PHYS 414 Problem Set 2: Turtles all the way down

This problem set explores the common structure of dynamical theories in statistical physics as you pass from one length and time scale to another. Brownian motion is an excellent model system for this: in Problem 1 we move seamlessly from the stochastic description of the Fokker-Planck equation down to classical mechanics in the form of the Liouville equation; in Problem 2 we go from Liouville to the quantum scale, and enter the strange world of the quantum phase space representation. Here probabilities become quasiprobabilities, taking on negative values, and Dirac delta functions are outlawed by the Heisenberg uncertainty principle.

Problem 1: From Fokker-Planck to Liouville

The derivation of the Fokker-Planck equation in Problem 2 of the first homework set was for a particular potential energy $U(x) = \frac{1}{2}k_{\text{trap}}x^2$ due to the optical tweezers, with its corresponding trap force $-U'(x) = -k_{\text{trap}}x$. If we allowed $U(x)$ to be an arbitrary function, the same method would give us the general Fokker-Planck time evolution equation for $\mathcal{P}(x,p,t)$. For later convenience we express the distribution in terms of x and $p = Mv_x$ rather than x and v_x. The Fokker-Planck equation is:

$$\frac{\partial \mathcal{P}}{\partial t} = -\frac{1}{M}\frac{\partial}{\partial x}(p\mathcal{P}) + \frac{\partial}{\partial p}\left[(\Gamma p + U'(x))\,\mathcal{P}\right] + M\Gamma k_B T \frac{\partial^2 \mathcal{P}}{\partial p^2}. \tag{1}$$

Here $\Gamma = \gamma/M$, where γ is the friction coefficient and M the mass of the Brownian particle.

a) Show that Eq. (1) can be rewritten in the following form:

$$\frac{\partial \mathcal{P}}{\partial t} = -\{\mathcal{P}, H\} + \Gamma \frac{\partial}{\partial p}\left[p\mathcal{P} + Mk_B T \frac{\partial \mathcal{P}}{\partial p}\right], \tag{2}$$

where $H(x,p) = p^2/2M + U(x)$ is the Hamiltonian of the Brownian particle and $\{A, B\}$ denotes the Poisson bracket of two functions $A(x,p)$ and $B(x,p)$:

$$\{A, B\} \equiv \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}. \tag{3}$$

The $\Gamma \to 0$ limit of Eq. (1) is the *Liouville equation*, describing the time evolution of a probability distribution under classical mechanics. This corresponds to diluting the gas surrounding the Brownian particle until it feels no collisions. We can get the same classical limit by looking at motion on time scales $t \ll \Gamma^{-1}$, when collisions have not yet had a substantial impact on the particle. Our Liouville equation is for a single particle of mass M moving in a potential $U(x)$, but the Liouville formulation can be easily generalized to many particles and an arbitrary Hamiltonian. Eq. (2) is nice because it shows that the stochastic time evolution of the Brownian particle is just classical mechanics plus "correction" terms proportional to Γ that lead to diffusive spreading of probability distributions.

b) Convince yourself that the Liouville equation describes classical trajectories: show that the probability distribution

$$\mathcal{P}(x,p,t) = \delta(x - x_c(t))\delta(p - p_c(t)) \tag{4}$$

is a solution to Eq. (2) when $\Gamma = 0$. Here $x_c(t)$ and $p_c(t)$ are functions of time that describe the motion of a classical particle with Hamiltonian $H(x,p) = p^2/2M + U(x)$. Hence they satisfy Hamilton's equations:

$$\frac{d}{dt}x_c(t) = \frac{\partial H}{\partial p}(x_c(t), p_c(t)), \qquad \frac{d}{dt}p_c(t) = -\frac{\partial H}{\partial x}(x_c(t), p_c(t)). \tag{5}$$

So for a distribution in phase space that starts as a delta function, $\mathcal{P}(x,p,0) = \delta(x-x_0)\delta(p-p_0)$, it will remain a delta function for all $t \geq 0$ centered at the corresponding classical trajectory. If $\Gamma \neq 0$, the delta function would broaden out over time under the diffusive effects of the gas environment. *Hint:* The following Dirac delta function properties may be useful: for any function $F(a)$ that is non-singular at $a = a_0$, we can write $F(a)\delta(a-a_0) = F(a_0)\delta(a-a_0)$ and $F(a)\delta'(a-a_0) = F(a_0)\delta'(a-a_0) - F'(a_0)\delta(a-a_0)$. Here $\delta'(a)$ is the first derivative of the Dirac delta function.

c) It is useful to compare the behavior of the mean energy $\langle H \rangle(t) = \int dx\, dp\, H(x,p)\mathcal{P}(x,p,t)$ in the stochastic ($\Gamma > 0$) versus classical ($\Gamma = 0$) regimes. Using Eq. (2) and integration by parts, show that:

$$\frac{d}{dt}\langle H \rangle = -\Gamma \int dx\, dp\, p \left[\frac{p}{M}\mathcal{P} + k_B T \frac{\partial \mathcal{P}}{\partial p} \right]. \tag{6}$$

Hence when $\Gamma = 0$, $d\langle H \rangle/dt = 0$ and the mean energy does not change with time: it is a constant of motion for classical trajectories. When $\Gamma > 0$, in general $d\langle H \rangle/dt$ does not have to be zero. The Brownian particle can gain or lose energy through collisions with the surrounding gas environment. In one special case $d\langle H \rangle/dt = 0$ even when $\Gamma > 0$: show that this is true when the Brownian particle has an equilibrium distribution $\mathcal{P}_{\text{eq}} \propto \exp(-H/k_B T)$. In equilibrium the mean energy $\langle H \rangle$ stays constant, since there is no net energy exchange with the environment on average (gain is balanced by loss).

d) Imagine that in addition to the force from the potential $U(x)$, there is an external force F_{ext} on the Brownian particle (imposed for example by an experimentalist). Find the extra term that appears on the right-hand-side of Eq. (2), and show this gives the following addition to Eq. (6):

$$\frac{d}{dt}\langle H \rangle = -\Gamma \int dx\, dp\, p \left[\frac{p}{M}\mathcal{P} + k_B T \frac{\partial \mathcal{P}}{\partial p} \right] + \frac{F_{\text{ext}}}{M} \int dx\, dp\, p\mathcal{P}. \tag{7}$$

Argue that this extra term is just the average rate of work done on the Brownian particle by the external force. Notice that this term is independent of Γ: it appears both in the classical and stochastic regime.

Problem 2: From Liouville to Quantum Mechanics

"Negative energies and probabilities should not be considered as nonsense. They are well-defined concepts mathematically, like a negative of money."

Paul Dirac, 1942

Let us now zoom in even further, studying the motion of our Brownian particle at time and length scales so small that quantum effects become important. We will assume that during these minuscule time intervals the gas particles have no time to reach and collide with the bead, so we are really just dealing with a single quantum particle of mass M in a potential $U(x)$. Ideally we would like a way of modifying our Liouville equation for the classical motion of the particle to include quantum correction terms, proportional to $\hbar$. In the classical limit, $\hbar$ could be assumed negligible compared to the distance/momentum scales of interest, and we would recover the Liouville equation.

There is one problem: in the standard formulation of quantum mechanics, we never speak of a probability density $\mathcal{P}(x,p,t)$ defined over the phase space of (x,p). There is a good reason for this: a delta function probability distribution in phase space, like the classical result in Eq. (4), would violate Heisenberg's uncertainty principle, since both x and p would be known simultaneously. The answer to this problem was developed by Weyl, Wigner, Groenewold, and Moyal through the 1930's and 1940's, and came to be known as the *phase space formulation* of quantum mechanics. It is an alternative to the two better known approaches to quantization: the standard Schrödinger-Heisenberg picture of operators in a Hilbert space, and the Feynman path integral representation. Though it is formally equivalent to both of them, it languished for many years (negative probabilities are freakish!), until recently it has been resurrected as a research tool for understanding quantum optics and the decoherence of quantum systems interacting with the environment (a major issue in quantum computing). For more historical background, there is a nice article by Thomas Curtright and Cosmas Zachos at: arxiv.org/abs/1104.5269. This problem will not do full justice to the quantum phase space picture, but it will explore some of its salient features, and the elegant relationship between the quantum and classical time evolution equations.

a) The basic tool to derive all the properties of the phase space representation is the *Wigner transformation*, a map W that converts any Hilbert space operator $\hat{A}$ in the standard picture of quantum mechanics to a corresponding scalar function $A(x,p) = W\{\hat{A}\}$ of x and p (which are the real-valued position and momentum of the particle):

$$A(x,p) = W\{\hat{A}\} \equiv 2\int_{-\infty}^{\infty} \langle x+y|\hat{A}|x-y\rangle e^{-2ipy/\hbar} dy. \tag{8}$$

Prove that $A(x,p)$ is real-valued if $\hat{A}$ is Hermitian. Also show that $A(x,p)$ can be expressed equivalently as an integral over momentum instead of position:

$$A(x,p) = W\{\hat{A}\} = 2\int_{-\infty}^{\infty} \langle p+q|\hat{A}|p-q\rangle e^{2ixq/\hbar} dq. \tag{9}$$

Hint: Standard quantum mechanics in a nutshell: $|x\rangle$ and $|p\rangle$ are eigenstates of the $\hat{x}$ and $\hat{p}$ operators respectively. In other words, $\hat{x}|x\rangle = x|x\rangle$, $\hat{p}|p\rangle = p|p\rangle$. Here are several useful properties of the eigenstates:

$$\begin{aligned} &\langle x|p\rangle = \langle p|x\rangle^* = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}, \qquad 1 = \int dx\, |x\rangle\langle x| = \int dp\, |p\rangle\langle p| \\ &\langle x|x'\rangle = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|x'\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{ip(x-x')/\hbar} = \delta(x-x'), \qquad \langle p|p'\rangle = \delta(p-p') \end{aligned} \tag{10}$$

You may also find the following identity useful: $\delta(ax) = |a|^{-1}\delta(x)$ for any constant a.

b) For a particle described by some quantum state $|\Psi\rangle$, define a Hermitian operator $\hat{\mathcal{P}} \equiv (2\pi\hbar)^{-1}|\Psi\rangle\langle\Psi|$ (this is proportional to what we will later call the *density operator*). The Wigner transformation $\mathcal{P}(x,p) = W\{\hat{\mathcal{P}}\}$ is the central quantity in the phase space formulation, and in the classical limit corresponds to the familiar phase space probability density. However, we have to be careful, because at the quantum level $\mathcal{P}(x,p)$ is almost (but not quite) a probability distribution. Hence it is called a *quasiprobability distribution*. To understand this, let us first discuss the good news. Derive the following properties of $\mathcal{P}(x,p)$:

$$\int dp\, \mathcal{P}(x,p) = |\langle x|\Psi\rangle|^2, \qquad \int dx\, \mathcal{P}(x,p) = |\langle p|\Psi\rangle|^2, \qquad \int dx\, dp\, \mathcal{P}(x,p) = 1. \tag{11}$$

So far everything looks great: the marginal probability density of finding the particle at position x is $|\langle x|\Psi\rangle|^2$, exactly as standard quantum mechanics predicts, and similarly the marginal probability density of finding the particle with momentum p is $|\langle p|\Psi\rangle|^2$. Moreover, these two properties guarantee that $\mathcal{P}(x,p)$ is properly normalized over all phase space.

c) Now the strangeness begins: from the definition of the Wigner transformation in Eq. (8), note that there is no guarantee that $\mathcal{P}(x,p)$ is actually positive. (All that you know from part b is that the integrals over $\mathcal{P}(x,p)$ in either coordinate have to be positive.) As it turns out, $\mathcal{P}(x,p)$ can take on negative values, though the negative regions are small (on the order of $\hbar$) and hence will not have observable consequences in the classical limit, where you look at phase space at scales $\gg \hbar$. To see this for yourself, calculate the Wigner transforms of the first two eigenstates $|\Psi_0\rangle$ and $|\Psi_1\rangle$ of the quantum harmonic oscillator, which has Hamiltonian $\hat{H} = \hat{p}^2/2m + M\omega^2\hat{x}^2/2$. These eigenstates with energies $E_0 = \hbar\omega/2$ and $E_1 = 3\hbar\omega/2$ have the x-space representation:

$$\langle x|\Psi_0\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}, \qquad \langle x|\Psi_1\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\, x e^{-\alpha x^2/2}, \tag{12}$$

where $\alpha \equiv M\omega/\hbar$. Show that the corresponding Wigner transforms are:

$$\mathcal{P}_0(x,p) = \frac{1}{\pi\hbar} e^{-\alpha x^2 - p^2/(\alpha\hbar^2)}, \qquad \mathcal{P}_1(x,p) = \frac{2p^2 + \alpha\hbar^2(2\alpha x^2 - 1)}{\alpha\pi\hbar^3} e^{-\alpha x^2 - p^2/(\alpha\hbar^2)}. \tag{13}$$

The function $\mathcal{P}_0(x,p)$ is everywhere positive, but $\mathcal{P}_1(x,p)$ has a pronounced negative dip around $(x,p) = (0,0)$. The fact that $\mathcal{P}(x,p)$ can become negative is one reason it is called a quasiprobability distribution.

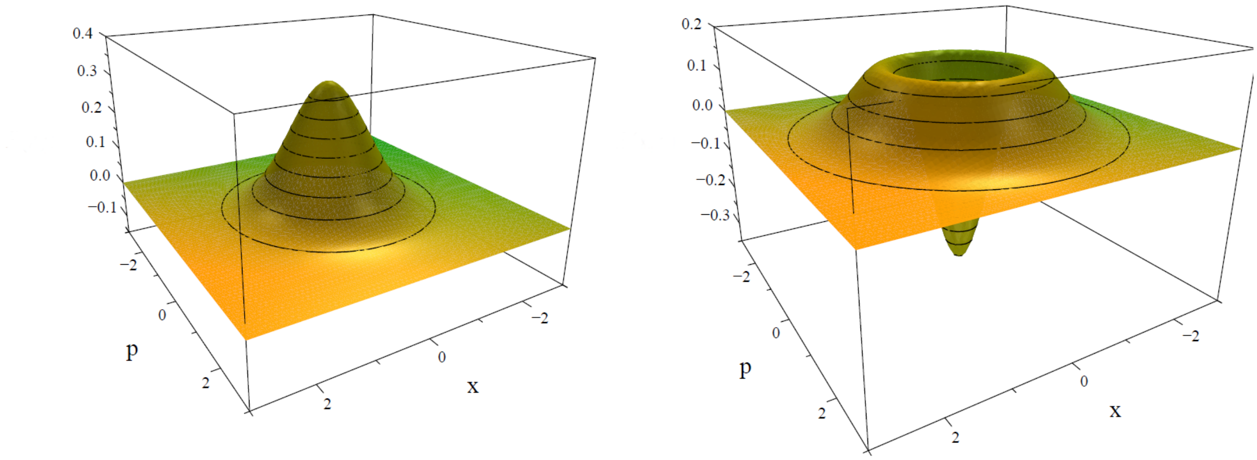

Figure 1: Simple harmonic oscillator eigenstates $\mathcal{P}_0(x,p)$ [left] and $\mathcal{P}_1(x,p)$ [right] in the phase space representation. Images courtesy of Curtright and Zachos, arxiv.org/abs/1104.5269.

d) Another reason $\mathcal{P}(x,p)$ is a quasiprobability is that it is strictly bounded in magnitude, something not true of actual probability distributions in the classical limit (think of Dirac delta functions with their infinite peaks). Show that $\mathcal{P}(x,p)$ must satisfy:

$$|\mathcal{P}(x,p)| \leq \frac{1}{\pi\hbar}. \tag{14}$$

This is a direct reflection of the Heisenberg uncertainty principle: probabilities cannot become arbitrarily concentrated (spiked) in regions of phase space on the order of $\hbar$, since that would allow both x and p to be determined simultaneously with arbitrary accuracy. As $\hbar \to 0$, these height restrictions become relaxed. *Hint:* Use the Cauchy-Schwarz inequality, which states that for any square-integrable complex functions $F(x)$ and $G(x)$, the following holds:

$$\left| \int dx\, F(x) G^*(x) \right|^2 \leq \left(\int dx\, |F(x)|^2 \right) \left(\int dx\, |G(x)|^2 \right). \tag{15}$$

Experimental interlude: The harmonic oscillator Wigner functions shown in Fig. 1 are extremely important in quantum optics. It turns out that quantizing the electric field leads to a Hamiltonian which has exactly the same form as a harmonic oscillator, with $\hat{x}$ and $\hat{p}$ mapped to the real and imaginary parts of the complex electric field amplitude. The ground state $\mathcal{P}_0$ is called the vacuum state: it represents a state with no photons, but there is still a finite probability of nonzero (x,p) due to quantum fluctuations. The first excited state $\mathcal{P}_1$ represents a single photon. Amazingly, this single photon Wigner function can be experimentally measured using a technique called homodyne tomography. For more details see the experimental paper by A.I. Lvovsky *et al.*, Phys. Rev. Lett. **87**, 050402 (2001) [posted on the course website]. There is also a nice overview at the group's website [http://www.iqst.ca/quantech/research/fock.php] along with a gallery of Wigner functions (check out the Schrödinger cat state!).

e) The final step in surveying the phase space picture is time evolution. First, use the time-dependent Schrödinger equation, $i\hbar(\partial/\partial t)|\Psi\rangle = \hat{H}|\Psi\rangle$, to derive the time evolution of the density operator $\hat{\mathcal{P}}$ introduced above. Show that:

$$\frac{\partial}{\partial t}\hat{\mathcal{P}} = \frac{1}{i\hbar}[\hat{H}, \hat{\mathcal{P}}]. \tag{16}$$

Here $\hat{H} = \hat{p}^2/2m + U(\hat{x})$ is the Hamiltonian operator, and $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator. Though this is often called the quantum version of the Liouville equation, it is not transparent what the classical limit $\hbar \to 0$ means in this operator form. You will now transform Eq. (16) into the phase space representation, where the connection to the classical Liouville equation is more apparent.

f) In order to make the transformation easier, derive the following Wigner transforms:

$$\begin{aligned} W\{\hat{H}\} &= \frac{p^2}{2m} + U(x) \equiv H(x,p), \qquad W\{[\hat{p}^2, \hat{\mathcal{P}}]\} = -2i\hbar p \frac{\partial}{\partial x}\mathcal{P}(x,p) \\ W\{[\hat{x}, \hat{\mathcal{P}}]\} &= i\hbar \frac{\partial}{\partial p}\mathcal{P}(x,p), \qquad W\{[\hat{x}^2, \hat{\mathcal{P}}]\} = 2i\hbar x \frac{\partial}{\partial p}\mathcal{P}(x,p) \\ W\{[\hat{x}^3, \hat{\mathcal{P}}]\} &= \left(3i\hbar x^2 \frac{\partial}{\partial p} - \frac{1}{4} i\hbar^3 \frac{\partial^3}{\partial p^3}\right)\mathcal{P}(x,p) \end{aligned} \tag{17}$$

When carrying out the derivations, make sure to use the appropriate definition of the Wigner transform, either Eq. (8) or Eq. (9). The former is more convenient with $\hat{x}$ operators, while the latter is easier with $\hat{p}$ operators.

g) Now apply the Wigner transform to both sides of Eq. (16). To make life simpler, expand $U(\hat{x})$ in a Taylor series to third-order, $U(\hat{x}) \approx v_0 + v_1\hat{x} + v_2\hat{x}^2 + v_3\hat{x}^3$, and ignore higher-order contributions. The end result should look like:

$$\frac{\partial \mathcal{P}}{\partial t} = -\{\mathcal{P}, H\} - \frac{v_3\hbar^2}{4}\frac{\partial^3 \mathcal{P}}{\partial p^3} + \cdots, \tag{18}$$

where $\{\cdot,\cdot\}$ is just the classical Poisson bracket of Eq. (3). If you had included more terms in the Taylor series for $U(\hat{x})$, you would end up with higher-order terms in $\hbar$. Remarkably the structure of the equation is analogous to Eq. (2): you have a classical Liouville equation plus correction terms that lead to additional "diffusive" broadening of the probability distribution. Instead of being proportional to Γ as in Problem 1, here the correction terms depend on $\hbar$. The "diffusion" term (with the odd third derivative) is not because of the environment, but rather because of the inherent stochastic nature of quantum mechanics. When the higher-order terms in Eq. (18) are included (don't try this at home!), you can get a closed-form expression for the right-hand side known as the *Wigner-Moyal equation*. If you want to see Wigner-Moyal time evolution in action, the Wikipedia article [http://en.wikipedia.org/wiki/Wigner_quasiprobability_distribution] has several instructive animations: Wigner functions are among the nicest ways to visualize the dynamics of quantum particles.

Interestingly, if your Hamiltonian only has terms up to second order in x (like the harmonic oscillator), so $v_i = 0, \forall i \geq 3$, Eq. (18) predicts a purely classical Liouville time evolution. For such a system, the quantum effects come not from the time evolution equation, but from the fact that your initial distribution $\mathcal{P}(x,p)$ at $t = 0$ has to satisfy Eq. (14) (as well as the various normalization conditions in Eq. (11)). You cannot start out with Dirac delta functions as in classical mechanics.