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# **Lecture Models for heavy-ion collisions: (Part I): transport models - Vlasov EoM**

**SS2024: , Dynamical models for relativistic heavy-ion collisions'** 

## **Basic models for heavy-ion collisions**



#### • **Statistical models:**

**basic assumption: system is described by a (grand) canonical ensemble of non-interacting fermions and bosons in thermal and chemical equilibrium**   $=$  thermal hadron gas at freeze-out with common T and  $\mu_B$ 

**[ - : no dynamical information]**

#### • **Hydrodynamical models:**

**basic assumption: conservation laws + equation of state (EoS);** 

**assumption of local thermal and chemical equilibrium** 

**- Interactions are 'hidden' in properties of the fluid described by transport coefficients (shear and bulk viscosity** h, z, ..), **which is 'input' for the hydro models**

**[ - : simplified dynamics]**

#### • **Microscopic transport models:**

**based on transport theory of relativistic quantum many-body systems**

- **- Explicitly account for the interactions of all degrees of freedom (hadrons and partons) in terms of cross sections and potentials**
- **- Provide a unique dynamical description of strongly interaction matter in- and out-off equilibrium:**
- **- In-equilibrium: transport coefficients are calculated in a box – controled by lQCD**
- **- Nonequilibrium dynamics – controled by HIC**

**Actual solutions: Monte Carlo simulations** 



**The goal: to study the properties of strongly interacting matter under extreme conditions from a microscopic point of view**

**Realization: dynamical many-body transport approaches**

#### **Plan:**

**1) Dynamical transport models (nonrelativistic formulation): from the Schrödinger equation to Vlasov equation of motion** ➔ **BUU EoM**

- **2) Density-matrix formalism: Correlation dynamics**
- **3) Quantum field theory** ➔ **Kadanoff-Baym dynamics** ➔ **generalized off-shell transport equations**
- **4) Transport models for HIC**

## **1. From the Schrödinger equation to the Vlasov equation of motion**

#### **Quantum mechanical description of the many-body system**

**Dynamics of heavy-ion collisions is a many-body problem!**

**Schrödinger equation for the system of N particles in three dimensions:**

$$
i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) = H(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)
$$

*nonrelativistic formulation*

 $\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, t) = A \prod_{i=1}^N \psi_i(\vec{r}_i, t)$ **Hartree-Fock approximation: • many-body wave function** → **antisym. product of single-particle wave functions**

•**many-body Hamiltonian** <sup>→</sup> **single-particle Hartree-Fock Hamiltonian**

J

$$
H(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, t) = \sum_{i=1}^N T(\vec{r}_i) + V(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, t)
$$
  
\n
$$
T(\vec{r}) = -\frac{\hbar}{2m} \vec{\nabla}_r^2
$$
  
\n
$$
(\text{approximation}) \approx \sum_{i=1}^N T(\vec{r}_i) + \sum_{i < j}^N V_{ij} (\left| \vec{r}_i - \vec{r}_j \right|, t) \approx \sum_{i=1}^N h_i(\vec{r}_i, t)
$$
  
\n
$$
\text{kinetic term} \qquad \text{2-body potential}
$$

**Time-dependent Hartree-Fock equation for a single particle** *i***:**

$$
i\hbar \frac{\partial}{\partial t} \psi_i(\vec{r},t) = \hat{h} \psi_i(\vec{r},t)
$$

**Single-particle Hartree-Fock Hamiltonian operator:**  $\hat{\bm{h}} = \hat{\bm{T}} + \hat{\bm{U}}_{\bm{\mu}} - \hat{\bm{U}}_{\bm{\kappa}}$ 

$$
•\text{Hartree term:}\quad \hat{U}_H = \sum_{i(occ)}\int d^3r' \psi_i^*(\vec{r}\,',t)V(\vec{r}-\vec{r}\,')\psi_i(\vec{r}\,',t)\qquad\qquad \hat{T}=-\frac{\hbar}{2m}\vec{\nabla}_r^2
$$

**self-generated local mean-field potential** 

**8** For the same generalized local integral field potential  
\n**8** Fock term: 
$$
\hat{U}_F = \sum_{i < N} \psi_i^*(\vec{r}',t) V(\vec{r},\vec{r}',t) \psi_i(\vec{r},t)
$$
\nnon-local mean-field exchange potential (quantum statistics)

➔ **Equation-of-motion (EoM): propagation of particles in the self-generated mean-field:**

$$
i\hbar \frac{\partial}{\partial t} \psi_i(\vec{r},t) = (T(\vec{r},t) + U_H(\vec{r},t)) \psi_i(\vec{r},t) - \int d^3\vec{r} \cdot (\vec{U}_F(\vec{r},\vec{r}\cdot t)) \psi_i(\vec{r}\cdot t)
$$
  
local potential

**We'll neglected the exchange (Fock) term** *local potential*

**Note: TDHF approximation describes only the interactions of particles with the time-dependent mean-field !**

**In order to describe the collisions between the individual(!) particles, one has to go beyond the mean-field level ! (see Part 2: Correlation dynamics)**

### **Single particle density matrix**

❑ **Introduce the single particle density matrix:**

$$
\rho(\vec{r},\vec{r}',t) \equiv \sum_{\beta_{occ}} \psi_{\beta}^*(\vec{r}',t) \psi_{\beta}(\vec{r},t)
$$

**Thus, the single-particle Hartree-Fock Hamiltonian operator can be written as**

$$
h(\vec{r},t) = T(\vec{r}) + \sum_{\beta_{occ}} \int d^3r' V(\vec{r}-\vec{r}',t) \rho(\vec{r}',\vec{r}',t) = T(\vec{r}) + U(\vec{r},t)
$$

❑ **Consider equation:**

 $\alpha$ 

$$
i\hbar \frac{\partial}{\partial t} \psi_{\alpha}(\vec{r}, t) = h(\vec{r}, t) \psi_{\alpha}(\vec{r}, t)
$$
 (1)

$$
\psi_{\alpha}^*(\vec{r}',t) * (1): \psi_{\alpha}^*(\vec{r}',t) i\hbar \frac{\partial}{\partial t} \psi_{\alpha}(\vec{r},t) = \psi_{\alpha}^*(\vec{r}',t) h(\vec{r},t) \psi_{\alpha}(\vec{r},t)
$$
 (2)

$$
(1)^{+}|_{for\,\vec{r}'} * \psi_{\alpha}(\vec{r},t):
$$
  
\n
$$
-i\hbar \left[ \frac{\partial}{\partial t} \psi_{\alpha}^{*}(\vec{r}',t) \right] \psi_{\alpha}(\vec{r},t) = h(\vec{r}',t) \psi_{\alpha}^{*}(\vec{r}',t) \psi_{\alpha}(\vec{r},t)
$$
 (3)

#### **Wigner transform of the density matrix**

$$
i\hbar \frac{\partial}{\partial t} \rho(\vec{r}, \vec{r}', t) = [h(\vec{r}, t) - h(\vec{r}', t)] \rho(\vec{r}, \vec{r}', t)
$$
 (4)

**The single-particle Hartree-Fock Hamiltonian:**

$$
\rho(\vec{r},\vec{r}',t) \equiv \sum_{\beta_{occ}} \psi_{\beta}^*(\vec{r}',t) \psi_{\beta}(\vec{r},t)
$$

$$
h(\vec{r},t) = T(\vec{r}) + \int d^3r' V(\vec{r} - \vec{r}',t) \rho(\vec{r}',\vec{r}',t)
$$

$$
= T(\vec{r}) + U(\vec{r},t)
$$

#### **kinetic term + potential (local) term**

➔**EoM:**

$$
\left[\frac{\partial}{\partial t}\rho(\vec{r},\vec{r}',t)+\frac{i}{\hbar}\left[\frac{\hbar^2}{2m}\vec{\nabla}_r^2+U(\vec{r},t)-\frac{\hbar^2}{2m}\vec{\nabla}_{r'}^2-U(\vec{r}',t)\right]\rho(\vec{r},\vec{r}',t)=0\right]
$$
 (5)

**Rewrite (5) using** *x* **instead of** *r*

$$
\frac{\partial}{\partial t}\rho(\vec{x},\vec{x}',t) + \frac{i}{\hbar}\left[\frac{\hbar^2}{2m}\vec{\nabla}_x^2 + U(\vec{x},t) - \frac{\hbar^2}{2m}\vec{\nabla}_{x'}^2 - U(\vec{x}',t)\right]\rho(\vec{x},\vec{x}',t) = 0
$$

#### **Wigner transform of the density matrix**

$$
\frac{\partial}{\partial t} \rho(\vec{x}, \vec{x}', t) + \frac{i}{\hbar} \left[ \frac{\hbar^2}{2m} \vec{\nabla}_x^2 + U(\vec{x}, t) - \frac{\hbar^2}{2m} \vec{\nabla}_{x'}^2 - U(\vec{x}', t) \right] \rho(\vec{x}, \vec{x}', t) = 0
$$

 $□$  Instead of considering the density matrix  $\rho$ , let's find the equation of motion **for its Fourier transform, i.e. the Wigner transform of the density matrix:** 

$$
\frac{1}{\partial t} \rho(\vec{x}, \vec{x}', t) + \frac{1}{\hbar} \left[ \frac{1}{2m} \nabla_x^2 + U(\vec{x}, t) - \frac{1}{2m} \nabla_x^2 - U(\vec{x}', t) \right] \rho(\vec{x}, \vec{x}', t) = 0
$$
\ntead of considering the density matrix  $\rho$ , let's find the equation of motion  
\nits Fourier transform, i.e. the Wigner transform of the density matrix:  
\n
$$
f(\vec{r}, \vec{p}, t) = \int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) \rho\left(\vec{r} + \frac{\vec{s}}{2}, \vec{r} - \frac{\vec{s}}{2}, t\right)
$$
\n
$$
old : \vec{x} = \vec{x}'
$$
\n
$$
\frac{f(\vec{r}, \vec{p}, t) \text{ is the single-particle phase-space distribution function}}{f(\vec{r}, \vec{p}, t) \text{ is the single-particle phase-space distribution function}}
$$
\nDensity in coordinate space:  $\rho(\vec{r}, t) = \frac{1}{(2\pi\hbar)^3} \int d^3 p \ f(\vec{r}, \vec{p}, t)$   
\nDensity in momentum space:  $g(\vec{p}, t) = \int d^3 r \ f(\vec{r}, \vec{p}, t)$ 

**New variables:**

$$
\vec{r}=\frac{\vec{x}+\vec{x}'}{2}, \quad \vec{s}=\vec{x}-\vec{x}'
$$

 $f(\vec{r},\vec{p},t\,)$  is the single-particle phase-space distribution function

Density in coordinate space: 
$$
\rho(\vec{r},t) = \frac{1}{(2\pi\hbar)^3} \int d^3p \ f(\vec{r},\vec{p},t)
$$

 $g(\vec{p}, t) = \int d^{3}r \ f(\vec{r}, \vec{p}, t)$ 

## **Uncertainty principle**

### $f$  (  $\vec{r}$  ,  $\vec{p}$  ,  $t$  )

**Is it consistent with Quantum Mechanics?**

**What about uncertainty principle?** *2*  $x \cdot \Delta p$ ħ  $\varDelta x \cdot \varDelta p \geq$ 

**Consider the case when disturbance varies only over macroscopic distances:**  $\;\varDelta x\sim\lambda\; ,$ 

where  $\lambda$  is a wave length of the particle: *2*D*p*  $\lambda$ ħ  $\geq$ 

**→ We can specify the momentum of the particle with microscopic accuracy**  $\Delta p$ *!* 

## **Wigner transformation + Taylor expansion**

$$
\frac{\partial}{\partial t}\rho(\vec{r}+\frac{\vec{s}}{2},\vec{r}-\frac{\vec{s}}{2},t) + \frac{i}{\hbar} \left[ \frac{\hbar^2}{2m} \vec{\nabla}_{\vec{r}+\frac{\vec{s}}{2}}^2 + U(\vec{r}+\frac{\vec{s}}{2},t) - \frac{\hbar^2}{2m} \vec{\nabla}_{\vec{r}-\frac{\vec{s}}{2}}^2 - U(\vec{r}-\frac{\vec{s}}{2},t) \right] \rho(\vec{r}+\frac{\vec{s}}{2},\vec{r}-\frac{\vec{s}}{2},t) = 0 \quad (1)
$$

❑ **Make Wigner transformation of eq.(1)**

$$
\int d^3s \exp\left(-\frac{i}{\hbar}\vec{p}\vec{s}\right) \frac{\partial}{\partial t} \rho\left(\vec{r} + \frac{\vec{s}}{2}, \vec{r} - \frac{\vec{s}}{2}, t\right)
$$
 (2)

$$
+\frac{i}{2m} \frac{\hbar^2}{\hbar} \int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) \left[ \vec{\nabla}^2_{\vec{r}+\frac{\vec{s}}{2}} - \vec{\nabla}^2_{\frac{\vec{r}}{2}-\frac{\vec{s}}{2}} \right] \rho \left(\vec{r}+\frac{\vec{s}}{2},\vec{r}-\frac{\vec{s}}{2},t\right) + \frac{i}{\hbar} \int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) \left[ U(\vec{r}+\frac{\vec{s}}{2},t) - U(\vec{r}-\frac{\vec{s}}{2},t) \right] \rho \left(\vec{r}+\frac{\vec{s}}{2},\vec{r}-\frac{\vec{s}}{2},t\right) = 0
$$

*r s 2 2 s r 2 2*  $\vec{r} + \frac{s}{c}$  $\frac{2}{\bar{s}}$   $\nabla$   $\frac{2}{\bar{s}}$   $=$   $2\nabla$   $_{\vec{r}}$   $\cdot$   $\nabla$   $_{\vec{s}}$  $\vec{\nabla}^{\,2}\,$  =  $- \vec{\nabla}^{\,2}\,$  =  $2 \vec{\nabla}$  =  $\cdot \vec{\nabla}$ □ Use that  $\vec{\nabla}^2_{\vec{r}+\vec{\underline{s}}}-\vec{\nabla}^2_{\vec{r}-\vec{\underline{s}}}=2\vec{\nabla}_{\vec{r}}\cdot\vec{\nabla}_{\vec{s}}$  (see Task 1) (3)

Consider 
$$
U(\vec{r} + \frac{\vec{s}}{2}, t) - U(\vec{r} - \frac{\vec{s}}{2}, t)
$$
 Make Taylor expansion around  $r; s \rightarrow 0$ 

\n
$$
= \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{1}{2} \vec{s} \cdot \vec{\nabla}_{\vec{r}} \right)^n U \Big|_{s=0} - \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{1}{2} \vec{s} \cdot \vec{\nabla}_{\vec{r}} \right)^n U \Big|_{s=0} = 2 \sum_{odd} \left( \frac{1}{2} \vec{s} \cdot \vec{\nabla}_{\vec{r}} \right)^n U \Big|_{s=0} \frac{1}{n!}
$$
\n
$$
\approx \vec{s} \cdot \vec{\nabla}_{\vec{r}} U(\vec{r}, t)
$$
\nterms even in *n* cancel

**Classical limit: keep only the first term** *n=1* **(good approximation for hadronic potentials)**

## **Vlasov equation-of-motion**

**From (2) and (3),(4) obtain**

$$
\frac{\partial}{\partial t} f(\vec{r}, \vec{p}, t) + \frac{i}{2m} \frac{\hbar^2}{\hbar} \int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) 2 \vec{\nabla}_{\vec{r}} \cdot \vec{\nabla}_{\vec{s}} \rho \left(\vec{r} + \frac{\vec{s}}{2}, \vec{r} - \frac{\vec{s}}{2}, t\right)
$$
(5)

$$
\mathbf{J} + \frac{i}{\hbar} \int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) \vec{s} \cdot \vec{\nabla}_{\vec{r}} U(\vec{r}, t) \rho \left(\vec{r} + \frac{\vec{s}}{2}, \vec{r} - \frac{\vec{s}}{2}, t\right) = 0
$$
 (see Task 2)  
\n
$$
\int d^3 s \exp\left(-\frac{i}{\hbar} \vec{p} \vec{s}\right) \rho \left(\vec{r} + \frac{\vec{s}}{2}, \vec{r} - \frac{\vec{s}}{2}, t\right)
$$

**Vlasov equation** 

**- free propagation of particles in the self-generated HF mean-field potential:**

$$
\frac{\partial}{\partial t} f(\vec{r}, \vec{p}, t) + \frac{\vec{p}}{m} \vec{\nabla}_{\vec{r}} f(\vec{r}, \vec{p}, t) - \vec{\nabla}_{\vec{r}} U(\vec{r}, t) \vec{\nabla}_{\vec{p}} f(\vec{r}, \vec{p}, t) = 0
$$
\n(6)

**Eq.(6) is entirely classical (lowest order in** *s* **expansion). Here** *U* **is a self-consistent potential associated with** *f* **phase-space distribution:** 

$$
U(\vec{r},t) = \frac{1}{(2\pi\hbar)^3} \int d^3r' d^3p V(\vec{r} - \vec{r}',t) f(\vec{r}',\vec{p},t)
$$
 (7)

## **Vlasov EoM**

#### **Vlasov equation of motion**

**- free propagation of particles in the self-generated HF mean-field potential:**

$$
\frac{\partial}{\partial t} f(\vec{r}, \vec{p}, t) + \frac{\vec{p}}{m} \vec{\nabla}_{\vec{r}} f(\vec{r}, \vec{p}, t) - \vec{\nabla}_{\vec{r}} U(\vec{r}, t) \vec{\nabla}_{\vec{p}} f(\vec{r}, \vec{p}, t) = 0
$$

**Vlasov EoM is equivalent to:**

$$
\frac{d}{dt} f(\vec{r}, \vec{p}, t) = 0 = \left[ \frac{\partial}{\partial t} + \dot{\vec{r}} \vec{\nabla}_{\vec{r}} + \dot{\vec{p}} \vec{\nabla}_{\vec{p}} \right] f(\vec{r}, \vec{p}, t) = 0
$$

**with**



**Note: the quantum physics plays a role in the initial conditions for** *f***:** 

## **Numerical solution of Vlasov EoM**

#### **Testparticle method or method of parallel ensembles :**

**the distribution functions of the system of N particles can be described as a sum of point-like particles (** $\delta$  **−functions)** 

In the limit of large number of parallel ensembles  $\,N_t^{\,} \rightarrow \infty$ 

$$
f(\vec{r}, \vec{p}, t) = \frac{1}{N_t} \sum_{i=1}^{N \cdot N_t} \delta(\vec{r} - \vec{r}_i(t)) \delta(\vec{p} - \vec{p}_i(t))
$$

**is a solution of Vlasov EoM**





➔ **Propagation of test-particles in time following 'classical' EoM:**

$$
\vec{r}_i = \frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m_i}
$$
\n
$$
\dot{\vec{p}}_i = \frac{d\vec{p}_i}{dt} = -\vec{\nabla}_{\vec{r}_i} U(\vec{r}_i, t)
$$

## **Mean-field potential**

❑ **Testparticle method provides a smooth density distribution for calculation of mean-field potential for particle propagation (No exchange of particles between the parallel ensembles)**



**Mean-field potential:** 

$$
U(\vec{r},t) = \frac{1}{(2\pi\hbar)^3} \int d^3r' d^3p V(\vec{r} - \vec{r}',t) f(\vec{r}',\vec{p},t)
$$

❑ **Effective two-body interaction with a finite-range Yukawa, Skyrme-type and Coulomb interactions:**

$$
v(\mathbf{x} - \mathbf{x}_2) = -A_0 \frac{\exp(-\mu|\mathbf{x} - \mathbf{x}_2|)}{\mu|\mathbf{x} - \mathbf{x}_2|} + B_0 \delta^3(\mathbf{x} - \mathbf{x}_2)\rho(\mathbf{x} - \mathbf{x}_2)^2 + \frac{e^2}{4\pi} \frac{\delta_{pp}}{|\mathbf{x} - \mathbf{x}_2|}
$$



### **Density distribution: Vlasov equation**



#### **Ca+Ca, 40 A MeV**



## **Useful literature**

**L. P. Kadanoff, G. Baym, '***Quantum Statistical Mechanics'***, Benjamin, 1962**

**M. Bonitz, '***Quantum kinetic theory'***, B.G. Teubner Stuttgart, 1998**

**W. Cassing, `Transport Theories for Strongly-Interacting Systems', Springer Nature: Lecture Notes in Physics 989, 2021; DOI: 10.1007/978-3-030-80295-0**

1) Show that

$$
\vec{\nabla}_x^2 - \vec{\nabla}_{x'}^2 = \vec{\nabla}_{\mathbf{r} + \mathbf{s}/2}^2 - \vec{\nabla}_{\mathbf{r} - \mathbf{s}/2}^2 = 2\vec{\nabla}_{\mathbf{s}} \cdot \vec{\nabla}_{\mathbf{r}},
$$
  
where  $\mathbf{x} = \mathbf{r} + \mathbf{s}/2$ ,  $\mathbf{x'} = \mathbf{r} - \mathbf{s}/2$ .

#### ❖ Solution:

1) We have  $(i=1,2,3)$ 

 $\rightarrow \infty$ 

$$
\frac{\partial}{\partial x_i} = \frac{\partial}{\partial r_i} \frac{\partial r_i}{\partial x_i} + \frac{\partial}{\partial s_i} \frac{\partial s_i}{\partial x_i} = \frac{1}{2} \frac{\partial}{\partial r_i} + \frac{\partial}{\partial s_i},
$$

$$
\frac{\partial}{\partial x'_i} = \frac{\partial}{\partial r_i} \frac{\partial r_i}{\partial x'_i} + \frac{\partial}{\partial s_i} \frac{\partial s_i}{\partial x'_i} = \frac{1}{2} \frac{\partial}{\partial r_i} - \frac{\partial}{\partial s_i}.
$$

This leads to

$$
\vec{\nabla}_x^2 - \vec{\nabla}_{x'}^2 = \vec{\nabla}_{\mathbf{r} + \mathbf{s}/2}^2 - \vec{\nabla}_{\mathbf{r} - \mathbf{s}/2}^2 = \sum_{i=1}^3 \left( (\frac{1}{2} \frac{\partial}{\partial r_i} + \frac{\partial}{\partial s_i})^2 - (\frac{1}{2} \frac{\partial}{\partial r_i} - \frac{\partial}{\partial s_i})^2 \right)
$$
  
= 
$$
\sum_{i=1}^3 \left( \frac{1}{4} \frac{\partial^2}{\partial r_i^2} + \frac{\partial}{\partial r_i} \frac{\partial}{\partial s_i} + \frac{\partial^2}{\partial s_i^2} - \frac{1}{4} \frac{\partial^2}{\partial r_i^2} + \frac{\partial}{\partial r_i} \frac{\partial}{\partial s_i} - \frac{\partial^2}{\partial s_i^2} \right) = 2 \vec{\nabla}_{\mathbf{r}} \cdot \vec{\nabla}_{\mathbf{s}}.
$$

2) What is the Wigner transform of  $\vec{\nabla}_s \cdot \vec{\nabla}_r \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)$  when assuming that  $\rho(\mathbf{r}, \mathbf{s})$ vanishes at  $s_i \to \pm \infty$  for  $i = x, y, z$ ?

#### **Solution:**  $\frac{1}{2}$

The Wigner transform of  $\vec{\nabla}_s \cdot \vec{\nabla}_r \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)$  is given by

$$
\int d^3s \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \vec{\nabla}_s \cdot \vec{\nabla}_r \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \n= \vec{\nabla}_r \cdot \int d^3s \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \vec{\nabla}_s \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2).
$$
\n(4)

Use that

$$
\frac{d}{dx}[f(x)g(x)] = f(x)\frac{dg(x)}{dx} + g(x)\frac{df(x)}{dx}.
$$

Then

$$
\vec{\nabla}_{s} \left( \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \right) =
$$
\n
$$
= \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \vec{\nabla}_{s} \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) + \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \vec{\nabla}_{s} \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}).
$$

Since

$$
\vec{\nabla}_{\mathbf{s}} \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) = -\frac{i}{\hbar} \mathbf{p} \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}),
$$

we obtain that

$$
\exp(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{s})\vec{\nabla}_{\mathbf{s}}\,\rho(\mathbf{r}+\mathbf{s}/2,\mathbf{r}-\mathbf{s}/2)
$$
\n
$$
=\vec{\nabla}_{\mathbf{s}}\left(\exp(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{s})\,\rho(\mathbf{r}+\mathbf{s}/2,\mathbf{r}-\mathbf{s}/2)\right)+\frac{i}{\hbar}\mathbf{p}\exp(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{s})\,\rho(\mathbf{r}+\mathbf{s}/2,\mathbf{r}-\mathbf{s}/2).
$$
\n(5)

Substitute  $(5)$  to eq. $(4)$ :

(4): 
$$
= \vec{\nabla}_{\mathbf{r}} \cdot \int d^{3} s \vec{\nabla}_{\mathbf{s}} \left( \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \right)
$$

$$
- \vec{\nabla}_{\mathbf{r}} \cdot \int d^{3} s \left( \vec{\nabla}_{\mathbf{s}} \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \right) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)
$$
(6)

The first term in (6) is vanishing in the limits of partial integration since  $\rho(\mathbf{r}, \mathbf{s}) \to \mathbf{0}$ when  $s_i \to \pm \infty$  for all components  $i = 1, 2, 3$ :

$$
\int d^3 s \vec{\nabla}_s \left( \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \right) \to 0
$$
  
since 
$$
\int_{-\infty}^{\infty} ds_i \frac{\partial}{s_i} \left( \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2) \right)
$$

$$
\to \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)|_{s_i \to -\infty}^{s_i \to \infty}
$$

Thus,

$$
\frac{\int d^3 s \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \vec{\nabla}_s \cdot \vec{\nabla}_r \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)}{4}.
$$
\n
$$
(4): = -\vec{\nabla}_r \cdot \int d^3 s \left(-\frac{i}{\hbar} \mathbf{p} \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)\right)
$$
\n
$$
= \frac{i}{\hbar} \mathbf{p} \cdot \vec{\nabla}_r \int d^3 s \exp(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}) \rho(\mathbf{r} + \mathbf{s}/2, \mathbf{r} - \mathbf{s}/2)
$$
\n
$$
= \frac{i}{\hbar} \mathbf{p} \cdot \vec{\nabla}_r f(\mathbf{r}, \mathbf{p}).
$$

 $(7)$