doublings : The extended wave function $\rho_2(x,p,X,P,t)$ (and the corresponding extended Wigner function $W_2(x,p,X,P,t)$) and the corresponding $\tilde{\rho}_2(x',p',X',P',t)$ (and the corresponding extended Weyl function $W_2(x',p',X',P',t)$) are related via 4-D Fourier transform $\Rightarrow$ clearly we can continue this process to introduce an 8D phase space $x-p-X-P-x'-p'-X'-P'$ and corresponding 8D extended distribution functions $(\rho_3, \tilde{\rho}_3, W_3, \tilde{W}_3, \cdots)$
More generally we can introduce 2^N-dimensional phase spaces with corresponding distribution functions of N^{th}-order
→ each doubling describes higher-order quantum noise (via ρ_N or W_N, etc.) plus higher-order quantum correlations (via $\tilde{\rho}_N$ or $\tilde{W}_N$, etc.)

(and loosely : noise ⟷ entropy
correlations ⟷ entanglement)

[Note : also recall that mixed states in $\mathcal{H}$ can correspond to entangled pure states in $\mathcal{H} \otimes \mathcal{H}$

e.g., $\hat{\rho} = \sum_{m,n} \rho_{mn} |m\rangle\langle n|$ in $\mathcal{H}$ (with $\mathrm{Tr}(\hat{\rho}^2) \leq 1$)

can map onto

$|\Psi\rangle = \sum_{m,n} \rho'_{mn} |m,n\rangle$ in $\mathcal{H} \otimes \mathcal{H}$

with $\rho'_{mn} = \dfrac{\rho_{mn}}{\sqrt{\mathrm{Tr}(\hat{\rho}^2)}}$]

■ 5. D-state quantum systems

: So far, what we've done is applicable to bosons (or oscillators)

$$\hat{a} = \sqrt{\tfrac{1}{2\hbar}}(\hat{x}+i\hat{p}) \; ; \; \hat{a}^\dagger = \sqrt{\tfrac{1}{2\hbar}}(\hat{x}-i\hat{p}) \qquad (m=\omega=1)$$

with coherent states $|z\rangle \equiv |x,p\rangle$

$$\hat{a}|z\rangle = z|z\rangle \; ; \; z = \tfrac{1}{\sqrt{2\hbar}}(x+ip)$$

$$\Rightarrow \quad |z\rangle = \hat{D}(z)|0\rangle \leftrightarrow |x,p\rangle = \hat{D}(x,p)|0\rangle$$

$$\hat{D}(z) \equiv \exp\left[z\hat{a}^\dagger - z^*\hat{a}\right] \Leftrightarrow \hat{D}(x,p) = \exp\left[\tfrac{i}{\hbar}(p\hat{x} - x\hat{p})\right]$$

– Can repeat for D-state quantum systems (quDits) with
- displacement operator $\hat{D}(x,p)$ replaced by finite displacement operators
- Fourier transform → finite Fourier transform

■ 6. Nonzero temperatures ($T \neq 0$)

Bishop and Vourdas have generalized above pure coherent states to mixed thermal coherent states at $T \neq 0$, via the density operator $\hat{\rho}_{x,p}(T)$

$$\hat{\rho}_{x,p}(T) \equiv \frac{e^{-\beta \hat{H}_{x,p}}}{\mathrm{Tr}\left[e^{-\beta \hat{H}_{x,p}}\right]} \quad : \; \beta = (k_B T)^{-1}$$

$$\hat{H}_{x,p} = \hat{D}(x,p)\,\hat{H}_0\,\hat{D}^\dagger(x,p) = \frac{(\hat{p}-p)^2}{2m} + \tfrac{1}{2}m\omega^2(\hat{x}-x)^2$$

- clearly $\hat{\rho}_{x,p}(T) \xrightarrow[T\to 0]{} |x,p\rangle\langle x,p|$
- and we proved $\displaystyle\iint \frac{dx\,dp}{2\pi\hbar}\,\hat{\rho}_{x,p}(T) = \hat{1}$
- hence temp-dependent Q, P, … representations

etc. !

<u>To conclude</u>: returning finally to my initial motivations, I believe this formal apparatus provides a rich arena in which the important aspects of QIP, <u>viz.</u>,

- quantum $\leftrightarrow$ classical interface (or quantum $\to$ classical limit)
- coherence versus decoherence (or pure versus mixed states; dissipation ($T \neq 0$))
- quantum entanglement

can be discussed consistently