Non-equilibrium physics WS 20/21 – Exercise Sheet 5:

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1 Discussion:

i) What is the Wigner-Weyl transform of a quantum mechanical operator? What are similarities and differences between the quantum mechanical Wigner function and the classical phase space distribution? What are *reduced phase space distributions* and how can they be used to calculate observables?

2 In-class problems:

2.1 Quantum vs. classical dynamics of simple systems

We consider a single particle whose dynamics in one-dimension ($d = 1$) is governed by the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{\lambda}{4!}x^4$. We will now analyze the dynamics in the Wigner-Weyl formalism.

i) Calculate the Wigner-Weyl transform $H_W(x,p)$ of the Hamiltonian

ii) Write down the explicit form of the quantum evolution equation for the Wigner function $\rho_W(x,p)$. Compare your result with the Liouville equation for the evolution of the classical phase-space density $f(x,p)$. What differences do you observe?

iii) Calculate the Wigner function for the ground state of the harmonic oscillator $\hat{\rho} = |0\rangle\langle 0|$. What is the difference compared to the phase-space distribution of a classical system in the classical ground state?

iv) Calculate the Wigner function for the first excited state of the harmonic oscillator $\rho = |1\rangle\langle 1|$. What differences do you observe in comparison to the ground state?

Formulae

In coordinate space the wave-functions of the ground state and first excited state of the harmonic oscillator are given by

$$\langle x|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} \,, \tag{1}$$

$$\langle x|1\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\, x\, e^{-\frac{m\omega x^2}{2\hbar}} \,. \tag{2}$$

Some useful integrals include

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int dx\, e^{ipx} e^{-\frac{x^2}{2\sigma^2}} = e^{-\frac{\sigma^2}{2}p^2} \,, \tag{3}$$

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int dx \; e^{ipx} \; \frac{x^2}{\sigma^2} \; e^{-\frac{x^2}{2\sigma^2}} \quad = \quad (1 - p^2\sigma^2) \; e^{-\frac{\sigma^2}{2} p^2} \; . \tag{4}$$

3 Homework problems:

3.1 Extreme quantum limit

Consider again the dynamics of a single particle in one-dimension ($d = 1$) governed by the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{\lambda}{4!}x^4$. Now consider the extreme quantum limit, by keeping only the terms of highest order in $\hbar$ in the evolution equation of the Wigner function, i.e. $\partial_t \rho(t,x,p) = -\frac{\hbar^2}{24}V'''(x)\frac{\partial^3}{\partial p^3}\rho(t,x,p)$

i) Expressing the Wigner distribution as $\rho_W(t,x,p) = \int dk\ \tilde{\rho}_W(t,x,k)\ e^{ikp}$, solve the evolution equation for the Fourier transform of the Wigner distribution $\tilde{\rho}_W(t,x,k)$ in the extreme quantum limit.

ii) Consider $\rho(t=0,x,p) = \frac{(2\pi\hbar)}{L}\ \delta(p-p_0)$ as an initial condition for the Wigner distribution and determine the initial condition for $\tilde{\rho}_W(t=0,x,k)$

iii) Based on the solution for the Fourier transform of the Wigner function $\tilde{\rho}_W(t,x,k)$ in i) and the initial conditions in ii), calculate the evolution of the Wigner function $\rho_W(t,x,p)$.
$\left(\text{Hint: } \frac{1}{\pi}\int_0^\infty dk\ \cos\left(\frac{k^3}{3} + xk\right) = Ai(x) \text{ where } Ai(x) \text{ denotes the Airy function}\right)$

iv) Visualize your result for the Wigner function $\rho_W(t,x,p)$ and comment on the observed features.

3.2 Reduced phase-space distributions in an ideal gas

Consider a classical ensemble of non-interacting identical particles described by the Hamiltonian $H_N = \sum_{i=1}^N \frac{p_i^2}{2m}$. We first consider the system to be in thermal equilibrium in the canonical ensemble, such that the N-body phase space distribution is given by

$$f_N(\{x_i\},\{p_i\}) = \frac{1}{Z_N}e^{-\beta H_N}\ , \qquad Z_N = \int d^{6N}\mathcal{V}\ e^{-\beta H_N}\ , \qquad \int d^{6N}\mathcal{V} = \frac{1}{N!}\int\left(\prod_{i=1}^N \frac{d^3x_i d^3p_i}{(2\pi\hbar)^3}\right)\ . \quad (5)$$

where, recalling the results from exercise sheet one, $Z_N = \frac{Z_1^N}{N!}$ with $Z_1 = V\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}$.

i) Calculate the single particle distribution $f_1^{(N)}(x_1,p_1)$ (where the superscript (N) denotes the fact that the single particle distribution is calculated in an ensemble of N particles)

ii) Calculate the two-particle distribution $f_2^{(N)}(x_1,p_1,x_2,p_2)$. How does the result compare to the product of single particle distributions $f_1^{(N)}(x_1,p_1)f_1^{(N)}(x_2,p_2)$?

Next we consider the system to be in thermal equilibrium in the grand-canonical ensemble, where the number of particles N is allowed to vary, such that the probability to find the system in a state with N particles is given by

$$P_N = \frac{1}{Z_{GC}} Z_N e^{\frac{\mu}{k_BT}N} \quad (6)$$

where Z_{GC} denotes the grand-canonical partition function

$$Z_{GC} = \sum_{N=0}^{\infty} Z_N e^{\frac{\mu}{k_BT}N} = \exp\left(Z_1 e^{\frac{\mu}{k_BT}}\right)\ , \quad (7)$$

iii) Calculate the one and two particle distributions $f_1^{(GC)}(x_1,p_1)$ and $f_2^{(GC)}(x_1,p_1,x_2,p_2)$ in the grand canonical ensemble, by carefully summing the contributions $f_1^{(N)}(x_1,p_1)$ and respectively

$f_2^{(N)}(x_1, p_1, x_2, p_2)$ of all states with a given particle number N weighted by their probability P_N. How does the grand canonical result for the two particle distribution compare to the product of single particle distributions $f_1^{(GC)}(x_1, p_1) f_1^{(GC)}(x_2, p_2)$?