

FREE TRANSPORT - HAMILTONIAN SYSTEMS

Formulate transport of a single particle as a Hamiltonian system. Yields in the classical case the Hamilton-Jacobi equations for the density function.

Observations are made by integrating the observable quantity against this density function.

In the quantum mechanical transport picture observations are made by computing the trace of an observation operator with respect to a basis given by the state of the system.

It is convenient to use three different formulations at the same time:

1. The Schrödinger equation for the wave function.
2. The Liouville equation for the density matrix of a mixed state (an ensemble of particles).
3. The Wigner equation for the Wigner function.

The advantage of the Wigner function is that it relates the quantum mechanical picture to the classical one in the limit $\hbar \rightarrow 0$.

More importantly, observations are made by integrating the classical observable quantity against the Wigner function.

functions is given by the Wigner - Weyl transform.

CLASSICAL HAMILTONIAN SYSTEMS

Conservation of an energy $\mathcal{E}(x, p)$

x : position, p : momentum

$f(x, p)$: density of particles

The Hamilton - Jacobi equations

$$\partial_t f + [\mathcal{E}, f]_c = 0,$$

The classical commutator:

$$[\mathcal{E}, f]_c := \nabla_p \mathcal{E} \cdot \nabla_x f - \nabla_x \mathcal{E} \cdot \nabla_p f$$

The classical commutator conserves any function of the energy \mathcal{E} and any function of f . This is a consequence of the cyclicity of the commutator.

We have in general

$$\int a[\mathcal{E}, f]_c dxp = \int [a, \mathcal{E}]_c f dxp \quad \forall a, \mathcal{E}, f$$

Setting $a = \phi(\mathcal{E})$ and using $[\phi(\mathcal{E}), \mathcal{E}] = 0$ gives

$$\partial_t \int \phi(\mathcal{E}) f \, dxp = - \int [\phi(\mathcal{E}), \mathcal{E}]_c f \, dxp = 0$$

So, the expectation of any function $\phi(\mathcal{E})$ of the energy under the density f is conserved in time.

The classical energy in a vacuum:

$$\mathcal{E}(x, p) = \frac{1}{2m}|p|^2 + V(x) = \mathcal{E}_{kin} + \mathcal{E}_{pot}$$

$$\partial_t f + \frac{p}{m} \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = 0 \quad (1)$$

Particles:

Equation (1) has distributional solutions of the form

$$f(x, p, t) = \sum_n \delta(x - y_n(t)) \delta(p - q_n(t))$$

with y_n, q_n satisfying Newton's second law equations

$$y'_n = v_n := \frac{q_n}{m}, \quad q'_n = -\partial_x V$$

(y_n, q_n) are the classical particle paths in (x, p) phase space.

HAMILTONIAN SYSTEMS IN THE SCHRÖDINGER PICTURE

The Schrödinger equation for the evolution of the wave function $\psi(x, t)$ under the Hamiltonian H .

$$i\hbar\partial_t\psi(r, t) = H\psi = -\frac{\hbar^2}{2m}\Delta_r\psi + V(r, t)\psi$$

$\psi(r, t)$ (the state of the system) plays the role of a (time variant) coordinate system.

Observable quantities are replaced by self - adjoint operators.

A : Self adjoint operator.

$$E(A) = \int \psi(r, t)^* A[\psi](r, t) dr$$

A self adjoint $\Rightarrow E(A) \in \mathbb{R}$

c.f. : The local mass density at $r = y$.

$$A[\psi](r, t) = \delta(r - y)\psi(r, t)$$

$$\Rightarrow n(y, t) = E(A) = |\psi(y, t)|^2$$

DENSITY MATRICES AND INTEGRAL KERNELS OF OPERATORS

$\rho(r, s, t)$: density matrix , $A_d(r, s)$: integral kernel of the operator A .

$$\rho(r, s, t) = \psi(r, t)\psi(s, t)^*, \quad A[\psi](r, t) = \int A_d(r, s)\psi(s, t) ds$$

Expectation of A expressed via the density matrix:

$$E(A) = Tr(A_d \cdot \rho) = \int A_d(r, s)\rho(s, r, t) drs$$

Evolution of the density matrix:

$$i\hbar\partial_t\psi(r, t) = H\psi(r, t) = \int H_d(r, s)\psi(s, t) ds,$$

$$H_d(r, s) = -\frac{\hbar^2}{2m}\Delta\delta(r - s) + V(r, t)\delta(r - s)$$

The quantum Liouville (Heisenberg) equation for the density matrix:

$$i\hbar\partial_t\rho = H_d \cdot \rho - \rho \cdot H_d =: [H_d, \rho]_d := [H, \rho] \quad (2)$$

[.,.]: Commutator

$$[H, \rho] = \frac{\hbar^2}{2m}(\Delta_s - \Delta_r)\rho + (V(r) - V(s))\rho$$

The density matrix for a mixed state (an ensemble of particles)

There are many possible states of the system, or the system consists of many subsystems which we do not know precisely. We make an assumption about the probabilities of the possible states. State n occurs with probability P_n .

$$\rho(r, s, t) = \sum_n P_n \psi_n(r, t) \psi_n(s, t)^*,$$

satisfies the same equation (2) as the single state density matrix.

Again we have conservation because of the cyclicity of the commutator under the trace:

$$\text{Tr}(\Phi_d \cdot [H_d, \rho]) = \text{Tr}([\Phi_d, H_d] \cdot \rho), \quad \forall \Phi_d, H_d, \rho$$

Any (operator) function of the of H_d or ρ is conserved

$$\partial_t \text{Tr}(\Phi_d \rho) = -\frac{i}{\hbar} \text{Tr}([\Phi_d, H_d] \cdot \rho) = 0$$

if $\Phi_d = \phi(H_d)$: function of the self adjoint operator (density matrix) H_d ; defined via diagonalization over an orthonormal basis

$$H_d(r, s) = \sum_j \psi_j(r) \lambda_j \psi_j(s)^*, \quad \phi(H_d)(r, s) = \sum_j \psi_j(r) \phi(\lambda_j) \psi_j(s)^*,$$

$$\Rightarrow [\phi(H_d), H_d] = 0 \quad \Rightarrow \quad \text{Tr}(\phi(H_d) \cdot [H_d, \rho]) = \text{Tr}([\phi(H_d), H_d] \cdot \rho) = 0$$

WIGNER FUNCTIONS

Given a density matrix ρ for a pure or a mixed state, we define the Wigner function $f(x, \xi, t)$

$$f(x, \xi, t) = (2\pi)^{-3} \int \rho\left(x - \frac{1}{2}y, x + \frac{1}{2}y, t\right) e^{iy \cdot \xi} dy \quad (3)$$

ξ : wave vector, $\hbar\xi$: momentum

Local density:

$$\int f(x, \xi, t) d\xi = \rho(x, x, t) = n(x, t)$$

The Wigner Equation

Most easily written in terms of pseudo differential operators (PDO).

$A(\xi, y)$: Symbol of the (PDO)

$$A(\xi, -i\nabla_\xi) f(\xi) = (2\pi)^{-3} \int A(\xi, y) f(\xi') \exp[iy \cdot (\xi - \xi')] dy \xi'$$

If $\rho(r, s, t)$ satisfies the Heisenberg equation (2) then $f(x, \xi, t)$ satisfies the Wigner equation

$$\partial_t f = -\frac{\hbar}{m} \xi \cdot \nabla_x f + \Theta[V] f, \quad \Theta[V] = \frac{i}{\hbar} [V(x + \frac{1}{2i} \nabla_\xi) - V(x - \frac{1}{2i} \nabla_\xi)] \quad (4)$$

Relation to the classical case:

Rename momentum $p = \hbar \xi$ ($\hbar \xi$: momentum) and compare to (1):

$$\partial_t f_c = -\frac{\hbar}{m} \xi \cdot \nabla_x f_c + \frac{1}{\hbar} \nabla_x V \cdot \nabla_\xi f_c \quad (5)$$

Remark: (4) coincides with (5) for quadratic V .

This allows to define the quantum equivalent (= operator A) of any observable quantity $\kappa(x, \xi)$ in the classical case by requiring

$$\text{Tr}(A_d \cdot \rho) = \int \kappa(x, \xi) f(x, \xi, t) dx \xi$$

WIGNER TRANSFORM AND WEYL QUANTIZATION

The Wigner transform:

Given any linear operator a with an integral kernel (a density matrix) $a_d(x, y)$, i.e. $a(\psi)(x) = \int a_d(x, y)\psi(y) dy$, we define the corresponding Wigner function

$$W[a](x, \xi) = \int a(x - \frac{1}{2}y, x + \frac{1}{2}y)e^{iy \cdot \xi} dy, \quad f(x, \xi, t) = W[\rho](x, \xi, t)$$

Conversely, given any function $g(x, \xi)$ we define the corresponding density matrix and operator via the inverse Wigner transform

$$W^{-1}[g](r, s) = (2\pi)^{-3} \int g(\frac{r+s}{2}, \xi)e^{i\xi \cdot (r-s)} d\xi$$

Self adjoint operators and density matrices correspond to real functions.

$$a_d(r, s) = a_d(s, r)^* \iff W[a](x, \xi) \in \mathbb{R}$$

Traces of matrix products become L^2 products

$$\text{Tr}(a \cdot b) = \int a_d(r, s) b_d(s, r) drs = (2\pi)^{-3} \int W[a](x, \xi) W[b](x, \xi) dx\xi$$

Expectations of operators:

$$E(a) = \text{Tr}(a_d \cdot \rho) = \int W[a] W[f](x, \xi) dx\xi$$

A self adjoint (observable) operator a and a observable function $\kappa(x, \xi)$ are related by

$$\kappa = W[a], \quad a = W^{-1}[\kappa], \quad W^{-1}[\kappa](r, s) = (2\pi)^{-3} \int \kappa\left(\frac{r+s}{2}, \xi\right) e^{i\xi(r-s)} d\xi$$

Real functions κ correspond to self adjoint operators with integral kernels $W^{-1}[\kappa]$

Positive observables correspond positive definite operators but NOT to positive functions

\Rightarrow The Wigner function $f = W[\rho]$ is not positive and therefore not a probability.

Example: Local moment densities, operators corresponding to powers of ξ

$$m_j^{class}(z) = \int \xi^{\otimes j} f_c(z, \xi, t) d\xi, \quad m_j^{quant}(z) = \int \delta(x-z) \xi^{\otimes j} f(x, \xi, t) dx \xi,$$

So the local moment density $m_j^{class}(z)$ corresponds to the expectation of $\delta(x-z)\xi^{\otimes j}$ under the Wigner function and to the expectation of the operator $a = W^{-1}[\delta(x-z)\xi^{\otimes j}]$ in the density matrix and Schrödinger picture.

$$a(r, s) = (-i)^j \delta\left(\frac{r+s}{2} - z\right) \nabla^{\otimes j} \delta(r-s),$$

$j = 0$: mass density

$$a(r, s) = \delta\left(\frac{r+s}{2} - z\right) \delta(r-s), \quad m_0(z) = \rho(z, z)$$

$j = 1$: momentum density

$$a(r, s) = (-i) \delta\left(\frac{r+s}{2} - z\right) \nabla \delta(r-s), \quad m_1(z) = \frac{i\hbar}{2} (\nabla_s - \nabla_r) \rho(z, z)$$

In the Schrödinger picture:

$$\int \phi(r) A[\psi](r) dr = (-i)^j \nabla_y^{\otimes j} [\phi(z - \frac{1}{2}y) \psi(z + \frac{1}{2}y)]|_{y=0}$$

$$E(A) = (-i)^j \nabla_y^{\otimes j} [\psi^*(z - \frac{1}{2}y) \psi(z + \frac{1}{2}y)]|_{y=0}$$

THE HAMILTONIAN STRUCTURE OF THE WIGNER EQUATION

The commutator in the Wigner picture can be conveniently expressed in terms of the operator product of two functions. Given two Wigner functions $f(x, \xi)$, $g(x, \xi)$, we define the operator product of f and g as the Wigner transform of the matrix product of the inverse Wigner transforms of f and g :

$$f \circ g = W[W^{-1}[f] \cdot W^{-1}[g]]$$

This can be written in pseudo differential operator notation as

$$f \circ g(x, \xi) = f\left(x + \frac{i}{2}\nabla_{\xi}, \xi - \frac{i}{2}\nabla_x\right)g(x, \xi) = g\left(x - \frac{i}{2}\nabla_{\xi}, \xi + \frac{i}{2}\nabla_x\right)f(x, \xi)$$

Note: \circ is, like the matrix product, not commutative! Therefore the Wigner equation can be written in terms of the Wigner commutator as

$$\partial_t f + [\mathcal{E}, f]_w = 0$$

$$[\mathcal{E}, f]_w = \frac{i}{\hbar}(\mathcal{E} \circ f - f \circ \mathcal{E}) = \sum_{\nu=\pm 1} \mathcal{E}(x + \frac{\nu i}{2} \nabla_{\xi}, \xi - \frac{\nu i}{2} \nabla_x) f(x, \xi)$$

Because of the cyclicity of the trace we have

$$\int \Phi(\mathcal{E})[\mathcal{E}, f] dx \xi = 0, \quad \int \Phi(f)[\mathcal{E}, f] dx \xi = 0$$

for any **operator** function Φ of \mathcal{E} or f

$$\Phi(\mathcal{E}) = W[\phi(W^{-1}[\mathcal{E}])]$$

For the classical energy in a vacuum we get

$$[\frac{\hbar^2}{2m}|\xi|^2 + V(x), f]_w = \frac{\hbar}{m}\xi \cdot \nabla_x f - \frac{i}{\hbar}[V(x + \frac{1}{2i}\nabla_{\xi}) - V(x - \frac{1}{2i}\nabla_{\xi})]f$$

or, written in terms of the momentum $p = \hbar\xi$

$$[\frac{\hbar^2}{2m}|\xi|^2 + V(x), f]_w = \frac{1}{m}p \cdot \nabla_x f - \frac{i}{\hbar}[V(x + \frac{\hbar}{2i}\nabla_p) - V(x - \frac{\hbar}{2i}\nabla_p)]f$$

For $\hbar \rightarrow 0$ (formally) this reduces to the classical commutator $[\cdot, \cdot]_c$.