Wave packet dynamics of double-well condensates, and cold atoms in optical lattices

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Outline of the course

Part I: Propagation of wavepackets in phase space

Part II: Dynamics of a BEC in a double-well potential

Part III: Dynamics of cold atoms in an optical lattice
Part I:
Propagation of wavepackets in phase space
Outline of part 1

1.1 Semiclassical operators — the Wigner-Weyl representation

1.2 Semiclassical states — states localized at a point and on a curve

1.3 Dynamics of localized wave packets

1.4 Dynamics of WKB states

1.5 Stationary WKB states — semiclassical quantization rules

1.6 Example: Wave packet dynamics in an anharmonic oscillator
1.1 The Heisenberg-Weyl group

- **Particle moving on a line**
- **Observables:** Position $\hat{q}$, momentum $\hat{p}$
- **Canonical commutator:** $[\hat{q}, \hat{p}] = i\hbar$
- **Translation:** $\exp\left(\frac{q_0\hat{p}}{\hbar}\right)$
- **Momentum translation (boost):** $\exp\left(-\frac{p_0\hat{q}}{\hbar}\right)$
- **Heisenberg operator:** $T(q_0, p_0) = \exp\left(\frac{q_0\hat{p} - p_0\hat{q}}{\hbar}\right)$

Phase-space shift $T^\dagger \hat{q} T = \hat{q} + q_0$  
$T^\dagger \hat{p} T = \hat{p} + p_0$
1.1 The Heisenberg-Weyl group

- The group law: (projective representation of the phase-space translation group)
  \[ T(q_1, p_1)T(q_2, p_2) = e^{i\frac{S}{\hbar}} T(q_1 + q_2, p_1 + p_2) \]
  \[ S = \frac{1}{2}(q_1p_2 - p_1q_2) \]
  symplectic product

- Action on wave functions:
  \[ \langle q \mid T(0, p_0)T(q_0, 0) \mid \psi \rangle = e^{-\frac{p_0q}{\hbar}} \langle q \mid \psi \rangle \]

- Remark: Obvious generalization to motion in three dimensions
1.1 The Wigner-Weyl representation

• Phase space representation of operator $\hat{O} \leftrightarrow O(q, p)$ such that

1. $\hat{O} = \int \frac{dq dp}{2\pi\hbar} O(q, p) \hat{\Delta}(q, p)$ Basis operators

2. $O(q, p) = \text{Tr} \hat{\Delta}(q, p) \hat{O}$ Weyl representation (symbol):

3. $\hat{\Delta}(q, p) = \int \frac{dq dp}{2\pi\hbar} \exp \left( \frac{pq - qp}{i\hbar} \right) T(\bar{q}, \bar{p})$

• Properties:

1. $T^\dagger (q_0, p_0) \hat{\Delta} (q_0, p_0) \leftrightarrow O(q + q_0, p + p_0)$ (equivariance)

2. $\text{Tr} \hat{\Delta}_1 \hat{\Delta}_2 = \int \frac{dq dp}{2\pi\hbar} O_1(q, p) O_2(q, p)$ (inner product)

3. $\hat{O}^\dagger \leftrightarrow O(q, p)^*$ (conjugation)

4. $f(q_0 \hat{p} - p_0 \hat{q}) \leftrightarrow f(q_0 p - p_0 q)$
1.1 The Weyl-Groenewold-Moyal product formula

- Representation of operator product $\hat{O}_3 = \hat{O}_1 \hat{O}_2$:

  $O_3(q, p) = O_1(q, p) \exp(\frac{i\hbar}{2} (\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overrightarrow{\partial}_q \overleftarrow{\partial}_p))O_2(q, p) = O_1O_2 + \frac{i\hbar}{2} \{O_1, O_2\} + O(\hbar^2)$

  classical Poisson bracket

- Classical limit of the commutator: $\frac{1}{i\hbar} [\hat{O}_1, \hat{O}_2] \leftrightarrow \{O_1, O_2\}_M = \{O_1, O_2\} + O(\hbar^2)$

  Moyal bracket
1.1 Semiclassical observables

• Non-Weyl ordering $\longrightarrow$ explicit $\hbar$-dependent symbol

• Example: $\hat{q}\hat{p} \leftrightarrow qp + \frac{i\hbar}{2}$ vs. $\frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}) \leftrightarrow qp$

• Definition: **Classically smooth operator** $\hat{O}$

$$O(q,p) \sim \lim_{\hbar \to 0} O_{\text{cl}}(p,q) + \hbar O_1(p,q) + \cdots$$

with **smooth** $O_{\text{cl}}(p,q), \hbar O_1(p,q), \ldots$

• Classically smooth operators: $\hat{q}\hat{p}, \frac{1}{2m}\hat{p}^2 + U(q)$

• Classically **singular** operators: $e^{\frac{i\hbar}{\hbar}(q_0\hat{p} - p_0\hat{q})}$ sign($\hat{q}$)
1.2 The Wigner function

- Weyl representation of the density matrix $\rho \leftrightarrow W(q, p), \ \ket{\psi} \bra{\psi} \leftrightarrow W(q, p)$ for a pure state $\ket{\psi}$. Quasi-distribution of a quantum state in phase space.

- Properties:

  1. $\int \frac{dp}{2\pi\hbar} W(q, p) = |\bra{q} \psi \rangle|^2$, $\int dq W(q, p) = |\bra{p} \psi \rangle|^2$ (marginals)

  2. $\langle \hat{O} \rangle = \int \frac{dq dp}{2\pi\hbar} W(q, p) O(q, p)$ (expectation values)

  3. $W(q, p)$ is real but can be negative
1.2 Wavepackets localized at a point

- State $|\psi\rangle$ is phase space localized:
  - $\langle q | \psi \rangle$ localized at $q_0$ with uncertainty $\Delta q$
  - $\langle p | \psi \rangle$ localized at $p_0$ with uncertainty $\Delta p$
  - with $\Delta q, \Delta p \xrightarrow{h \to 0} 0$
- Wigner function localized at $(q_0, p_0)$

\[18,26\]
1.2 Wavepackets localized in phase space

**Example**: Coherent states

\[ |q_0, p_0\rangle = T(q_0, p_0) |0, 0\rangle \]

\[ |0, 0\rangle = \text{harmonic oscillator ground state} \]

\[ \langle q |0, 0\rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega q^2}{2\hbar}} \]
\[ \langle p |0, 0\rangle = \left( \frac{1}{m\omega\pi\hbar} \right)^{1/4} e^{-\frac{p^2}{2m\omega\hbar}} \]

**Balanced wavepacket** \( \Delta q, \Delta p \sim \sqrt{\hbar} \)

**Inner product**: \( |\langle q_1, p_1 | q_2, p_2 \rangle|^2 = e^{-\frac{1}{\hbar} (m\omega(q_1 - q_2)^2 + \frac{1}{m\omega}(p_1 - p_2)^2)} \)

**Wigner function**

\[ W(q, p) = \left( \frac{1}{\pi\hbar} \right)^{1/2} e^{-\frac{1}{\hbar} (m\omega q^2 + \frac{1}{m\omega} p^2)} \]
1.2 Wavepackets localized on a phase-space curve — WKB wavefunctions

- Phase-space curve \(q(r), p(r)\),
  \[dr = \text{probability of interval } [r, r + dr]\]

- **Projected** probability densities
  \[ |\langle q | \psi \rangle|^2 = \frac{1}{q'(r)} \quad \frac{1}{2\pi\hbar} |\langle p | \psi \rangle|^2 = \frac{1}{p'(r)} \]

- WKB wavefunctions:
  \[
  \langle q | \psi \rangle = |\langle q | \psi \rangle| e^{i\frac{\hbar}{\hbar}S(q)} \\
  \langle p | \psi \rangle = |\langle p | \psi \rangle| e^{i\frac{\hbar}{\hbar}\tilde{S}(p)} \text{sign}(q'(p)) \frac{i\pi}{4}
  \]

- Classical action \( S(q) = \int p \, dq \), \( \tilde{S}(q) = -\int q \, dp \)

[3,4,30]
1.2 Multibranched WKB wavefunctions

- \( q(s_1) = q(s_2) \) branches \( r_1(q), r_2(q) \)

- WKB wavefunctions:
  \[
  \langle q \mid \psi \rangle = a_1(q)e^{i\frac{\bar{\hbar}}{\hbar} S_1(q)} + a_2(q)e^{i\frac{\bar{\hbar}}{\hbar} S_2(q)} - \frac{i\pi}{2} k
  \]
  \[
  \langle p \mid \psi \rangle = \tilde{a}(p)e^{i\frac{\bar{\hbar}}{\hbar} \tilde{S}(p)} - \text{sign}(q'(p)) \frac{i\pi}{4}
  \]

- Maslov index: an integer
  \[
  k = \frac{1}{2} (\text{sign}(p'_1(q)) - \text{sign}(p'_2(q)))
  \]

- \( a_{1,2}(q) = (q'(r_{1,2}))^{-\frac{1}{2}} \)
  \( \tilde{a}(p) = (p'(r))^{-\frac{1}{2}} \)
  \[
  S_{1,2}(q) = \int_{r_{1,2}} p dq \quad \tilde{S}(q) = -\int q dp
  \]
1.2 WKB wavefunctions on a loop: Quantization

• Branches can be reached in 2 ways

\[ S^+_2(q) = \int_{\text{counter-cw}}^{(q,p_2(q))} pdq \quad S^-_2(q) = \int_{\text{clockwise}}^{(q,p_2(q))} pdq \]

• WKB wavefunction must be consistent:

\[ \langle q | \psi \rangle = a_1(q)e^{\frac{i}{\hbar}S_1(q)} + a_2(q)e^{\frac{i}{\hbar}S^+_2(q) - \frac{i\pi}{2}k^+} \]

\[ = a_1(q)e^{\frac{i}{\hbar}S_1(q)} + a_2(q)e^{\frac{i}{\hbar}S^-_2(q) - \frac{i\pi}{2}k^-} \]

\[ S^+_2 - S^-_2 - \frac{\hbar \pi}{2} (k^+ - k^-) = 2\pi\hbar (\text{integer}) \]

\[ \oint pdq = 2\pi\hbar (n + \frac{1}{4} k) \]

Classical action

Loop Maslov index: A topological invariant

• Loop Maslov index: an even integer

• Maslov index of a topological circle = 2

Bohr-Sommerfeld quantization

[3,4,30]
1.3 Dynamics of localized wavepackets

- von Neumann equation, possibly time-dependent Hamiltonian

\[ i\hbar \partial_t \rho = [\hat{H}, \rho] \]

\[ \partial_t W(q, p) = \{H, W\}_M \]

- Classically smooth Hamiltonian

- \( H(q, p) \) varies slowly on the scale of \( W \)

- Can approximate \( H(q, p) \) by a quadratic Taylor expansion

\[
\begin{align*}
H(q, p) &\to H_Q^{(q_0, p_0)}(q, p) = H(q_0, p_0) + (q - q_0)\partial_q H + (p - p_0)\partial_p H \\
&\quad + \frac{1}{2}((q - q_0)^2\partial_q^2 + 2(q - q_0)(p - p_0)\partial_q\partial_p + (p - p_0)^2\partial_p^2)H
\end{align*}
\]
1.3 Dynamics of localized wavepackets

- High-order terms in the Moyal bracket involve 3rd-order and higher derivatives

\[ \partial_t W(q, p) \sim \{ H_Q, W \}_M = \{ H_Q, W \} \]

- \( W \) evolves as a classical phase-space distribution under the flow of \( H \)

- **Important:** \( H^{(q_0, p_0)}_Q \) is time-dependent through \( q_0, p_0 \) even if \( H \) is not
1.3 The evolution of the Wigner function

- The wavepacket center is governed by the Hamilton equations:
  \[
  \begin{align*}
  \frac{\partial_t q_0}{\partial p} &= \partial p H = v(q_0, p_0) \\
  \frac{\partial_t p_0}{\partial q} &= -\partial q H = F(q_0, p_0)
  \end{align*}
  \]

- Other points follow linearized equations:
  \[
  (q, p) = (q_0, p_0) + (\delta q, \delta p)
  \]
  \[
  \frac{\partial_t}{\partial q} = \begin{pmatrix} \partial_q v & \partial_p v \\ \partial_q F & \partial_p F \end{pmatrix} (\delta q)
  \]

- The time-dependent Wigner function
  \[
  W_t(q_t, p_t) = W(q, p)
  \]
  \[
  (q_t, p_t) = (q_{0,t}, p_{0,t}) + S_t((q, p) - (q_0, p_0))
  \]
  \[
  S_t = T \exp \int_0^t \begin{pmatrix} \partial_q v & \partial_p v \\ \partial_q F & \partial_p F \end{pmatrix} dt'
  \]
1.3 The evolution of the *expectation values*

- The time-dependent Wigner function
  \[ W_t(q_t, p_t) = W(q, p) \]
  \[ (q_t, p_t) = (q_0, p_0) + S_t((q, p) - (q_0, p_0)) \]
  Hamiltonian flow linearized at center

- Position & momentum uncertainties
  \[ \langle (\hat{q}_t, \hat{p}_t) \otimes (\hat{q}_t, \hat{p}_t) \rangle = \langle (\hat{q}, \hat{p}) \cdot S_t \otimes S_t \cdot (\hat{q}, \hat{p}) \rangle \]
  \[ = \hat{q} - \langle \hat{q} \rangle \]
  \[ = \hat{p} - \langle \hat{p} \rangle \]

- \( S \) is area-preserving \( \Rightarrow S^\dagger S \) has eigenvalues \( \lambda, 1/\lambda \) with eigenvectors \( v_+, v_- \)

- Let \( \hat{z}_\pm = v_\pm \cdot (\hat{q}, \hat{p}) \). If \( \lambda > 1 \) then
  \[ \Delta z_- = \Delta z_0 e^{-\frac{1}{2} \lambda t} \]

- Fluctuations of \( \hat{z}_- \) are *squeezed*. [18,26]
1.3 The evolution of the state

- Q: How does $|\psi\rangle$ evolve under a quadratic (time-dependent) Hamiltonian?

- A: Phase-space translation following a unitary operator $M(S_t)$ that realizes $S_t$ on Hilbert space

  $$M(S)^\dagger (\hat{q}, \hat{p}) M(S) = S \cdot (\hat{q}, \hat{p})$$

- Phase ambiguity determined up to sign by

  $$M(S_1) M(S_2) = M(S_1 S_2)$$

- Wigner function determines $|\psi\rangle$ up to phase

  $$|\psi\rangle_t = e^{i\gamma} T(q_t, p_t) M(S_t) |\psi\rangle_0$$ (choosing $q_0 = p_0 = 0$)

- Substituting in Schrödinger equation

  $$i\hbar \partial_t |\psi\rangle = H_Q |\psi\rangle$$

  $$\hbar \gamma = \frac{1}{2} \int (qd^p - pdq) - \int Hdt$$

  = classical action for a closed orbit
1.4 Dynamics of WKB wavefunctions

- WKB wavefunction $\langle q | \psi \rangle_t = a_t(q)e^{\frac{i}{\hbar}S_t(q)}$

- Schrödinger equation $i\hbar \partial_t |\psi\rangle = \hat{H}|\psi\rangle$

- Hamilton-Jacobi equation: $\partial_t S + H(q, \partial_q S) = 0$

- The continuity equation: $\partial_t (a^2) + \partial_q(a^2v) = 0$

- State curves follow classical flow
  
  $(q(r), p(r)) \rightarrow (q_t(r), p_t(r))$

  Solution of Hamilton’s equation

  $S_t(q) = \int p_t dq$  \hspace{1cm} $a_t(q) = (q'_t(r))^\frac{1}{2}$
1.5 **Stationary** WKB wavefunctions: Energy states

- Stationary WKB states localized on invariant phase-space curve $H(q, p) = E$
- Invariant density $\propto$ propagation time $dt$
- Confining Hamiltonian closed equal-energy curves
- Propagation time $\propto \frac{\theta}{\omega}$
  - Canonical angle variable
  - Angular frequency
- Quantization rule $A(E_n) = \oint pdq = 2\pi\hbar(n + \frac{k}{4})$
  - Action variable
1.6 Example: Dynamics of an anharmonic oscillator wavepacket

- $\hat{H} = \frac{1}{2m}\hat{p}^2 + U(\hat{q})$. Initial coherent state $|q_0p_0\rangle$

- Classical action-angle variables $H(I, \theta) = h(I)$
  $$(q_0, p_0) \longrightarrow (\theta_0, I_0)$$
  $$q - q_0 = \partial_I q(I - I_0) + \partial_\theta q(\theta - \theta_0)$$
  $$p - p_0 = \partial_I p(I - I_0) + \partial_\theta p(\theta - \theta_0)$$

- Oscillation frequency $\omega(E) = \omega(I(E)) = h'(I)$

- Wavepacket at time $t = \frac{2\pi}{\omega(E_0)}$: $e^{i\gamma M(S)}|q_0p_0\rangle$

  $S = \begin{pmatrix} \partial_q I & \partial_q \theta \\ \partial_p I & \partial_p \theta \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \omega'(I) \end{pmatrix}$

  - $\gamma = \frac{2\pi}{\hbar}(I_0 - E_0/\omega(E_0))$
1.6 Example: Dynamics of an anharmonic oscillator wavepacket

- Long-time dynamics: Wigner function spreads over energy contour
- Linearized dynamics becomes invalid

**Nevertheless:** Expectation values follow classically-advected Wigner function

- Oscillations in $\langle \hat{q}, \hat{p} \rangle$ suppressed on time-scale

\[
t_c = \frac{1}{\Delta \omega} = \frac{1}{\omega'(E) \Delta E} = O(\hbar^{-1/2})
\]

- Collapse of oscillation at the Ehrenfest time = time needed for quantum fluctuations to become macroscopic

- Revival of oscillations at

\[
t_r = \frac{1}{2\pi \hbar \omega'(E) \omega(E)} = O(\hbar^{-1})
\]

Level spacing stepping

- Discreteness of spectrum manifest at the Heisenberg time
Summary of part 1

• Observables that change slowly on quantum scales — smooth observables — can be approximated classically, using a phase-space representation.

• Classical dynamics is a good approximation for the evolution of states if they are phase-space localized, near a point or a curve (WKB states).

• The area of a closed curve supporting a semiclassical state is quantized.

• The center of a wavepacket follows the classical trajectory, its shape is deformed linearly, i.e. squeezed, by the local classical flow, and the overall phase is proportional to the classical action.

• The curve and density of WKB states evolve by classical advection.

• Propagating wavepackets typically become delocalized on time scales that diverge in the classical limit.