Homework set 7

Math 444

This final assignment won't be collected. You should read it in detail by Thursday (12/08/22) so that we can discuss it in class. It concerns the classical harmonic oscillator and its quantization.

Let us first recall the following basic facts about Hamiltonian systems already discussed in class. We assume for simplicity that the mechanical system has a configuration manifold which is an open subset $\mathcal{U}$ of $\mathbb{R}^n$. We say that n is the number of *degrees of freedom* of the system. Let $\mathcal{S} = \mathcal{U} \times \mathbb{R}^n$ be the *phase space*. The points (q, p) in $\mathcal{S}$ represent the generalized positions, q, and momenta, p. The dynamic is specified by a choice of Hamiltonian, which is a (continuously differentiable as many times as needed) function $H : \mathcal{S} \to \mathbb{R}$. I'll denote the set of such nice functions by $\mathcal{O}$ and generally refer to functions in $\mathcal{O}$ as (classical) *observables*. Thus the Hamiltonian is an observable. We write

$$H(q, p) = H(q_1, \ldots, q_n, p_1, \ldots, p_n).$$

The equations of motion are then given by *Hamilton's equations*:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad i = 1, \ldots, n.$$

As our main example, the Hamiltonian for the 1-dimensional harmonic oscillator if

$$H(q, p) = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 q^2,$$

where m indicates the mass of a point particle and both m and $\omega > 0$ are constants. Hamilton's equations are

$$\frac{dq}{dt} = \frac{1}{m} p, \quad \frac{dp}{dt} = -m\omega^2 q.$$

Note that the first equation gives $p = mv$ where $v = dq/dt$ is the particle's velocity. The second is Newton's equation: on the left side is the familiar mass × acceleration term and on the right side is the Newtonian force that acts on the particle.

More generally, if $f \in \mathcal{O}$ we may define $f_t(q, p) := f(q(t), p(t))$. It then turns out that

$$\frac{df_t}{dt} = \{H, f_t\}, \tag{1}$$

where the *Poisson bracket* $\{\cdot, \cdot\} : \mathcal{O} \times \mathcal{O} \to \mathcal{O}$ is defined as

$$\{f, g\} = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} - \frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} \right).$$

Remark: Using the chain rule and Hamilton's equations, it is not difficult to show that $\frac{df_t}{dt} = \{H, f\}_t$. In order to obtain Equation (1) we need further $\{f, g\}_t = \{f_t, g_t\}$. (It is easy to check that $H_t = H$.) See the notes on Hamiltonian mechanics in Canvas (Pages, item 37) for more details on this calculation. (Those notes are still in rather rough form!)

Note that

$$\{H,q_j\} = \frac{\partial H}{\partial p_j},\ \ \{H,p_j\} = -\frac{\partial H}{\partial q_j}.$$

So the Poisson equation implies Hamilton's equations. The Poisson bracket on $\mathcal{O}$ turns this vector space into a Lie algebra as you will check in Exercise 1.

1. *The Poisson Lie algebra.* We have introduced above the Poisson bracket $\{\cdot,\cdot\}:\mathcal{O}\times\mathcal{O}\to\mathcal{O}$ where $\mathcal{O}$ is the space of functions on $\mathbb{R}^{2n}$ which are continuously differentiable to all orders. (This is often denoted $C^\infty(\mathbb{R}^n)$.)

   (a) Show that $(\mathcal{O},\{\cdot,\cdot\})$ is a Lie algebra. It is clear that $\{f,g\}=-\{g,f\}$ and that $f\mapsto\{f,g\}$ is linear. You only need to check that the *Jacobi identity* holds:

   $$\{f,\{g,h\}=\{\{f,g\},h\}+\{g,\{f,h\}\}.$$

   In addition, check that $\{f,gh\}=\{f,g\}h+g\{f,h\}$. (The concept of Lie algebra does not require this relation.)

   (b) Verify the *Canonical Commutation Relations* (CCR):

   $$\{q_i,q_j\}=\{p_i,p_j\}=0,\ \ \{p_i,q_j\}=\delta_{ij}.$$

   (c) Let us consider the 1-dimensional harmonic oscillator example. Let $\mathbf{1}$ denote the constant function equal to 1. Check that

   $$\{p,q\}=\mathbf{1},\ \ \{H,q\}=p/m,\ \ \{H,p\}=-m\omega^2q.$$

   Naturally, $\{q,q\}=\{p,p\}=\{H,H\}=\{\mathbf{1},\cdot\}=0$. The (real) 4-dimensional subspace of $\mathcal{O}$ (for $\mathbb{R}^2$) spanned by $\{q,p,H,\mathbf{1}\}$ thus defines a Lie algebra, called the *harmonic oscillator Lie algebra*.

   (d) It is useful to introduce complex valued coordinates:

   $$z=\frac{1}{\sqrt{2m\omega\hbar}}\big(m\omega q+ip\big),\quad \overline{z}=\frac{1}{\sqrt{2m\omega\hbar}}\big(m\omega q-ip\big).$$

   Introducing Planck's constant $\hbar$ here only serves the purpose of making z dimensionless. (The term $\omega\hbar$ has physical dimension of energy so $\sqrt{m\omega\hbar}$ has the physical dimension of momentum.) Check that, in terms of $z,\overline{z}$, the harmonic oscillator Hamiltonian becomes

   $$H\big(z,\overline{z}\big)=\omega\hbar|z|^2.$$

   We can extend the Poisson bracket to complex-valued functions by complex linearity:

   $$f+ig\mapsto\{f+ig,\cdot\}=\{f,\cdot\}+i\{g,\cdot\}.$$

   Verify that the harmonic oscillator Poisson Lie algebra satisfies the bracket relations:

   $$\{z,\overline{z}\}=\frac{i}{\hbar}\mathbf{1},\ \ \{H,z\}=-\omega iz,\ \ \{H,\overline{z}\}=\omega i\overline{z}.$$

2. Quantizing the harmonic oscillator is interpreted as obtaining an operator representation of the Poisson Lie algebra of the classical (1-dimensional) harmonic oscillator. Thus we wish to replace the classical phase space $\mathbb{R}^2$ with a Hilbert space $\mathcal{H}$ and the observables q,p,H with self-adjoint operators Q,P,H on $\mathcal{H}$. There are issues

of domain definition that need to be taken into account, but let us ignore them for the moment. The Poisson bracket is replaced with the operator commutator:

$$\{f,g\} \rightsquigarrow \frac{i}{\hbar}[F,G] = \frac{i}{\hbar}(FG-GF),$$

where F, G are the operator observables to be associated to the classical observables f, g, respectively. The imaginary i needs to be added so that $i[F,G]$ can still be self-adjoint. Let us denote by Q, P and H the self-adjoint operators to be associated to the classical obsevables q, p and H, where

$$H = \frac{1}{2m}\left(P^2 + (m\omega Q)^2\right).$$

The commutation relations are now

$$[P,Q] = \frac{\hbar}{i}I, \ \ [H,Q] = -\frac{\hbar i}{m}P, \ \ [H,P] = -im\omega^2\hbar Q.$$

We may also consider the non-self-adjoint operators a, a^* associated to the complex valued functions $z, \overline{z}$:

$$a := \frac{1}{\sqrt{2m\omega\hbar}}(m\omega Q + iP), \ \ a^* := \frac{1}{\sqrt{2m\omega\hbar}}(m\omega Q - iP).$$

Check that the following identities hold:

$$[a,a^*] = I, \ \ [a^*a, a] = -a, \ \ [a^*a, a^*] = a^*, \ \ H = \omega\hbar\left(a^*a + \frac{1}{2}I\right). \tag{2}$$

Notice the presence of the term $(1/2)I$ in H, which didn't appear in the corresponding classical expression

$$H = \omega\hbar z\overline{z}$$

due to commutativity for functions.

As we discussed in class, the central problem in solving the Schrödinger equation $\frac{du_t}{dt} = -\frac{i}{\hbar}Hu_t$ for a given Hamiltonian H is to determine the spectral resolution of H. For the harmonic oscillator, this is equivalent to determining the spectral resolution of a^*a. We investigate this next.

3. *Spectrum of a^*a assuming the existence of an eigenvector.* Prove the following statements using the commutation relations $[a,a^*] = I, [a^*a,a] = -a, [a^*a,a^*] = a^*$. These are operators on a given Hilbert space $\mathcal{H}$. We assume that the self-adjoint operator a^*a admits an eigenvector $u \neq 0$: $a^*au = \lambda u$. (In finite dimensions, every self-adjoint operator admits an eigenvector, but one of the conclusions to be drawn from the results of this exercise is that the Lie algebra of CCR, at least for the harmonic oscillator, does not admit a representation by operators on a finite-dimensional Hilbert space. And in infinite dimensions it is not necessarily the case that self-adjoint operators have eigenvectors. For example, the operator of multiplication by x, $f(x) \mapsto xf(x)$, on the Hilbert space $L^2(\mathbb{R}, dx)$ does not admit eigenvectors.)

   (a) Show that
   $$a^*a(au) = (\lambda-1)au, \quad a^*a(a^*u) = (\lambda+1)a^*u.$$
   (Note: $a^*aa = aa^*a + [a^*a,a]$.) It follows by induction that
   $$a^*aa^m u = (\lambda - m)a^m u, \quad a^*a(a^*)^m u = (\lambda+m)a^*u.$$

(b) Show that $\lambda = \|au\|^2/\|u\|^2 \geq 0$. Thus every eigenvalue of a^*a is nonnegative.

(c) Using the first item of this exercise, show that there must be a smallest nonnegative integer n such that

$$a^{n+1}u = 0, \;\; a^n u \neq 0.$$

Let us write $u_0 := a^n u$. Thus $au_0 = 0$. Observe that

$$0 = a^*au_0 = a^*aa^n u = (\lambda - n)(\lambda - n)a^n u = (\lambda - n)u_0.$$

Since $u_0 \neq 0$, we can conclude that $\lambda = n$.

(d) For $m = 1, 2, \dots$ let us define the sequence $u_m := (a^*)^m u_0$. Thus $u_{m+1} = a^* u_m$ for each m. Show that

$$a^*au_m = mu_m.$$

This can be show by a simple induction. Note first that $a^*au_0 = 0$. Then use the first item to show that if $a^*au_m = mu_m$ then $a^*au_{m+1} = (m+1)u_{m+1}$.

(e) Without loss of generality, we may suppose that u_0 is a unit vector. Show that for positive integers m, m',

$$\langle u_m, u_{m'} \rangle = m!\delta_{mm'}.$$

Note: For nonnegative integers m, m',

$$\begin{aligned}(m - m')\langle u_m, u_{m'}\rangle = \langle mu_m, u_m'\rangle - \langle u_m, m'u_{m'}\rangle = \langle a^*au_m, u_{m'}\rangle - \langle u_m, a^*au_{u_m}\rangle \\ = \langle au_m, au_{m'}\rangle - \langle au_m, au_{m'}\rangle = 0.\end{aligned}$$

Conclude from this that if $m \neq m'$ then $\langle u_m, u_{m'}\rangle = 0$. When $m = m'$, use induction, starting from the assumption that $\langle u_0, u_0\rangle = 1$. Note:

$$\langle u_{m+1}, u_{m+1}\rangle = \langle a^* u_m, a^* u_m\rangle = \langle u_m, aa^* u_m\rangle = \langle u_m, (a^*a + [a, a^*])u_m\rangle.$$

From this one obtains $\langle u_{m+1}, u_{m+1}\rangle = (m+1)\langle u_m, u_m\rangle$. The initial claim can now be seen to follow from a simple induction.

(f) Show that $au_{m+1} = (m+1)u_m$ for all nonnegative integer m. Note: $au_{m+1} = aa^* u_m = (a^*a + [a, a^*])u_m$.

(g) Note that the harmonic oscillator Lie algebra does not admit a representation in a finite dimensional Hilbert space. If fact, from the above discussion we have: $\mathcal{H}$ admits an orthonormal system $\{v_0, v_1, v_2 \cdots\}$ consisting of eigenvectors of a^*a such that $v_m := u_m/\sqrt{m!}$ for each nonnegative integer m, with corresponding eigenvalues $0, 1, 2 \dots$. Furthermore, $av_{m+1} = \sqrt{m+1}\,v_m$ and $a^* v_m = \sqrt{m+1}\,v_{m+1}$. In particular, the eigenvalues of the Hamiltonian H (see Equation (2) for the expression of H in terms of a, a^*) are

$$E_m := \left(m + \frac{1}{2}\right)\omega\hbar.$$

The eigenvector v_0 associated to the least energy $E_0 = \omega\hbar/2$ is called the *ground state*. The *ladder operators* a^* and a are also known as the *creation* and *annihilation* operators.

4. *The Schrödinger representation of the canonical commutation relations.* The discussion in the previous exercise is purely algebraic and abstract. It shows what the operators associated to the Harmonic oscillator, in particular

the Hamiltonian, should look like in a diagonalizing basis, but we still need to contend with the assumption that an eigenvector exists. Let us look for a concrete representation of these operators in a specific Hilbert space. I will omit issues related to domains of definition of these operators, at least for the moment. Let the Hilbert space be the space of square integrable functions on the real line with the Lebesgue (i.e., the standard $\mu(A) := \int_A dx$) measure: $L^2(\mathbb{R}, dx)$ and inner product $\langle \varphi_1, \varphi_2 \rangle := \int_{-\infty}^{\infty} \overline{\varphi_1(x)} \varphi_2(x)\, dx$. Let us define $x := q/D$ where $D = \sqrt{\hbar/m\omega}$, so that $d/dx = D d/dq$. Let us also write

$$a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \quad a^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

These operators are note defined on the entire Hilbert space. Their domains contain all functions that are infinitely continuously differentiable and decay sufficiently fast to 0 as $x \to \pm\infty$. In particular, the function

$$\psi_0(x) := Ce^{-x^2/2}$$

is in the domain of any polynomial function of the operators a and a^*. The constant $C = 1/\pi^{1/4}$ is a normalization constant. Expressed in terms of q,

$$\psi_0(q) = \left(\frac{\pi m\omega}{\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}q^2}.$$

(a) Show that the above a^* is indeed the adjoint of a and that $[a, a^*] = I$.

(b) Show that $\psi_0(x)$ is an eigenfunction for a^*a with eigenvalue 1.

(c) Argue that the space of all functions of the form $P(x)e^{-x^2/2}$ where $P(x)$ is any polynomial in x is invariant under an arbitrary (finite) number of applications of the operators a and a^*. Therefore the conclusions of the previous exercise hold and all the eigenfunctions $\psi_m(x)$ of a^*a associated to eigenvalue m are of this form. That is,

$$\psi_m(x) = H_m(x)e^{-x^2/2}.$$

The functions $H_m(x)$ are known as the *Hermite polynomials*. Without regard to normalization, show (based on the relation $u_{m+1} = a^* u_m$ of the previous exercise) that

$$H_{m+1}(x) = \frac{1}{\sqrt{2}}\left(2xH_m(x) - H_m'(x)\right).$$

This provides one way of iteratively obtaining all $H_m(x)$.

(d) Think about the following statement: The functions $\psi_0(x), \psi_1(x), \ldots$ (properly normalized) constitute an orthonormal basis of $L^2(\mathbb{R}, dx)$. The notion of a basis for an infinite dimensional Hilbert space should now be understood in the sense that the linear span of these vectors (i.e., all the finite linear combinations) is a dense subspace of the Hilbert space. To say that the subspace is dense means that any vector in the Hilbert space can be written as a converging sequence of elements in the subspace. This can be argued based on the Weierstrass approximation theorem (for approximating continuous functions by polynomials) and the fact that square integrable functions can be approximated by continuous functions in the natural norm on the Hilbert space. We can, after the fact, argue that all the manipulations used in the previous exercise make rigorous mathematical sense and indeed solve the problem of quantizing the harmonic oscillator.