# M393C NOTES: TOPICS IN MATHEMATICAL PHYSICS

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These notes were taken in UT Austin's M393C (Topics in Mathematical Physics) class in Fall 2017, taught by Thomas Chen. I live-TEXed them using `vim`, so there may be typos; please send questions, comments, complaints, and corrections to a.debray@math.utexas.edu. Thanks to Yanlin Cheng for fixing some typos.

## Contents



Lecture 1.

## The Lagrangian formalism for classical mechanics: 8/31/17

The audience in this class has a very mixed background, so this course cannot and will not assume any physics background. We'll first discuss classical and Lagrangian mechanics. Quantum mechanics is, of course, more fundamental, and though historically people obtained quantum mechanical mechanics from classical mechanics, it should be possible to go in the other direction.

We'll start, though, with classical and Lagrangian mechanics. This involves understanding symplectic and Poisson structures, and the principle of least action, the beautiful insight that classical mechanics can be formulated variationally; there is a Lagrangian $L$ and an action functional

$$S = \int_{t_0}^{t_1} L \, \mathrm{d}t,$$

and the system evolves through paths that extremize the action functional.

The history of the transition from classical mechanics to quantum mechanics to quantum field theory happened extremely quickly in the historical sense, all fitting into one lifetime. JJ Thompson discovered the electron in 1897, and in 1925, GP Thompson, CJ Dawson, and LH Germer discovered that it had mass. This led people to discover some inconsistencies with classical physics on small scales, ushering in quantum mechanics, with all of the famous names: Einstein, Schrödinger, Heisenberg, and more. The basic equations

of quantum mechanics fall in linear dispersive PDE for functions living in the Hilbert space, typically $L^2$ or the Sobolev space $H^1$ (since energy involves a derivative).

One of the key new constants in quantum mechanics is *Planck's constant* $\hbar := h/2\pi$. It has the same units as the classical action $S$, and therefore they are comparable. There is a sense in which quantum mechanics is the regime in which $S/\hbar \approx 1$, and classical mechanics is the regime in which $S/\hbar \gg 1$. In this sense, quantum mechanics is the physics of very small scales. Sometimes people take a "semiclassical limit," and say they're letting $\hbar \to 0$, but this makes no sense: $\hbar$ is a physical quantity. Instead, it's more accurate to say taking a semiclassical limit lets $(S/\hbar)^{-1} \to 0$.

If you want to analyze a fixed number of electrons, life is good. They will always be there, and so on. But this is a problem for photons, as there are physical processes which create photons, and processes which destroy photons. Thus imposing a fixed number of quantum particles is a constraint — and the theory which describes the quantum physics of arbitrary numbers of quantum particles, quantum field theory, was worked out a little later. In this case, the Hilbert space is a direct sum over the Hilbert subspace of 1-particle states, 2-particle states, etc., and is called *Fock space*. The symplectic and Poisson structures of classical mechanics, transformed into commutation relations of operators in quantum mechanics, is again interpreted as commutation relations of creation and annihilation operators.

The mathematics of quantum field theory is rich and diverse, drawing in more PDE as well as large amounts of geometry and topology. But there's a problem — many important integrals and power series don't converge. And this is not a formal series problem: it's too central. Physicists have used renormalization as a formal trick to solve these divergences; it feels like a dirty trick that produces incredibly accurate results agreeing with experiment. But again there are problems: renormalization expresses Fock space and the commutation relations in terms of the noninteracting case, and the results you get don't necessarily agree with what you did *a priori*.

For example, quantum field theory contains a Hamiltonian $H$ whose spectrum is of interest. One can imagine starting with the noninteracting Hamiltonian $H_0$ and perturbing it by some small operator $W$: $H := H_0 + W$. You're often interested in the resolvent

$$\begin{aligned} R(z) &= (H - z)^{-1} \\ &= (H_0 - z)^{-1} \sum_{\ell=0}^{\infty} \Big( W(H_0 - z)^{-1} \Big)^{\ell}. \end{aligned}$$

The issue is that adding $W$ does not do nice things to the spectrum, and this is part of the complexity of quantum field theory.

Let $\lambda$ denote the interaction, and $N$ denote the number of particles, and suppose $\lambda \sim 1/N$ as we let $N \to \infty$. Then, the equations describing the mean field theory for this system are complicated, typically nonlinear PDEs. Typical examples include the nonlinear Schrödinger equation, the nonlinear Hartree equation, the Vlasov equation, or the Boltzmann equation. We'll hopefully see some of these equations in this class.

This is a lot of stuff that's tied together in complicated and potentially confusing ways, and hopefully in this class we'll learn how to make sense of it.

**Classical mechanics and symplectic geometry** In classical mechanics, we think of objects in idealized ways, e.g. thinking of a stone as a point mass at its center of mass. Thus, we're studying the motion of idealized point masses (or particles, in the strictly classical sense). We do this by letting time be $t \in \mathbb{R}$; at a time $t$, the particles $x_1, \dots, x_N$ have positions $\mathbf{q}(t) := (q_1(t), \dots, q_N(t))$, with $q_i(t) \in \mathbb{R}^d$; these are called "generalized coordinates."

Classical mechanics says that the kinematics of particles can be completely described by their position and velocity. Thus the motion of a system is completely determined by $\mathbf{q}(t)$ and $\dot{\mathbf{q}}(t) := \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t}$.

The next question: what determines the motion? The answer is the Newtonian equations of motion: $\ddot{\mathbf{q}}$ is expressed as a function of $\dot{\mathbf{q}}$ and $\mathbf{q}$ using *Hamilton's principle*, also known as the *principle of least action*.

(1) Let $\mathbf{q} \in C^2([t_0, t_1], \mathbb{R}^{Nd})$ be a curve in $\mathbb{R}^{Nd}$. We associate to $\mathbf{q}$ a weight function $L(\mathbf{q}, \dot{\mathbf{q}})$ called the *Lagrangian*.

(2) Given $\mathbf{q}$ as above, define the *action functional*

$$S[\mathbf{q}] := \int_{t_0}^{t_1} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\,\mathrm{d}t.$$

(3) Then, among all $C^2$ curves with $\mathbf{q}(t_0)$ and $\mathbf{q}(t_1)$ fixed, the curve that minimizes $S$ is the one that satisfies the equations of motion.

Now let $\mathbf{q}_\bullet(t)$ be a $C^2$ family of curves $[t_0, t_1] \times \mathbb{R} \to \mathbb{R}^{Nd}$ and that $\mathbf{q}_0$ minimizes $S$. Then,

$$\partial_s|_{s=0}\, S[\mathbf{q}_s] = 0.$$

We can apply this to the Lagrangian to derive the equations of motion.

$$\begin{aligned}\partial_s|_{s=0}\, S[\mathbf{q}_s] &= \int_{t_0}^{t_1} \left((\nabla_{\mathbf{q}_s} L)\cdot \partial_s \mathbf{q}_s(t) + (\nabla_{\dot{\mathbf{q}}_s} L)\cdot \partial_s \dot{\mathbf{q}}_s(t)\right)\mathrm{d}t\Big|_{s=0} \\ &= \int_{t_0}^{t_1} \left(\nabla_{\mathbf{q}_s} L - (\nabla_{\dot{\mathbf{q}}_s} L)^\bullet\right)\big|_{s=0} \cdot \underbrace{\partial_s|_{s=0}\,\mathbf{q}_s(t)}_{\delta\mathbf{q}(t)}\,\mathrm{d}t + (\nabla_{\dot{\mathbf{q}}_0} L)\cdot \underbrace{(\partial_s|_{s=0}\mathbf{q}(t))}_{=0}\Big|_{t_0}^{t},\end{aligned}$$

where $\delta\mathbf{q}(t)$ is the variation. For all variations, this is nonzero. Thus, minimizers of $S$ satisfy the *Euler-Lagrange equations*

$$\nabla_{\mathbf{q}} L - (\nabla_{\dot{\mathbf{q}}} L)^\bullet = 0. \tag{1.1}$$

We'll now impose some conditions on $L$ that come from reasonable physical principles.

**Additivity:** if we analyze a system $A \cup B$ which is a union of two subsystems $A$ and $B$ that don't interact, then

$$L_{A\cup B} = L_A + L_B.$$

**Uniqueness:** Assume $L_1$ and $L_2$ differ only by a total time derivative of a function $f(\mathbf{q}(t), t)$; then, they should give rise to the same equations of motion:

$$\begin{aligned}S_2 &= S_1 + \int_{t_0}^{t_1} \partial_t f(\mathbf{q}(t), t)\,\mathrm{d}t \\ &= S_1 + f(\mathbf{q}(t_1), t_1) - f(\mathbf{q}(t_0), t_0),\end{aligned}$$

so the minimizers for $S_1$ and $S_2$ are the same.

**Galilei relativity principle:** The physical laws of a closed system are invariant under the symmetries of the *Galilei group* parameterized by $a, v \in \mathbb{R}^d$, $t \in \mathbb{R}$, and $R \in \mathrm{SO}(d)$, the group element $g_{a,v,R,b}$ acts by

$$\begin{aligned}\mathbf{q} &\longmapsto a + vt + Rq \\ t &\longmapsto t + b.\end{aligned}$$

That is, in each component $j$, $q_j \mapsto a + vt + Rq_j$.

This actually determines $L$ for a system consisting of a single particle. By homogeneity of space (by the Galilei group contains translations), $L$ can only depend on $V = \dot{q}$. Since space is isotropic (because the Galilei group contains rotations), $L$ should depend on $v^2$. Next, the Euler-Lagrange equations imply

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} - \frac{\partial L}{\partial q} = 0,$$

and since $L$ does not depend on $q$, $\frac{\partial L}{\partial q} = 0$, so $\frac{\partial L}{\partial v}$ must be a constant.

Now we consider Galilei invariance of $v$ If $v \mapsto v + \varepsilon$, the equations of motion must be invariant, so

$$L[(v')^2] = L[(v+\varepsilon)^2] = L(v^2) + \frac{\partial L}{\partial v^2} 2v\cdot e + O(\varepsilon),$$

and this should only differ by a total time derivative $\dot{q}$:

$$F(\dot{q})\cdot\dot{q} = \partial_t G,$$

where $F(\dot{q})$ is a constant, and $\frac{\partial L}{\partial v^2}$ is also constant. This latter constant is denoted $m$, and called the *mass*, and the Lagrangian expresses its kinetic energy:

$$L(v) = \frac{1}{2}mv^2.$$

Now imagine adding $N$ particles, which we assume don't interact. Then additivity tells us they have masses $m_1, \dots, m_N$, and the Lagrangian is

$$L = \frac{1}{2}\sum_{j=1}^{N} m_j v_j^2.$$

If the particles are interacting, there's some potential function $U(q_1, \dots, q_N)$, and the Lagrangian is instead

$$L = \frac{1}{2}\sum_{j=1}^{N} m_j v_j^2 - U(q_1, \dots, q_N).$$

Now, by (1.1),

$$m_j \ddot{q}_j = -\partial_{q_j} U = F,$$

and this is called the *force*. This is Newton's second law $F = ma$.

**Symmetries and conservation laws** There's a general result called Noether's theorem which shows that any symmetry of a physical system leads to a conserved quantity. We'll see the presence of symmetry in classical mechanics and then how it changes in quantum mechanics.

For example, the systems we saw above had symmetries under time translation invariance $t \mapsto t + b$, so the Lagrangian doesn't depend on $t$, just on $\mathbf{q}$ and $\dot{\mathbf{q}}$. Therefore

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}L &= \sum_j \left(\frac{\partial L}{\partial q_j}\dot{q}_j + \frac{\partial L}{\partial \dot{q}_j}\ddot{q}_j\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=1}^{N}\left(\frac{\partial L}{\partial \dot{q}_j}\right)\cdot \dot{q}_j,\end{aligned}$$

and therefore

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{j=1}^{N}\frac{\partial L}{\partial \dot{q}_j}\cdot\dot{q}_j - L\right)}_{E} = 0.$$

The quantity $E$ is the *energy* of the system, and time translation invariance tells is that energy is conserved. The component $p_j := \frac{\partial L}{\partial \dot{q}_j}$ is called the $j^{\text{th}}$ *canonical momentum*.

The homogeneity of space, told to us by invariance under the Galilei translations $q_j \mapsto q_j + \varepsilon$, tells us that

$$\begin{aligned}\delta L &= \sum_i \frac{\partial L}{\partial \dot{q}_j}\cdot\varepsilon \\ &= \varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\sum\frac{\partial L}{\partial \dot{q}_j} = 0.\end{aligned}$$

Thus, the quantity

$$\mathbf{p} := \sum_{j=1}^{N}\frac{\partial L}{\partial \dot{q}_j}$$

is conserved, and is constant. This is called the *total momentum*, so translation-invariance gives you conservation of momentum. In the same way, rotation-invariance around any center gives you conservation of angular momentum around any center.

**Hamiltonian dynamics** The Euler-Lagrange equations express $\ddot{\mathbf{q}}$ as a second-order ODE. One might want to reformulate this into a first-order ODE; there are many ways to do this. There's one that's particularly important. Since

$$p_j = \frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}),$$

then it looks like one could solve for $\dot{\mathbf{q}}$ in terms of $\mathbf{p}$ and $\mathbf{q}$.

**Lemma 1.2.** *Let $f \in C^2(\mathbb{R}^n, \mathbb{R})$ be such that its Hessian $D^2 f$ is uniformly positive definite, i.e. there's an $\alpha > 0$ such that*

$$D^2 f(x)(h,h) = \sum_{i,j} \frac{\partial^2 f}{\partial x_j \partial x_\ell} h_j h_\ell \geq \alpha \|h\|^2$$

*uniformly in $x \in \mathbb{R}^n$, then there is a unique solution to*

$$Df(x) = y$$

*for every $y \in \mathbb{R}^n$.*

*Proof.* Let $g(x,y) \coloneqq f(x) - \langle x, y\rangle$. Then, $\nabla_x g(x,y) = \nabla f - y$, and $D^2 g = D^2 f$. Hence it suffices to check for $y = 0$.

The positive definite assumption on $D^2 f$ means $f$ is strictly convex, and hence has at most a single critical point, at which $\nabla f = 0$. Thus it remains to check that there's at least one solution.

If you Taylor-expand, you get that

$$f(x) = f(0) + \langle Df(0), x\rangle + \frac{1}{2} D^2 f(sx)(x,x) + \cdots,$$

so for all $x$,

$$f(x) \geq f(0) - |\nabla f(0)||x| + \frac{\alpha}{2}|x|^2.$$

Thus, there's an $R > 0$ such that if $|x| \geq R$, then $f(x) \geq f(0)$, so $f$ has at most one minimum in the ball $\overline{B_R(0)}$, so by compactness, it has a minimum $x_0$, which must be the global minimum, so $Df(x_0) = 0$. ⊠

**Definition 1.3.** Suppose $f$ is continuous on $\mathbb{R}^n$. Then, its *Legendre transform* or *Legendre-Fenchel transform* is

$$f^*(y) \coloneqq \sup_{x \in \mathbb{R}^n} (\langle y, x\rangle - f(x)).$$

You can think of this as measuring the distance from the graph of $f$ to the line cut out by $\langle y, x\rangle$ (i.e. between the two points with minimum distance).

Lecture 2.

## The Hamiltonian formalism for classical mechanics: 9/5/17

Last time, we discussed Lemma 1.2, that if $f\colon \mathbb{R}^n \to \mathbb{R}$ is $C^2$ and its Hessian is uniformly positive definite, then there's a unique solution to $\nabla f(x) = y$ for all $y \in \mathbb{R}^n$. We then defined the Legrendre-Fenchel transform of $f$: $f^*(y)$ geometrically means the minimal distance from $f(x)$ to the hyperplane $\langle y, x\rangle = 0$. It has the following key properties:

**Theorem 2.1.** *Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be a $C^2$ function with uniformly positive definite Hessian. Then,*

(1) $$f^*(y) = \langle y, x(y)\rangle - f(x(y)),$$
*where $x(y)$ is the unique solution to $\nabla f(x) = y$ guaranteed by Lemma 1.2, and*

(2) *$f^*(y)$ is $C^2$ and strictly convex.*

(3) *If $n = 1$, $\nabla(f^*) = (\nabla f)^{-1}$.*

(4) *For all $x, y \in \mathbb{R}^n$,*
$$f(x) + f^*(y) \geq \langle y, x\rangle,$$
*with equality iff $x = x(y)$ is the unique solution to $\nabla f(x) = y$.*

(5) *The Legendre-Fenchel transform is involutive, i.e. $(f^*)^* = f$.*

We'll use this in the Hamiltonian formalism of classical mechanics. One motivation for the Hamiltonian formalism is that the Lagrangian formalism produces second-order ODEs, and it would be nice to have an approach that gives first-order equations. There are many ways to do that, but this one has particularly nice properties.

Suppose we have generalized coordinates $\mathbf{q}$ and $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$. You might ask whether we can solve for $\dot{q}_i = \dot{q}_i(\mathbf{q}, \mathbf{p})$. If we assume $D^2_{\mathbf{v}} L(\mathbf{q}, \mathbf{v})$ is uniformly positive definite, then $\mathbf{p} = \nabla_{\dot{\mathbf{q}}} L(\mathbf{q}, \dot{\mathbf{q}})$ has a unique solution.

**Definition 2.2.** The *Hamiltonian* $H$ is the Legendre-Fenchel transform of $L$ for $\mathbf{q}$ fixed, i.e.

$$\begin{aligned} H(\mathbf{q}, \mathbf{p}) &:= \sup_{\mathbf{v} \in \mathbb{R}^n} \left( \langle \mathbf{p}, \mathbf{v} \rangle - L(\mathbf{q}, \mathbf{v}) \right) \\ &= \langle \mathbf{p}, \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p}) \rangle - L(\mathbf{q}, \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p})). \end{aligned}$$

**Theorem 2.3.** *Assume the matrix*

$$\left[ \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \right] \tag{2.4}$$

*is uniformly positive definite. Then, the Euler-Lagrange equations*

$$\left( \frac{\partial L}{\partial \dot{\mathbf{q}}} \right)^{\bullet} - \frac{\partial L}{\partial \mathbf{q}} = 0$$

*are equivalent to*

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{2.5}$$

(2.4) is called the *mass matrix* of the system, and (2.5) is called the *Hamiltonian equations of motion*.

*Proof.* Since $p_j = \frac{\partial L}{\partial \dot{q}_j}$,

$$\begin{aligned} \frac{\partial H}{\partial p_i} &= \dot{q}_i + \sum_{j=1}^{n} \left( p_j \frac{\partial \dot{q}_j}{\partial p_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial p_i} \right) \\ &= \dot{q}_i. \end{aligned}$$

Similarly, since $\frac{\partial q_j}{\partial q_i} = \delta_{ij}$ and $\frac{\partial L}{\partial \dot{q}_j} = p_j$, then

$$\begin{aligned} \frac{\partial H}{\partial q_i} &= \sum_{j=1}^{n} \left( p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial q_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} \right) \\ &= -\left( \frac{\partial L}{\partial \dot{q}_i} \right)^{\bullet} = \dot{p}_i. \end{aligned}$$

⊠

This leads to the Hamiltonian formalism, which starts with the Hamiltonian and works towards the physics from there. We begin on a phase space $\mathbb{R}^{2n}$ with coordinates $(\mathbf{q}, \mathbf{p})$, and a Hamiltonian $H \colon \mathbb{R}^{2n} \to \mathbb{R}$. Let

$$J := \begin{bmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{bmatrix}$$

denote the *symplectic normal matrix*.[1]

The *Hamiltonian vector field* for this system is

$$X_H := J \nabla H = \begin{bmatrix} \nabla_{\mathbf{p}} H \\ -\nabla_{\mathbf{q}} H \end{bmatrix}.$$

Then, the Hamiltonian equations of motion (2.5) may be expressed in terms of the flow for $X_H$.

[1] More generally, one can formulate this system on any symplectic manifold, in which case $J$ is the symplectic form in Darboux coordinates. But we won't worry about this right now.

This "Hamiltonian structure" on $\mathbb{R}^{2n}$ is closely related to a complex structure: $J^2 = -1$ is closely reminiscent of $i^2 = -1$. Indeed, if

$$\mathbf{z} := (\mathbf{q} + i\mathbf{p}),$$

then

$$\begin{aligned} i\dot{\mathbf{z}} &= i(\dot{\mathbf{q}} + i\dot{\mathbf{p}}) \\ &= i(\nabla_{\mathbf{p}} H - i\nabla_{\mathbf{q}} H) \\ &= (\nabla_{\mathbf{q}} + i\nabla_{\mathbf{p}})H. \end{aligned}$$

This is an example of a *Wirtinger derivative*:

$$\begin{aligned} \partial_z &= \frac{1}{2}(\partial x - i\partial y) \\ \partial_{\overline{z}} &= \frac{1}{2}(\partial x + i\partial y) \end{aligned}$$

**Example 2.6** (Harmonic oscillator)**.** Let

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

so

$$H(z,\overline{z}) = \frac{1}{2}z\overline{z}.$$

In this case, the Hamiltonian equations of motion are

$$\begin{aligned} i\dot{z} &= 2\partial_{\overline{z}} H = z \\ z(0) &= z_0, \end{aligned}$$

so we recover

$$z(t) = z_0 e^{it},$$

as usual for a harmonic oscillator. ◁

We can also study Hamiltonian PDEs, which include several interesting systems of equations. But they got erased before I could write them down. :( One of them includes the *nonlinear Schrödinger equation*: for $x \in \mathbb{R}^d$, the system

$$\mathcal{H}[u,\overline{u}] = \int \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{2p}|u|^{2p}\right) \mathrm{d}x,$$

which leads to the equations of motion (the Schrödinger equation)

$$i\dot{u} = -\Delta u + |u|^{2p-2}u.$$

The solutions of these equations tend to be interesting: Hamiltonian flow (the flow generated by $X_H$) isn't a gradient flow, but rather gradient flow twisted by $J$. We call this flow $\Phi_t \colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, with $x(t) = \Phi_t(x_0)$ and $x(t) = \Phi_{t,s}(x(s))$.

**Theorem 2.7.** *$H$ is conserved by $\Phi_t$.*

*Proof.*

$$\frac{\mathrm{d}}{\mathrm{d}t}H(x(t)) = \nabla_{\mathbf{x}} H \cdot \dot{\mathbf{x}} = \nabla_{\mathbf{x}} H \cdot J\nabla_{\mathbf{x}} H = 0,$$

because $J$ is skew-symmetric. ⊠

**Definition 2.8.** In this situation, the *symplectic form* is the skew-symmetric form $\omega \in \Lambda^2((\mathbb{R}^{2n})^*)$ defined by

$$\omega(X,Y) := \langle Y, JX\rangle.$$

The pair $(\mathbb{R}^{2n},\omega)$ is a symplectic vector space; the space of invertible matrices preserving this form is called the *symplectic group*

$$\mathrm{Sp}(2n,\mathbb{R}) := \{M \in \mathrm{GL}_{2n}(\mathbb{R}) \mid M^{\mathrm{T}}JM = J\}.$$

Now we can prove some properties of the Hamiltonian flow.

**Theorem 2.9.** *Let $\Phi_t$ be the Hamiltonian flow generated by $X_H$. Then,*

(1) $x(t) = \Phi_{t,s}(x(s))$,
(2) $\Phi_{s,s} = \mathrm{id}$, *and*
(3) $D\Phi_{t,s}(x) \in \mathrm{Sp}(2n, \mathbb{R})$.

*Conversely, if $\Phi_{t,s}$ is the local flow generated by a vector field $X$ such that locally (in $x$) (3) holds, then $X$ is locally Hamiltonian, in that there's a $G$ such that $X = X_G$.*

**Definition 2.10.** A diffeomorphism $\phi\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ with $D\phi \in \mathrm{Sp}(2n, \mathbb{R})$ is called a *symplectomorphism*.

*Proof sketch of Theorem 2.9.* Since

$$\partial_t D\Phi_{t,s}(x) = DX_H(\Phi_{t,s}(x)) \cdot D\Phi_{t,s}(x),$$

then it suffices to check that if

$$\Gamma(t, s, x) \coloneqq D\Phi_{t,s}^{\mathrm{T}}(x) J D\Phi_{t,s}(x),$$

then

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma = 0.$$

**Definition 2.11.** The *Liouville measure* $\mu_L$ on $\mathbb{R}^{2n}$ is the measure induced by $\omega^{\wedge n}$, i.e.

$$\int_{\mathbb{R}^{2n}} f \mathrm{d}\mu_L \coloneqq \int_{\mathbb{R}^{2n}} f\omega^{\wedge n}.$$

**Theorem 2.12** (Liouville)**.** *Let $\Phi_{t,s}$ be the Hamiltonian flow. Then, for every Borel set $B$, $|\Phi_{t,s}(B)| = |B|$. Hence $\Phi_{t,s}$ preserves the Lesbegue measure and the Liouville measure.*

*Proof.* If $\varphi\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is a diffeomorphism, then

$$\int_B f(x)\,\mathrm{d}x = \int_{\varphi^{-1}(B)} (f \circ \varphi)|\det D\varphi(x)|\,\mathrm{d}x,$$

and $\det D\Phi_t = 1$. ⊠

The next theorem is a conservation property.

**Theorem 2.13.** *Let $\Phi_{t,s}$ be the flow generated by an arbitrary vector field $X$, $D \subset \mathbb{R}^{2n}$ be a bounded region, and $D_{t,s} \coloneqq \Phi_{t,s}(D)$. Then, for every $f \in C^1(\mathbb{R}^n)$,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{D_{t,s}} f\,\mathrm{d}x = \int_{D_{t,s}} (\partial_t f + \mathrm{div}(fX))\,\mathrm{d}x.$$

*Proof.* By the group property ($\Phi_{t,s} = \Phi_{t,s_1} \circ \Phi_{s_1,s}$) it suffices to prove it for $s = 0$ and at $t = 0$. In this case

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\int_{D_t} f\,\mathrm{d}x = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\int_D (f \circ \Phi_t)\det D\Phi_t\,\mathrm{d}x$$

Since $D\Phi_t = \mathbf{1} + tDX + O(t^2)$, then $\det(D\Phi_t) = 1 + t\,\mathrm{tr}(DX) + O(t^2)$ and hence

$$\begin{aligned} &= \int_D ((\partial f + \nabla f \cdot X) + f\,\mathrm{div}\,X)\,\mathrm{d}x \\ &= \int_D (\partial_t f + \mathrm{div}\,fX)\,\mathrm{d}x. \end{aligned}$$

⊠

**Corollary 2.14.** *Any function $f(t, x)$ for which the* matter content

$$MC(f)(t) \coloneqq \int_{\Phi_{t,s}(D)} f(x, t)\,\mathrm{d}x$$

*remains constant (equivalently, $\frac{\mathrm{d}}{\mathrm{d}t}MC(f)(t) = 0$), must satisfy the* continuity equation

$$\partial_t f + \mathrm{div}(fX) = 0. \tag{2.15}$$

In physically interesting cases, the matter content actually represents how much mass is in the system. In the Hamiltonian case, $\operatorname{div} X_H = 0$, so

$$\partial_t f + \nabla f \cdot X_H = 0$$

is equivalent to

$$\partial_t f + \nabla f \cdot J\nabla H = 0.$$

We can rewrite this in terms of the *Poisson bracket*

$$\{f, H\} \coloneqq \langle \nabla f, J\nabla H \rangle,$$

producing the equation

$$\partial_t f + \{f, H\} = 0.$$

The Poisson bracket can also be defined as

$$\begin{aligned}\{f, H\} &= \omega(X_f, X_H) \\ &= \sum_{j=1}^{n} \left( \frac{\partial f}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial H}{\partial q_j}\frac{\partial f}{\partial p_j} \right).\end{aligned}$$

We'll see related phenomena in the quantum-mechanical case. What we talk about next, though, will not reappear in quantum mechanics, but it's too beautiful to ignore completely.

**Definition 2.16.** An *integral of motion* is a $C^1$ function $g\colon \mathbb{R}^{2n} \to \mathbb{R}$ constant along the orbits of the Hamiltonian. Equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t} g(x(t)) = \{g, H\} = 0.$$

Two integrals of motion $g_1$ and $g_2$ are *in involution* if $\{g_1, g_2\} = 0$.

Notice that $\{g, g\} = 0$ always.

Generally, Hamiltonian systems are incredibly difficult to solve. There are some cases where they can be solved by hand, e.g. by quadrature classically. It would be nice to know when such a solution exists. If you can find $n$ integrals of motion that are in involuton with each other, you can heuristically reduce the equations into something tractable; this is the contant of the Arnold-Yost-Liouville theorem.

**Theorem 2.17** (Arnold-Yost-Liouville)**.** *On the phase space $(\mathbb{R}^{2n}, \omega)$, assume we have $n$ integrals of motion $G_1, \dots, G_n$ which are in involution; further, assume $G_1 = H$. Let $\mathbf{G} = (G_1, \dots, G_n)\colon \mathbb{R}^{2n} \to \mathbb{R}^n$, and consider its level set*

$$\mathcal{M}_{\mathbf{G}}(\mathbf{c}) \coloneqq \{x \in \mathbb{R}^{2n} \mid \mathbf{G}(x) = \mathbf{c}\},$$

*for some $\mathbf{c} \in \mathbb{R}^n$. Assume that the 1-forms $\{\mathrm{d}G_j\}$ are linearly independent (equivalently, the gradients $\nabla G_j$ are linearly independent). Then,*

(1) *$\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is a smooth manifold that's invariant under the flow generated by $X_H$, and*
(2) *if $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is compact and connected, it is diffeomorphic to an $n$-torus $T^n \coloneqq S^1 \times \cdots \times S^1$.*
(3) *The Hamiltonian flow of $H$ determines a quasiperiodic motion*

$$\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}t} = \boldsymbol{\eta}(\mathbf{c}), \qquad \frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t} = \mathbf{0} \tag{2.18}$$

*with initial data $(\boldsymbol{\varphi}_0, \mathbf{I}_0)$.*

(4) *The Hamiltonian equations of motion can be integrated by quadrature:*

$$\begin{aligned}\mathbf{I}(t) &= \mathbf{I}_0 \\ \boldsymbol{\varphi}(t) &= \boldsymbol{\varphi}_0 + \boldsymbol{\eta}(\mathbf{c})t.\end{aligned} \tag{2.19}$$

*Here $\mathbf{I}$ and $\boldsymbol{\varphi}$ are the new coordinates for phase space in which the system can be solved.*

We'll prove this next lecture, then move to quantum mechanics.

Lecture 3.

## The Arnold-Yost-Liouville theorem and KAM theory: 9/7/17

Today, we're going to prove the Arnold-Yost-Liouville theorem, Theorem 2.17. We keep the notation from that theorem and the notes before it.

One key takeaway from the theorem is that the Hamiltonian equations can be explicitly solved. That is, going from (2.18) to (2.19) is a particularly simple system of ODEs.

*Proof sketch of Theorem 2.17.* By assumption, $\{\nabla G_j\}$ is linearly independent on $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$. By the implicit function theorem, $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is an $n$-dimensional submanifold of $\mathbb{R}^{2n}$. The gradients $\{\nabla G_j\}$ span the normal bundle of $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ because it's a level set for them.

Consider $X_{G_j} \coloneqq J\nabla G_j$. It's a tangent vector:

$$\begin{aligned} \langle X_{G_j}, \nabla G_\ell \rangle &= \langle J\nabla G_j, \nabla G_\ell \rangle \\ &= -\langle J\nabla G_j, JJ\nabla G_\ell \rangle \\ &= \omega\Big(X_{G_j}, X_{G_\ell}\Big) \\ &= \{G_j, G_\ell\} = 0 \end{aligned} \tag{3.1}$$

for all $j$ and $\ell$. We've produced $n$ linearly independent tangent vectors at each point, so $\{X_{G_j}\}_{j=1}^n$ spans $T\mathcal{M}_{\mathbf{G}}(\mathbf{c})$. In particular, $X_H = X_{G_1}$ is tangent to $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$, so $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is invariant under its flow. This proves (1).

For part (2), we assume $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is compact and connected. Let $\varphi_{t_j}^j$ denote the flow generated by $X_{G_j}$, so $t_1, \dots, t_n \in \mathbb{R}$ are separate time variables. Because $\{G_j, G_\ell\} = 0$, then $G_\ell$ is invariant under $\varphi_{t_j}^j$ for any $j$ and $\ell$. Thus $\varphi_{t_j}^j$ and $\varphi_{t_\ell}^\ell$ commute, so we may define

$$\varphi_{\mathbf{t}} \coloneqq \varphi_{t_1}^1 \circ \cdots \circ \varphi_{t_n}^n.$$

Pick an $x_0 \in \mathcal{M}_{\mathbf{G}}(\mathbf{c})$ and define $\varphi\colon \mathbb{R}^n \to \mathcal{M}_{\mathbf{G}}(\mathbf{c})$ to send $\mathbf{t} \mapsto \varphi_{\mathbf{t}}(x_0)$. This is transitive in the sense that for all $x \in \mathcal{M}_{\mathbf{G}}(\mathbf{c})$, there's a $\boldsymbol{\tau} \in \mathbb{R}^n$ such that $\varphi_{\boldsymbol{\tau}}(x_0) = x$.

Since $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is compact but $\mathbb{R}^n$ isn't, $\varphi$ cannot be a bijection. Define

$$\Gamma_{x_0} \coloneqq \{\mathbf{t} \in \mathbb{R}^n \mid \varphi_{\mathbf{t}}(x_0) = x_0\},$$

the *stationary group* of $x_0$. This is indeed an abelian group, because if $\boldsymbol{\tau} \in \Gamma_{x_0}$, then $n\boldsymbol{\tau} \in \Gamma_{x_0}$ for all $n \in \mathbb{Z}$: if you iterate a loop again and again, you still end up back where you started with. And clearly $\mathbf{0} \in \Gamma_{x_0}$.

Let ${}_{\varepsilon_1}U$ be an $\varepsilon_1$-neighborhood of $\mathbf{0}$ in $\mathbb{R}^n$ and $V_{\varepsilon_2}$ be an $\varepsilon_2$-neighborhood of $x_0$ in $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$; then, there are $\varepsilon_1, \varepsilon_2 > 0$ such that $\varphi|_{U_{\varepsilon_1}} : U_{\varepsilon_1} \to V_{\varepsilon_2}$ is a diffeomorphism. Thus, for sufficiently small $\varepsilon_2$, there's no other fixed point in $V_{\varepsilon_2}$, which means $\Gamma_{x_0}$ is a discrete subgroup of $(\mathbb{R}^n, +)$.

This means there are vectors $\mathbf{e}_1, \dots, \mathbf{e}_n \in \mathbb{R}^n$ such that

$$\Gamma_{x_0} = \left\{ \sum_{i=1}^n m_i \mathbf{e}_i \mid m_1, \dots, m_n \in \mathbb{Z} \right\},$$

and that $\varphi$ establishes an isomorphism

$$T^n \cong \mathbb{R}^n / \Gamma_{x_0} \longrightarrow \mathcal{M}_{\mathbf{G}}(\mathbf{c}).$$

This proves (2).

Now we need to make the change-of-variables in (3); these new variables are called *action-angle variables*. First note that $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is a *Lagrangian submanifold*, i.e. it's half-dimensional and the restriction of $\omega$ to it is 0 (it's *isotropic*; an isotropic submanifold of $\mathbb{R}^{2n}$ can be at most $n$-dimensional). This is because $T\mathcal{M}_{\mathbf{G}}(\mathbf{c})$ is spanned by $\{X_{G_j}\}$, and in (3.1), we proved $\omega(X_{G_j}, X_{G_\ell}) = \{G_j, G_\ell\} = 0$ for all $j, \ell$.

Consider the 1-form

$$\Theta \coloneqq \sum_j p_j \, \mathrm{d}q_j.$$

Then,

$$\mathrm{d}\Theta = \sum_j \mathrm{d}p_j \wedge \mathrm{d}q_j = \omega,$$

so restricted to $\mathcal{M}_{\mathbf{G}}(\mathbf{c})$, $\Theta$ is a closed 1-form.

Let $\{\gamma_j\}_{j=1}^n$ be a set of cycles whose homology classes generate $H_1(\mathcal{M}_{\mathbf{G}}(\mathbf{c})) = H_1(T^n) \cong \mathbb{Z}^n$. Then, the *action variables*

$$I_j(\mathbf{c}) \coloneqq \frac{1}{2\pi} \oint_{\gamma_j} \Theta$$

is independent of the choice of cycle representative of the homology class of $\gamma_j$: if $D$ is a 2-chain with $\partial D = \gamma_j - \widetilde{\gamma}_j$ (a cobordism or homotopy from $\gamma_j$ to $\widetilde{\gamma}_j$), then by Stokes' theorem.

$$\oint_{\gamma_j} \Theta - \oint_{\widetilde{\gamma}_j} \Theta = \int_D \mathrm{d}\Theta = \int_D 0 = 0.$$

One can show that the assignment $(\mathbf{q}, \mathbf{p}) \mapsto (\boldsymbol{\varphi}, \mathbf{I})$ is symplectic, where $\varphi_j$ is a variable parameterizing $\gamma_j$ and is called an *angle variable* (since it's valued in $S^1$). In these coordinates, $H$ only depends on $\mathbf{I}$, not $\boldsymbol{\varphi}$, so

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}t} &= \frac{\partial H}{\partial \mathbf{I}} = \boldsymbol{\eta}(\mathbf{c}) \\ \frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t} &= -\frac{\partial H}{\partial \boldsymbol{\varphi}} = 0. \end{aligned}$$

⊠

Sometimes the entires of $\boldsymbol{\eta}(\mathbf{c})$ are irrational relative to each other. In this case you'll get dense orbits in the torus, corresponding to lines with irrational slope in $\mathbb{R}^{2n}$ before quotienting by the lattice $\Gamma_{x_0}$, and there will not be $n$ integrals of motion.

**Kolmogorov-Arnold-Moser (KAM) theory.** More generally, if one doesn't have complete integrability, one can make weaker but still interesting statements. For example, one can envision a problem which is completely integrable in the absence of perturbations, and one can study what happens when the dependence on $\boldsymbol{\varphi}$ is small:

$$H(\boldsymbol{\varphi}, \mathbf{I}) = H_0(\mathbf{I}) + \varepsilon H(\boldsymbol{\varphi}, \mathbf{I}).$$

Some systems will lose integrability, though understanding the precise ways they do so is very hard. Such a system is associated to a *frequency vector* $\boldsymbol{\eta}_0 \coloneqq \boldsymbol{\eta}(\mathbf{I}(t_0))$ satisfying the *Diophantine condition*

$$|\langle \boldsymbol{\eta}_0, \mathbf{n} \rangle| \geq \frac{1}{\langle \mathbf{n} \rangle^\tau}$$

for all $n \in \mathbb{Z}$ for some $\tau > 0$. Here $\langle \mathbf{x} \rangle \coloneqq \sqrt{1 + |\mathbf{x}|^2}$ is the *Japanese bracket*. This quantitatively captures the qualitative idea that "$\boldsymbol{\eta}_0$ is poorly approximated by rationals."

In this setup, there exists an invariant torus under the flow of $H$. The proof involves renormalization group flow, though it was not originally discovered in those terms. It's a kind of recursive proof style, and getting into the details would take a long time. It involves a great result called the *shadowing lemma*, which discusses the dynamics of a pendulum.

The pendulum has two equilibria: the bottom is stable ($\varphi = 0$), and the top is unstable (both with no velocity). The phase space is two-dimensional, in $\varphi$ and $\dot{\varphi}$, and some trajectories are shown in Figure 1. The curves with singularities are called *separatrices*.

Given a sequence of 0s and 1s, one may construct a parametric perturbation of the pendulum, regularly bumping it a small amount based on whether 0 or 1 is present.[2]. The shadowing lemma states that these trajectories uniformly approximate real trajectories. There's a rich theory here: the proof is a fixed-point argument, and there's interesting geometry of the *homoclinic points*, where two trajectories meet. These tend to be concentrated near the unstable equilibrium.

[2] TODO: did I get this right?

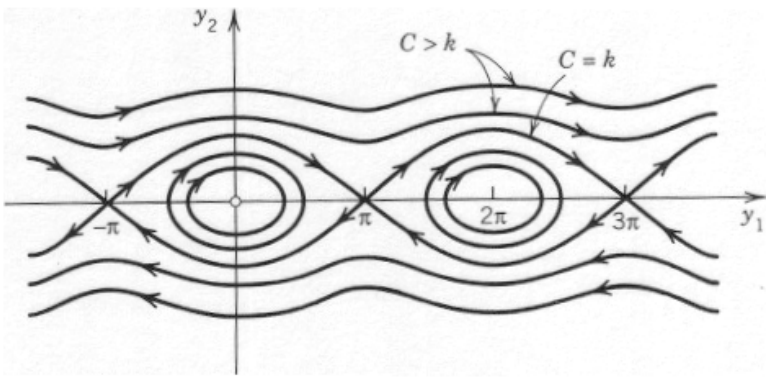


FIGURE 1. The phase diagram of a pendulum. Source: https://physics.stackexchange.com/q/162577.

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**Quantum mechanics.** Though quantum mechanics was discovered later than classical mechanics, it's actually much more fundamental. This suggests that one can derive classical mechanics as some sort of limit of quantum mechanics where Planck's constant is small, and indeed we can do this. We'll do this in three ways.

(1) The first is to use the Weiner transform to derive the Liouville equations from quantum mechanics in a semiclassical limit.
(2) The second case is to use a path integral to rediscover the principle of least action.
(3) The third way is to use observables and something called the Ehrenfest theorem.

Schrödinger discovered the *Schrödinger equation*, one of the cornerstones of quantum mechanics:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi,$$

where $\psi(t,x) \in L^2$ and

$$\|\psi\|_{L^2}^2 = \int |\psi(t,x)|^2 \,\mathrm{d}x = 1,$$

Schrödinger arrived at this equation by (somewhat heuristically) studying quantization. Electrons had been observed (by de Broglie) to sometimes behave as particles and sometimes behave as waves. If an electron behaves like a particle, it has momentum $\hbar k$, where $k$ is something called a *wave vector*. If you look at it as a wave, you get something like $i\hbar\nabla e^{-ikx}$, where $P := i\hbar\nabla$ is called the *momentum operator*. The Schrödinger equation (a guess within his PhD thesis) replaced the true momentum in the Hamiltonian

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

with the momentum operator $i\hbar\nabla$, giving is $-\hbar^2\Delta$.

Lecture 4.

## The Schrödinger equation and the Wigner transform: 9/12/17

Today we're going to begin by asking, how does one derive (well, guess) the Schrödinger equation? This involves an interesting and relevant digression on the Hamilton-Jacobi equation.

From the principle of least action, we know the Euler-Lagrange equations (1.1). Assume $q_0(t)$ is a solution to these equations. Take a one-parameter variation $(s, q_s)$ from $(t_0, q_0)$ to $(t, q)$. The *Hamilton principal function* is

$$S(t,q) = \int_{(t_0,q_0)}^{(t,q)} L(q(s), \dot{q}(s))\,\mathrm{d}s.$$

The variation with respect to $q$ is

$$\begin{aligned}\delta S &= \int_{t_0}^{t} \left( \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q} \right) \mathrm{d}s \\ &= \int_{t_0}^{t} \partial_s \left( \frac{\partial L}{\partial \dot{q}}\delta q \right) \mathrm{d}s \\ &= \frac{\partial L}{\partial \dot{q}}\delta q \Big|_{t_0}^{t}.\end{aligned}$$

Since $p = \frac{\partial L}{\partial \dot{q}}$ and $\delta q(t_0) = 0$, this is

$$= (p\delta q)(t).$$

Hence, $p = \frac{\partial S}{\partial q}$ and

$$L = \frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\partial S}{\partial t} + \sum_j \frac{\partial S}{\partial q_j}\dot{q}_j,$$

so

$$\begin{aligned}\frac{\partial S}{\partial t} &= L - \sum_j p_j \dot{q}_j \\ &= -H(q, \nabla_q S).\end{aligned}$$

This is called the *Hamilton-Jacobi equation*.

The link with the Schrödinger equation: let's take for an ansatz that we have a wavefunction

$$\psi(t,x) = a(t,x)e^{-iS(t,x)/\hbar}.$$

This does not come entirely out of left field: if you want to exponentiate the action, you have to make it dimensionless, and that's exactly what dividing by $\hbar$ accomplishes. Then,

$$\begin{aligned}i\hbar\partial_t\psi &= i\hbar\dot{a}e^{-iS/\hbar} + \frac{\hbar}{\hbar}\frac{\partial S}{\partial t}ae^{-iS/\hbar}. \\ &= -H(q,\nabla S)\psi + O(\hbar) \\ &= \left( -\frac{1}{2}(\nabla S)^2 + V(x) \right)\psi + O(\hbar).\end{aligned}$$

Compare with

$$\begin{aligned}-\frac{\hbar^2}{2}\Delta a e^{-iS/\hbar} &= -\frac{\hbar^2}{2}\left( -\frac{i}{\hbar}\Delta S + \left( \frac{i\nabla S}{\hbar} \right)^2 \right) a e^{-iS./\hbar} + O(\hbar) \\ &= \frac{1}{2}(\nabla S^2 a e^{-iS/\hbar} + O(\hbar).\end{aligned}$$

Putting these together, we arrive at

$$i\hbar\partial_t\psi = \left( -\frac{\hbar^2}{2}\Delta + V(x) \right)\psi + O(\hbar).$$

That is, the Schrödinger equation is an $O(\hbar)$-deformation of the Hamilton-Jacobi equations.

We'd like to solve this equation. Precisely, given a $\psi_0 \in L^2(\mathbb{R}^n)$, we'd like to find $\psi$ such that

$$\begin{aligned}i\partial_t\psi &= -\Delta\psi + V(x)\psi = H\psi \\ \psi(t=0) &= \psi_0.\end{aligned} \tag{4.1}$$

Here $H$ is the Hamiltonian.

We'd like to apply spectral theory to solve this, but $-\Delta$ is unbounded, with the domain

$$\{f \in L^2 \mid \|-\Delta f\|_{L^2} < \infty\},$$

which is dense in $L^2$. It is self-adjoint, in the formal sense, but because it (and pretty much every operator in quantum mechanics) is unbounded, the analysis is trickier. For the moment, we'll consider a regularized Hamiltonian.

Recall that we have a Fourier transform $\mathcal{F}\colon L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ given by

$$\widehat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(x) e^{-i\xi\cdot x}\, \mathrm{d}x$$
$$\check{g}(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} g(\xi) e^{i\xi\cdot x}\, \mathrm{d}\xi.$$

Here, $g \mapsto \check{g}$ is the inverse Fourier transform. This was defined on Schwartz-class functions by the formulas above, then using the Plancherel theorem and the density of Schwartz functions in $L^2$, it extends to $L^2$. The Laplacian turns into multiplication under the Fourier transform:

$$\mathcal{F}(-\Delta f)(\xi) = \xi^2 \widehat{f}(\xi).$$

Now we will regularize the Laplacian: define

$$\mathcal{F}(-\Delta_R f)(\xi) \coloneqq \xi^2 \chi_R(|\xi|) \widehat{f}(\xi),$$

where $R \gg 1$ and $\chi_R$ is a smooth bump function equal to 1 on $[0, R]$ and 0 on $[2R, \infty)$. Hence, for any finite $R$, Plancherel's theorem allows us to calculate that

$$\|-\Delta_R f\| \leq (2R)^2,$$

where we use the operator norm. If we assume that $V \in L^\infty(\mathbb{R}^n)$, then

$$\|V(x)\psi\|_{L^2} \leq \|V\|_{L^\infty} \|\psi\|_{L^2},$$

so the regularized Hamiltonian

$$H_R \coloneqq -\Delta_R + V$$

is bounded.

**Definition 4.2.** Let $A$ be an operator on $L^2$, possibly unbounded. We define the adjoint operator $A^*$ to satisfy $(\phi, A\psi) = (A^*\phi, \psi)$ for all $\phi, \psi \in L^2$. $A$ is *symmetric* if $(\phi, A\psi) = (A\phi, \psi)$ for all $\phi, \psi$ in the domain of $A$; if $A$ and $A^*$ have the same domain, this implies $A = A^*$, and $A$ is called *self-adjoint*.

**Theorem 4.3.** *If $A$ is bounded, then symmetric implies self-adjoint.*

**Theorem 4.4.** *If $A$ is a bounded, self-adjoint operator, then there is an $L^2$ solution to*

$$\begin{aligned} i\partial_t \psi &= -\Delta\psi + V(x)\psi = A\psi \\ \psi(t=0) &= \psi_0, \end{aligned} \tag{4.5}$$

*where $\psi_0 \in L^2$, which is given by*

$$\psi(t) = e^{-itA}\psi_0.$$

Here,

$$e^A \coloneqq \sum_{j=0}^{\infty} \frac{A^j}{j!}. \tag{4.6}$$

The particular case $e^{-itA}$ is really nice: it's an isometry, because

$$\|e^{itA}\psi_0\|_{L^2} = \|\psi_0\|_{L^2},$$

and it's unitary:

$$(e^{itA})^* = e^{-itA} = (e^{itA})^{-1}.$$

**Exercise 4.7.** Check that the infinite sum in (4.6) converges, so that $e^A$ is well-defined, and $\|e^{itA}\| \leq e^{t\|A\|}$ for all $t$.

Now, what does this all mean physically? Quantum mechanics considers a particle whose position and velocity at time $t$ are probabilistically given by some probability density $\psi(t,x)$, such that

$$\|\psi(t)\|_{L^2} = \|\psi_0\|_{L^2} = 1.$$

Measuring physical facts about this system is expressed through *observables*, self-adjoint operators $A\colon L^2 \to L^2$: the expected value of $A$ with respect to the distribution $\psi(t,x)$ is

$$\langle A\rangle_{\psi(t)} := \int \overline{\psi}(t,x)(A\psi)(t,x)\,\mathrm{d}x = (\psi, A\psi).$$

Because this system satisfies the Schrödinger equation (4.1), there are several conserved quantities. Consider

$$\begin{aligned}\partial_t(\psi, H\psi) &= \left(\frac{1}{i}H\psi, H\psi\right) + \left(\psi, H\left(\frac{1}{i}H\psi\right)\right)\\ &= -\left(H\psi, \frac{1}{i}H\psi\right) + \left(H\psi, \frac{1}{i}H\psi\right).\end{aligned}$$

In our case, we'd use $H_R$ instead of $H$. The *energy* of the system is

$$E[\psi] := \frac{1}{2}(\psi, H\psi),$$

and by the above, this is a conserved quantity. The $L^2$ *mass* is also conserved:

$$M[\psi] := \|\psi\|_{L^2}^2.$$

**The Wigner transform.** We'll now discuss the Wigner transform, a noncommutative version of the Fourier transform. As is customary with the Fourier transform and related phenomena, we will be cavalier about factors of $2\pi$ arising from the transform; if you don't like this, it's possible to avoid with the harmonic analysts' convention

$$\widehat{f}(\xi) = \int f(x)e^{-2\pi i\xi\cdot x}\,\mathrm{d}x,$$

where making these factors precise is easier. We'll also ignore some factors of $\hbar$.

Consider the function

$$\widehat{\rho}(t,\xi) := \langle e^{ix\cdot\xi}\rangle_{\psi(t)} = \int \underbrace{|\psi(t,x)|^2}_{\rho(t,x)} e^{-ix\cdot\psi}\,\mathrm{d}\xi,$$

so that $\rho(t,x)$ is a probability distribution in $x$ for a given $t$. The *momentum operator* $P = i\nabla_x$, on the other hand, satisfies

$$\langle P\rangle_{\psi(t)} = \int |\widehat{\psi}(t,\xi)|\xi\,\mathrm{d}\xi,$$

and hence defines another natural probability density $\mu(t,\xi)$ via

$$\langle e^{-iP\eta}\rangle_{\psi(t)} = \int \underbrace{|\widehat{\psi}(t,\xi)|^2}_{\mu(t,\xi)} e^{-i\xi\cdot\eta}\,\mathrm{d}\xi = \widehat{\mu}(t,\eta).$$

The two probability distributions $\widehat{\rho}$ and $\mu$ ought to be related, but they're not Fourier transforms from each other. Maybe in quantum mechanics, it doesn't make sense to separate the densities in $x$ (position) and $\xi$ (momentum), and to instead consider a probability density on the entirety of phase space of a solution $\psi$ to (4.1). In particular, let

$$\widehat{W}(t,\xi,\eta) := \left\langle e^{-i(x\cdot\xi + P\cdot\eta)}\right\rangle_{\psi(t)}.$$

Here $x$ and $P$ do not commute. Accordingly, the *Wigner transform* of $\psi$ is

$$W(t,x,v) := (\widehat{W})^{\vee}(t,x,v). \tag{4.8}$$

In the semiclassical limit, as $\hbar \to 0$, this will converge to the Liouville equation as in classical mechanics.

*Remark.* For a general solution $\psi$ of the Schrödinger equation, its Wigner transform is not positive definite, and hence doesn't define a probability density. However, we can make it positive definite: if

$$G(x,v) = e^{-c_1x^2-c_2v^2}$$

is a Gaussian, then the convolution

$$H(t,x,v) \coloneqq (W * G)(t,x,v)$$

is positive definite, and, suitably normalized, it defines a probability density function. The function $H$ is called a *Husini function*, and is very useful in applied math, specifically in the study of wave equations. ◂

The definition (4.8) is great for telling us what and why the Wigner transform is, but not so much how to calculate anything with it. Fortunately, there's an explicit formula.

**Lemma 4.9.**

$$W(t,x,v) = \int \overline{\psi(t,x-y/2)}\psi(t,x+y/2)e^{iy\cdot v}\,\mathrm{d}y.$$

This can be simplified using the density matrix $\Gamma_{xx'} \coloneqq \overline{\psi}(x)\psi(x')$. So the Wigner transform is the Fourier transform of a density matrix.

*Proof.* The proof is not fascinating, but will be good practice for a useful technique.

Let $A$ and $B$ be linear operators for which $e^A$ and $e^B$ are well-defined, and assume $[A,B] \coloneqq AB - BA$ is a scalar multiple of the identity. Then the higher commutators all vanish: $[A,[A,B]] = [[A,B],B] = 0$. Hence, the *Baker-Campbell-Hausdorff* formula for $e^{A+B}$ simplifies greatly to

$$e^{A+B} = e^Ae^Be^{-[A,B]/2}. \tag{4.10}$$

We're specifically interested in $x_i$ and $P_j$, and $[x_i,P_j] = -i\delta_{ij}$, so we may use (4.10):

$$e^{-i(x\cdot\xi+P\cdot\eta)} = e^{-ix\cdot\xi}e^{-iP\cdot\eta}e^{-\xi\cdot\eta/2}.$$

Next, observe that $e^{-iP\cdot\eta}$ acts through a translation by $\eta$:

$$\begin{aligned}\left(e^{-iP\cdot\eta}f\right)(x) &= e^{\eta\cdot\nabla}\int \widehat{f}(\xi)e^{i\xi\cdot x}\,\mathrm{d}\xi \\ &= \int \widehat{f}(\xi)e^{i(x+\eta)\cdot\xi}\,\mathrm{d}\xi \\ &= f(x+\eta).\end{aligned}$$

Therefore

$$\widehat{W}(t,\xi,\eta) = \int e^{-ix\xi}e^{-(i/2)\xi\cdot\eta}\overline{\psi(t,x)}\psi(t,x+\eta)\,\mathrm{d}x.$$

If you compute the inverse Fourier transform, which is mechanical, you'll get the desired formula. ⊠

**Convergence to the classical Liouville equation.** Taking a semiclassical limit means sending $\hbar$ to 0, more or less. Of course, this makes no sense: $\hbar$ is a nonzero physical constant! But it represents the idea that, relative to the scale of $\hbar$, everything is very large. Also, we'll call it $\varepsilon$ instead of $\hbar$, which makes it better.

Our Schrödinger equation is, given a potential $V \in C^2(\mathbb{R}^n)$,

$$i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V\psi^\varepsilon.$$

Now, the rescaled Wigner transform is

$$W^\varepsilon(t,x,p) = \frac{1}{\varepsilon^n}\int \overline{\psi^\varepsilon(t,x-y/2)}\psi^\varepsilon(t,x+y/2)e^{i(y\cdot P)/\varepsilon}\,\mathrm{d}y.$$

Scaling $y \to \varepsilon y$, this is

$$= \int \overline{\psi^\varepsilon(t,x-\varepsilon y/2)}\psi^\varepsilon(t,x+\varepsilon y/2)e^{iy\cdot P}\,\mathrm{d}y. \tag{4.11}$$

**Exercise 4.12.** Show that $\partial_t W^\varepsilon(t,x,p)$ is the sum of a *kinetic term* $(I)$ and a *potential term* $(II)$ where

$$(I) = -p \cdot \nabla_x W^\varepsilon(t,x,p) \tag{4.13a}$$

$$(II) = (\text{didn't get this in time}) \tag{4.13b}$$

The Wigner transform has the property that it turns a Schrödinger-like equation into a transport equation, and vice versa.

Lecture 5.

## The semiclassical limit of the Schrödinger equation: 9/14/17

*"Evaluating an object like (5.11) looks like it can be damaging to one's health. But it can be done"*

We've been working on the Schrödinger equation

$$\begin{aligned} i\varepsilon \partial_t \psi^\varepsilon(t,x) &= -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon(t,x) + V(x)\psi^\varepsilon(t,x) \\ \psi^\varepsilon(t=0) &= \psi_0^\varepsilon. \end{aligned}$$

Here, $V \in C^2(\mathbb{R}^n)$, and $\varepsilon = \hbar$, because it seems much more reasonable to say $\varepsilon \to 0$ rather than $\hbar \to 0$ (since $\hbar$ is a physical constant, not a variable!), as we will do when considering its semiclassical limit.[3]

To compute this, we introduced the rescaled Wigner transform Equation (4.11).

**Theorem 5.1.** *As $\varepsilon \to 0$, $W^\varepsilon \to F$, where*

$$(\partial_t + p \cdot \nabla_X) F(t,x,p) = (\nabla V)(x) \cdot \nabla_p F(t,x,p).$$

*Proof.* As in Exercise 4.12, we want to write $\partial_t W^\varepsilon(t,x,p)$ as a sum of a kinetic term $(I)$ (4.13a) and a potential term $(II)$ (4.13b). In more detail, if

$$\begin{aligned} (I) &= \frac{i\varepsilon}{2}\int \left( \overline{\psi^\varepsilon\left(t, x - \frac{\varepsilon y}{2}\right)} \Delta\psi^\varepsilon\left(t, x + \frac{\varepsilon y}{2}\right) - \overline{\Delta\psi^\varepsilon\left(t, x - \frac{\varepsilon y}{2}\right)} \psi^\varepsilon\left(t, x + \frac{\varepsilon y}{2}\right) \right) e^{ipy}\, \mathrm{d}y \\ &= i\int \nabla_x \cdot \nabla_y \left( \overline{\psi^\varepsilon\left(t, x - \frac{\varepsilon y}{2}\right)} \psi^\varepsilon\left(t, x + \frac{\varepsilon y}{2}\right) \right) e^{ipy}\, \mathrm{d}y. \end{aligned}$$

Then, the cross terms cancel, which is how you get (4.13a).[4]

The other term is

$$(II) = -\frac{i}{\varepsilon}\int \left( V\left(x + \frac{\varepsilon y}{2}\right) - V\left(x - \frac{\varepsilon y}{2}\right) \right) \overline{\psi^\varepsilon\left(t, x - \frac{\varepsilon y}{2}\right)} \psi^\varepsilon\left(t, x + \frac{\varepsilon y}{2}\right) e^{ipy}\, \mathrm{d}y.$$

For some $s_y \in (-1,1)$, this is

$$= -\frac{i}{\varepsilon}\int \left( \varepsilon \nabla V(x) \cdot y + \frac{1}{2} D^2 V\left(x + s_y \frac{\varepsilon y}{2}\right)(\varepsilon y, \varepsilon y) \right) \overline{\psi^\varepsilon(\cdots)} \psi^\varepsilon(\cdots) e^{ipy}\, \mathrm{d}y.$$

Splitting this along the red $+$ sign, call the first part $(II_1)$ and the second $(II_2)$. The first term is what we want, and the second is an error term.

$$\begin{aligned} (II_1) &= -i\int \nabla V(x) \frac{1}{i} \nabla_p \overline{\psi^\varepsilon\left(x - \frac{\varepsilon y}{2}\right)} \psi^\varepsilon\left(x + \frac{\varepsilon y}{2}\right) e^{ipy}\, \mathrm{d}y \\ &= \nabla V(x) \cdot \nabla p W^\varepsilon(t,x,p). \end{aligned}$$

We'd like the error term to go away, but because $y$ is unbounded (this integral is over $\mathbb{R}^n$) we need to make some assumptions. Let's assume $\operatorname{supp}(V) \subset B_R(0)$ is bounded. Then,

$$\left| x + \frac{\varepsilon y}{2} \right| < R,$$

so

$$|y| \le \frac{2}{\varepsilon}(R + |x|).$$

This is not strong enough: it's asymptotic to $1/\varepsilon$, which does not go away (rather the opposite, in fact).

[3] For this reason, $\varepsilon$ is sometimes known as a *semiclassical parameter*.

[4] TODO: I think... I didn't get this written down in time.

Instead, we'll have to show that $(II_2)$ converges *weakly* to 0, even when $V$ isn't compactly supported. Let $J(x,p) \in \mathcal{S}(\mathbb{R}^n \times \mathbb{R}^n)$ be a test function (Schwartz class), and recall that the Fourier transform sends Schwartz-class functions to Schwartz-class ones. This implies that for all $m$, $n$, $r$, and $s$,

$$\|x^m \nabla_x^n p^r \nabla_p^s J\|_{L^\infty} < C_{m,n,r,s}.$$

For any such $J$, its Fourier transform, also Schwartz class, satisfies

$$|\widehat{J}(x,y)| \le \frac{f(x)}{(R^2+y^2)^{m/2}} \tag{5.2}$$

for some $R$, where $f(x) \to 0$ rapidly as $|x| \to \infty$. Hence, when we integrate,

$$\frac{1}{\varepsilon}\int J(x,p) D^2V(\varepsilon y, \varepsilon y)\overline{\psi^\varepsilon(\cdots)}\psi^\varepsilon(\cdots)e^{ipy}\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}p$$
$$= \frac{1}{\varepsilon}\int \widehat{J}(x,y) D^2V(\varepsilon y, \varepsilon y)\overline{\psi^\varepsilon(\cdots)}\psi^\varepsilon(\cdots)\,\mathrm{d}y\,\mathrm{d}x.$$

Using (5.2),

$$|(\text{above})| \le \frac{1}{\varepsilon}\int |f(x)|\|D^2V\|_{L^\infty}|\varepsilon y^2| \frac{1}{(R^2+y^2)^m}\left|\overline{\psi^\varepsilon\left(t, x-\frac{\varepsilon y}{2}\right)}\right|\left|\psi^\varepsilon\left(t, x+\frac{\varepsilon y}{2}\right)\right|\mathrm{d}x\,\mathrm{d}y.$$

Since $V$ is $C^2$, $\||f|\cdot\|D^2V\|_{\text{matrix}}\|_{L^\infty}$ is bounded by some constant $C$. Here we need to assume $D^2V$ grows at most polynomially in $|x|$ as $|x| \to \infty$ and that $f$ is Schwartz. Then,

$$\le \frac{1}{\varepsilon}\int \frac{1}{(R^+y^2)^{n/2+1}}\,\mathrm{d}y\left(\int\left|\psi^\varepsilon\left(t, x-\frac{\varepsilon y}{2}\right)\right|^2\mathrm{d}x\right)^{1/2}\left(\int\left|\psi^\varepsilon\left(t, x+\frac{\varepsilon y}{2}\right)\right|^2\mathrm{d}x\right)^{1/2}.$$

Each of the $L^2$ terms is $O(\varepsilon)$, and therefore the whole thing goes as $\varepsilon^2/\varepsilon$, hence $O(\varepsilon)$, which goes to 0 as $\varepsilon \to 0$. ⊠

Hence the semiclassical limit of the Schrödinger equation is the Liouville equation, as promised. We're lucky in a sense, because the semiclassical limit came purely by rescaling; in general, one has to be more clever.

**Derivation of the principle of least action from the path integral.** There's another way to pass from quantum to classical without doing anything so strange as letting $\hbar \to 0$ (so in particular, we can call it $\hbar$ again).

First, let's simplify by removing the $V\psi$ term, obtaining the *free Schrödinger equation*

$$H_0 = -\frac{\hbar^2}{2}\Delta,$$

whose solution with $\psi(t=0) = \psi_0$ is

$$\psi(t,x) = \left(e^{-itH_0/\hbar}\psi_0\right)(x) \tag{5.3}$$
$$= \left(\frac{1}{2\pi i\hbar t}\right)^{d/2}\int e^{-i|x-q_0|^2/(2\hbar t)}\psi_0(q_0)\,\mathrm{d}q_0.$$

If it weren't for the $i$ in the exponent, this would look like a Gaussian. To solve it, we're going to discretize time $[0,t]$ into $N$ intervals of width $\Delta t := t/N$. Let $t_j := j\cdot\Delta t$ and $q_j$ be the variable corresponding to $t_j$.

$$= \left(\frac{1}{2\pi i\hbar\Delta t}\right)^{dN/2}\int \prod_{j=0}^{N-1} e^{-i|q_{j+1}-q_j|^2/(2\hbar\Delta t)}\Bigg|_{q_N=x}\psi_0(q_0)\prod_{j=0}^{N-1}\mathrm{d}q_j. \tag{5.4}$$

Thus, if you let $\mathbf{q}_N := (q_0,\dots,q_N)$ and

$$\mathcal{D}\mathbf{q}_N := \left(\frac{1}{\pi i\hbar\Delta t}\right)^{dN/2}\prod_{j=1}^{N-1}\mathrm{d}q_j,$$

which is a complex-valued measure, then (5.4) simplifies to

$$\int \exp\left(-\frac{i}{\hbar} S_{0,N}(t, \mathbf{q}_N, x)\right) \psi_0(q_0)\, \mathcal{D}\mathbf{q}_N. \tag{5.5}$$

Here $S_{0,N}$ is the discretization of the action:

$$S_{0,N} := \frac{1}{2} \sum_{j=0}^{N-1} \left(\frac{q_{j+1} - q_j}{\Delta t}\right)^2 \Delta t. \tag{5.6}$$

As $\Delta t \to 0$, this converges to $(1/2)\int_0^t (\dot{q}(s))^2\, \mathrm{d}s$, and (5.5) resembles more and more the integral of $e^{iS/\hbar}$ over all paths connecting $q_0$ to $x$, integrated against $\psi(q_0)$ with respect to $q_0$. This is an example of a *path integral* (after all, it's an integral over paths).

For the full Schrödinger equation, with $V \neq 0$, the idea is the same, just with more variables per line. Again subdivide

$$[0, t] = \bigcup_{j=0}^{N_1} [t_j, t_{j+1}],$$

and discretize the classical action, like in (5.6) but with a potential.

$$S_N(t, \mathbf{q}_N, x) := \sum_{j=0}^{N-1} \left(\frac{1}{2}\left(\frac{q_{j+1} - q_j}{\Delta t}\right)^2 + V(q_j)\right) \Delta t. \tag{5.7}$$

Then, define

$$\Psi_N(t, x) := \int e^{-iS_N(t, \mathbf{q}_N, x)/\hbar} \underbrace{\left[\frac{\det(\partial_t^2)}{\det(\partial_t^2 + D^2 V)}\right]}_{(*)} \psi_0(q_0)\, \mathcal{D}\mathbf{q}_N. \tag{5.8}$$

The quantity in (*) is called the *Van Vleck-Pauli-Morette determinant*, which is the correction to (5.5) dictated by the potential.

**Theorem 5.9.** *If $\Psi(t, x) := \lim_{N\to\infty} \Psi_N(t, x)$, then $\psi$ is a strong $L^2$ solution to the Schrödinger equation with $\Psi(t = 0) = \Psi_0$.*

*Partial proof.* Here s-lim denotes a strong limit. If $A$ and $B$ are two matrices which do not necessarily commute, *Trotter's product formula* establishes that

$$e^{A+B} = \lim_{N\to\infty} \left(e^{(1/N)A} e^{(1/N)B}\right)^N. \tag{5.10}$$

In particular, $H_0$ and $V$ don't necessarily commute, so if $\Delta t := t/N$,

$$\exp\left(-it\frac{H_0 + V}{\hbar}\right) = \operatorname*{s-lim}_{N\to\infty} \left(\exp -i\frac{\Delta t H_0}{\hbar} \exp\left(-i\frac{\Delta t V}{\hbar}\right)\right)^N.$$

Implicit in this composition of operators is a kernel transform.[5] Therefore

$$e^{-it\frac{H_0+V}{\hbar}}(x, q_0) = \operatorname*{s-lim}_{N\to\infty} \int \left(e^{-i\Delta t H_0/\hbar}\right)(x, q_{N-1}) e^{-i\Delta t V(q_{N-1})/\hbar} \left(e^{-i\Delta t H_0/\hbar}\right)(q_{N-1}, q_{N-2}) \cdots e^{-i\Delta t V(q_0)/\hbar}\, \mathrm{d}q_1 \cdots \mathrm{d}q_{N-1}. \tag{5.11}$$

If you insert

$$\left(e^{-i\Delta t H_0/\hbar}\right)(q_{j+1}, q_j) = \left(\frac{1}{2\pi i\hbar\Delta t}\right)^{d/2} e^{-i|q_{j+1} - q_j|^2/(2\hbar\Delta t)},$$

you get the desired expression for $\Psi_N$ in (5.8), except for the VV-P-M determinant. Now we need to actually evaluate (5.11), which is a very oscillatory integral on a high-dimensional space. Fortunately, we can use a trick from harmonic analysis called the stationary phase formula to assist us.[6]

[5] TODO: what is this explicitly referring to?

[6] For those of you who like topology and geometry, there's a geometric reformulation of this which is related to the Duistermaat-Heckman formula in symplectic geometry.

**Theorem 5.12.** *Assume $\Phi$ and $f$ are $C^2$ functions on $\mathbb{R}^n$, and let $y^*$ denote the unique solution to $\Delta\Phi(y) = 0$. Assume $D^2\Phi(y^*)$ is nondegenerate; then*

$$\int e^{-i\lambda\Phi(y)} f(y)\,dy = \left(\frac{2\pi i}{\lambda}\right)^{d/2} |\det D^2\Phi(y^*)|^{-1/2} e^{-i\pi\,\mathrm{sign}(D^2\Phi(y^*))/4} e^{-i\lambda\Phi(y^*)} f(y^*) + o\left(\left(\frac{1}{\lambda}\right)^{d/2}\right)$$

*as $\lambda \to \infty$.*

The cool idea is, since

$$e^{i\lambda cy} = \frac{1}{i\lambda c}\partial_y e^{icy},$$

you can use the regularity of $f$ to trade for factors of $1/\lambda$: the more regular $f$ is, the stronger convergence you can obtain.

Lecture 6.

## The stationary phase approximation: 9/19/17

To recap, we wanted to solve the Schrödinger equation, and in order to do so took a kind of path integral: we discretized the action (5.7) and integrated over all (piecewise-linear) possible paths (5.8) between $q_0$ and $q_N = x$, the point where we wanted to evaluate the answer. These discretized paths are approximations $\mathbf{q}_N^*$ to the classical paths which solve the Euler-Lagrange equations, and one has that

$$\Psi_N(t,x) = \left(\frac{1}{2\pi i\hbar t}\right)^{d/2} \int \exp\left(\frac{-iS_N(t,\mathbf{q}_N^*,x)}{\hbar}\right)\left[\frac{\det(\partial_t^2)}{\det(\partial_t^2 + D^2V)}\right]\psi_0(q_0)\,dq_0. \tag{6.1}$$

We then used Trotter's product formula (5.10) to prove that this converges to solutions $\psi(t)$ strongly (Theorem 5.9).

To prove (6.1), we have to use the *stationary phase formula*: that for $\lambda \gg 1$,

$$\int e^{i\lambda\Phi(x)} f(x)\,dx = \left(\frac{1}{2\pi i\lambda}\right)^{d/2} e^{i\lambda\Phi(x^*)} e^{i\pi\,\mathrm{sign}(D^2\Phi(x^*))/4}\left(\frac{1}{\det D^2\Phi(x^*)}\right)^{1/2} f(x^*) + o\left(\left(\frac{1}{\lambda}\right)^{d/2}\right), \tag{6.2}$$

where $x^*$ is the *stationary point*, i.e. the point where $\nabla\Phi(x^*) = 0$.

To use (6.2), we need to find the stationary point $\mathbf{q}_N^*$ of $S_N(t,\mathbf{q}_N,x)$, which must satisfy

$$\nabla_{\mathbf{q}_N^*}(t,\mathbf{q}_N^*,x) = 0. \tag{6.3}$$

The Hessian is

$$D^2 S_N(t,\mathbf{q}_N,x) = \frac{1}{\Delta t}\underbrace{\begin{pmatrix} 2\mathbf{1}_d & -\mathbf{1}_d & & & \\ -\mathbf{1}_d & 2\mathbf{1}_d & -\mathbf{1}_d & & \\ & -\mathbf{1}_d & \ddots & & \\ & & & \ddots & -\mathbf{1}_d \\ & & & -\mathbf{1}_d & 2\mathbf{1}_d \end{pmatrix}}_{M_{N,d}} + D_{\mathbf{q}}^2 V(\mathbf{q}_N^*)\Delta t.$$

Now, (6.3) is equivalent to the equation

$$\frac{-q_{j+1}^* + 2q_j^* - q_{j-1}^*}{(\Delta t)^2} = -(\nabla_{q_j} V)(q_j^*)$$

for $j = 1,\dots,N-1$, and this is precisely a discretization of the Newton equations

$$\ddot{q} = -\nabla V(q).$$

*Remark.* $1/(\Delta t)^2 M_{N,d}$ is a discretization of $\partial^2$. ◂

From the stationary phase equation,

$$\Psi_N(t,x) = \int K_N(t,\mathbf{q}_N^*,x)\psi_0(q_0)\,\mathrm{d}q_0 + \text{lower-order terms},$$

where

$$\begin{aligned} K_N(t,\mathbf{q}_N^*,x) &= \left(\frac{1}{2\pi i\hbar\Delta t}\right)^{Nd/2}(2\pi i\hbar)^{Nd/2}\left|\det\left(D^2_{\mathbf{q}_N}S_N(t,\mathbf{q}_N^*,x)\right)\right|^{-1/2}\exp\left(\frac{iS_N(t,\mathbf{q}_N^*,x)}{\hbar}\right)\\ &= \left|\det\left(\Delta t\, D_q^2 S_N(t,\mathbf{q}_N^*,x)\right)\right|^{-1/2}\exp\left(\frac{iS_N(t,\mathbf{q}_N^*,x)}{\hbar}\right)\\ &= \left|\det\left(M_{N,d}+D_q^2V(\mathbf{q}_N^*)(\Delta t)^2\right)\right|^{-1/2}\exp\left(\frac{iS_N(t,\mathbf{q}_N^*,x)}{\hbar}\right), \end{aligned} \tag{6.4}$$

and we know what the Hessian is. We'll use a strange-looking trick to simplify this next: observe that

$$\left(\frac{1}{2\pi i\hbar}\right)^{d/2} = \left(\frac{1}{2\pi i\hbar t}\right)^{d/2}\exp\left(-\frac{i|x-x|}{2\hbar t}\right),$$

which can be interpreted as a free propagator of $x$ with itself. This can be expressed as an action

$$= |\det(M_{N,d})|^{-1/2}\exp\left(\frac{i}{\hbar}S_{0,N}(t,x,x,\dots,x)\right).$$

Plugging the ratio of these terms back into (6.4),

$$K_N(t,\mathbf{q}_N^*,x) = \left(\frac{1}{2\pi i\hbar t}\right)^{d/2}\int\left|\frac{\det((1/(\Delta t)^2)M_{N,d})}{\det((1/(\Delta t)^2)M_{N,d}+D^2V)}\right|\exp\left(\frac{iS_N(t,\mathbf{q}_N^*,x)}{\hbar}\right).$$

This ratio of determinants is important — it's the discretization of the VV-P-M determinant that we alluded to last time.

**Ehrenfest theorem.** The Ehrenfest theorem is another link between the quantum and classical worlds.

**Theorem 6.5.** *Let $A(t)$ be a linear operator on $L^2$ and assume $\psi(t)$ is an $L^2$ solution of the Schrödinger equation, i.e.*

$$i\hbar\partial_t\psi = H\psi$$

*and $\psi(t=0)=\psi_0$ for some specified $\psi_0$. Then,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A(t)\rangle_{\psi(t)} = \frac{1}{i\hbar}\langle[H,A]\rangle_{\psi(t)} + \langle\partial_t A\rangle_{\psi(t)}.$$

(Recall that $\langle A\rangle_\psi = \langle\psi, A\psi\rangle$.) One special case of interest: let $A=x$ be a position variable. Then,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle_{\psi(t)} = \langle[H,x]\rangle_{\psi(t)},$$

and

$$[H,X] = \left[-\frac{\hbar^2}{2}\Delta + V, x\right].$$

If you calculate it out, this commutator is the gradient, so

$$[H,x]f = -\hbar^2\nabla f = -i\hbar Pf,$$

where $P := -i\hbar\nabla$ is the momentum operator.

If on the other hand you apply Theorem 6.5 to $P$, you get that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} = \frac{1}{i\hbar}\langle[H,P]\rangle_{\psi(t)},$$

and in a similar manner,

$$[H,P]f = [V,P]f = -i\hbar(\nabla V)\cdot f.$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} = -\langle\nabla V\rangle_{\psi(t)}.$$

What this means is that the classical Hamiltonian equations hold, in the operator sense, in expectation, with respect to $\psi(t)$.

**Spectral theory.** We're going to spend the next several lectures on spectral theory. We've done some before in the prelim classes, but the operators that arise in quantum physics are not always compact, and so we'll need a more advanced theory.

**Definition 6.6.** Let $A$ be a linear operator (possibly unbounded) on a Hilbert space $\mathcal{H}$. Its *spectrum* $\sigma(A)$ is the set of $\lambda \in \mathbb{C}$ such that $A - \lambda$ is noninvertible.[7] The *resolvent* $\rho(A) := \mathbb{C} \setminus \sigma(A)$.

The spectrum further subdivides into three types.

- The *point spectrum* $\sigma_p(A)$ is the subset of $\sigma(A)$ where $A - \lambda$ is not injective.
- The *continuous spectrum* $\sigma_c(A)$ is the subset of $\sigma(A)$ where $A - \lambda$ is injective, and the range of $A - \lambda$ is dense, but $(A - \lambda)^{-1}$ is not bounded.
- The *residual spectrum* is the subset of $\sigma(A)$ where the range of $A - \lambda$ is not dense.

**Theorem 6.7.** *These are all the spectral types: $\sigma(A) = \sigma_p(A) \cup \sigma_c(A) \cup \sigma_r(A)$. Moreover, if $A$ is self-adjoint, $\sigma_r(A) = \varnothing$ and $\sigma(A) \subset \mathbb{R}$.*

**Definition 6.8.** Assume $(A - \lambda)\psi = 0$ has a nonzero solution $\psi \in \mathcal{H}$. Then, $\lambda$ is called an *eigenvalue* and $\psi$ an *eigenvector*.

There are also cases that are "almost as good."

**Definition 6.9.** The sequence $\{\psi_n\} \in \mathcal{H}$ is called a *Weyl sequence* for $A$ and $\lambda$ if

(1) $\|\psi_n\|_{\mathcal{H}} = 1$,
(2) $\|(A - \lambda)\psi_n\|_{\mathcal{H}}$ goes to 0 as $n \to \infty$, and
(3) $\psi_n \rightharpoonup 0$ as $n \to \infty$.

The last condition means that $\psi_n$ *converges weakly* to 0, i.e. $(\phi, \psi_n) \to 0$ for all $\phi \in \mathcal{H}$.
Let $\sigma_d(A)$ denote the *discrete spectrum* of $A$, i.e. the set of isolated eigenvalues of $A$ with finite multiplicity.
We won't prove these theorems, but a proof will be posted (either on Canvas or the course website).

**Theorem 6.10** (Weyl criterion)**.** *$\sigma_c(A)$ is the set of $\lambda \in \mathbb{C}$ for which there exists a Weyl sequence.*

**Theorem 6.11.** *If $U\colon \mathcal{H} \to \mathcal{H}$ is unitary, then $\sigma(U^*AU) = \sigma(A)$.*[8]

*Proof.* This follows because $U^*AU - \lambda = U^*(A - \lambda)U$, which is true because $U^*U = \mathbf{1}$, and the fact that $U$ is an isometric isomorphism, hence preserves injectivity, surjectivity, and density. ⊠

Different authors use different conventions/definitions for these things, so be careful.

Lecture 7.

## Spectral theory: 9/21/17

*"Let me write this down in the hope that the errors today are new errors, not old ones."*

We started with a correction of a derivation from the last lecture. I don't know where it fits in the notes, unfortunately.

$$\left(\frac{1}{2\pi i\hbar t}\right)^{d/2} = \left(\frac{1}{2\pi i\hbar t}\right)^{d/2} \exp\left(-\frac{i|x-x|^2}{2\hbar t}\right)$$
$$= \left(\frac{1}{2\pi i\hbar \Delta t}\right)^{dN/2} \int \exp\left(-\frac{i}{\hbar} S_{0,N}(t, \mathbf{q}_N, x)\right) d\mathbf{q}_N.$$

$d\mathbf{q}_N$ is a product of $N-1$ integrands $dq_j$, rather than $N$ integrands.

$$= \left(\frac{1}{2\pi i\hbar \Delta t}\right)^{dN/2} (2\pi i\hbar)^{\frac{d(N-1)}{2}} \left|\det\left(\frac{1}{\Delta t}\right) M_{d,N}\right|^{-1/2},$$

[7] That is, if $\lambda \notin \sigma(A)$, $A - \lambda$ has not just an inverse, but a bounded inverse.

[8] TODO: this is also true for $\sigma_p$, $\sigma_c$, and $\sigma_r$, right?

and again, $M_{d,N}$ is an $(N-1)\times(N-1)$-matrix.

$$= \left(\frac{N}{2\pi i\hbar t}\right)^{d/2} \left|\det M_{d,N}\right|^{-1/2}.$$

As the determinant of the $(N-1)\times(N-1)$-matrix

$$A_{N-1} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & & & \\ & & \ddots & & \\ & & & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

is $N$, the determinant of $M_{d,N} = A_{N-1} \otimes \mathbf{1}_d$ is $N^d$. The good news is, in the limit the answer is the same. (There was also a correction in the spectral theory part of the notes, which has already been incorporated.)

**Example 7.1.**

(1) Let $\mathcal{H} = L^2(\mathbb{R}^d)$ and for a monotone continuous function $g\colon \mathbb{R} \to \mathbb{R}$ with range $[-M, M]$, let $A_g$ be the operator sending $f$ to $A_g f(x) = g(x)f(x)$. Then, $\sigma(A_g) = [-m, M]$.
   If $\lambda \notin \mathrm{Im}(g)$, then $(A_g - \lambda)^{-1} = 1/(g(x) - \lambda)$ is bounded.
   Now assume $\lambda \in \mathrm{Im}(g)$; since $g$ is monotone, $g^{-1}(\lambda)$ is either a point or an interval.
   - Suppose $|g^{-1}(\lambda)| = 0$. Then, $A_g - \lambda$ is injective, because $((A_g - \lambda)f)(x) = 0$ iff $(g(x) - \lambda)f(x) = 0$ implies $f = 0$ almost everywhere, so $\lambda \in \sigma_c(A_g)$.
   - Suppose $|g^{-1}(\lambda)| > 0$. Then, there functions $f \in L^2(\mathbb{R})$ not almost everywhere zero with $((A_g - \lambda)f)(x) = 0$, so $\lambda \in \sigma_p(A_g)$.

(2) Let $A$ be multiplication by $x$ acting on $L^2(\mathbb{R})$. Then, $\sigma(A) = \sigma_c(A) = \mathbb{R}$, essentially by the previous example. This is the spectrum of a position operator in quantum mechanics.

(3) Let $P = -i\nabla$, which is the momentum operator, again in $d = 1$. If $U$ denotes the Fourier transform, then $U^*PU = \xi$, so once again $\sigma(P) = \sigma_c(P) = \mathbb{R}$.

(4) Suppose $A\psi = -\Delta\psi$. Then, $U^*(-\Delta)U = \xi^2$, so we can just look at the spectrum of that, which is entirely the continuous spectrum, which is $\mathbb{R}_{\geq 0}$, so $\sigma(-\Delta) = \sigma_c(-\Delta) = \mathbb{R}_{\geq 0}$.

(5) If $A = -\Delta$ and $d > 1$, then

$$U^*(-\Delta)U = \sum_{j=1}^{d} \xi_j^2,$$

which has the same range, and therefore it's still true that $\sigma(-\Delta) = \sigma_d(-\Delta) = \mathbb{R}_{\geq 0}$. ◂

**Theorem 7.2.** *Suppose $H = -\Delta + V$ on $L^2(\mathbb{R}^d)$, where $V$ is a continuous function such that $V(x) \to 0$ as $|x| \to \infty$. Then, $\sigma_{\mathrm{ess}}(H) = \mathbb{R}_{\geq 0}$.*

This is tricky, because these operators do not commute. The proof is a nice application of a variant of Weyl sequences.

**Definition 7.3.** Let $A$ be a linear operator on $L^2(\mathbb{R}^d)$. A *spreading sequence* for $A$ and $\lambda$ is a sequence $\{\psi_n\}$ such that

- $\|\psi_n\| = 1$,
- for any bounded $B \subset \mathbb{R}^d$, there's an $N_B$ such that $\mathrm{supp}(\psi_n) \cap B = \varnothing$ for $n > N_B$, and
- $\|(A - \lambda)\psi_n\| \to 0$ as $n \to \infty$.

**Proposition 7.4.** *A spreading sequence for $A, \lambda$ is also a Weyl sequence.*

*Proof of Theorem 7.2.* Consider the sequence

$$\psi_n(x) := e^{i\sqrt{\lambda}x} \frac{1}{n^{d/2}} \phi\left(\frac{|x - 2n\,\mathrm{sign}(x)|}{n}\right),$$

where $\phi$ is a bump function with total integral 1 and supported on $(-1, 1)$. We're going to show this is a spreading sequence for $H$ when $\lambda \geq 0$.

We have

$$|x - 2n\,\mathrm{sign}(x)| \le n \iff n \le |x| \le 3n,$$

and therefore the support of $\psi_n$ is unbounded as $n \to \infty$. It's also quick to check tht $\|\psi_n\|^2 = 1$. Finally, let's compute

$$\|(H-\lambda)\psi_n\| \le \underbrace{\|(-\Delta - \lambda)\psi_n\|_{L^2}}_{(I)} + \underbrace{\|V\psi_n\|_{L^2}}_{(II)}. \tag{7.5}$$

Since the Fourier transform is norm-preserving,

$$(I) = \|(\xi^2 - \lambda)\widehat{\psi}_n\|,$$

and

$$\widehat{\psi}_n(\xi) = e^{2in|\xi|}\underbrace{n^{d/2}\widehat{\phi}\Big(n\Big(|\xi| - \lambda^{1/2}\Big)\Big)}_{\chi_n(\xi)}.$$

$|\chi_n|^2$ is concentrated around $|\xi| - \lambda^{1/2}$, and in fact converges weakly to a $\delta$-function supported there, which means that for any test function $g$, as $n \to \infty$,

$$\int g(|\xi|)\chi_n^2(|\xi|)\,\mathrm{d}|\xi| \longrightarrow g(\lambda^{1/2}).$$

Therefore, assuming $\lambda$ is in the image of $\xi^2$,

$$\int (\xi^2 - \lambda^2)|\chi_n(\xi)|^2\,\mathrm{d}\xi \longrightarrow 0.$$

The other piece of (7.5) also goes to 0:

$$\begin{aligned}(II)^2 &= \|V\psi_n\| \\ &= \int V(x)^2|\psi_n(x)|^2\,\mathrm{d}x \\ &\le \sup_{|x|\in[n,3n]} |V(x)|^2 \int |\psi_n|^2, \end{aligned} \tag{7.6}$$

and we know $\|\psi_n\| = 1$ and $V(x) \to 0$ as $|x| \to \infty$, so (7.6) does go to 0 as $n \to \infty$, and therefore for $\lambda \ge 0$, $\{\psi_n\}$ is a spreading sequence, hence a Weyl sequence by Proposition 7.4, and by Theorem 6.10, we're done. ⊠

Lecture 8.

## The spectral theory of Schrödinger operators: 9/26/17

Note: I came in 20 minutes late and may have missed some material.
References: Reed-Simon, Hislop-Sigal, Yoshida, Kato.

**Definition 8.1.** $T$ is *essentially self-adjoint* on $\mathcal{H}$ if its closure is self-adjoint.

**Theorem 8.2.** *Let $T$ be a symmetric operator on $\mathcal{H}$. Then, the following are equivalent:*

(1) *$T$ is essentially self-adjoint on $\mathcal{H}$.*
(2) $\ker(T^* \pm i) = \{0\}$.
(3) $\mathrm{Im}(T \pm i)$ *is dense in $\mathcal{H}$.*

Now we'll talk about the spectral theorem.

For motivation, consider an $n \times n$ matrix with complex entries. It has $n$ eigenvalues $\sigma(A) = \{\lambda_j\}$, and assume that it has $n$ linearly independent eigenvectors $v_j$, so that it may be diagonalized: let $T = (v_1 \ \dots \ v_n)$ and

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}.$$

Then,

$$A = T^{-1}\Lambda T = \sum \lambda_j P_j,$$

where if $E_j$ is the matrix with a 1 in position $(j,j)$ and 0 elsewhere, $P_j \coloneqq T^{-1}E_jT$.

The *operator norm* $\|A\|_{\text{op}}$ is defined to be the supremum of the set of eigenvalues of $A$. If $A = A^*$ (i.e. it's *Hermitian*), then $T^{-1} = T^*$, i.e. it's *unitary*.

Now suppose $f$ is a function with a convergent power series expansion $f = \sum a_n x^n$. For a matrix $A$ we can write

$$\begin{aligned} f(A) &= \sum a_n A^n \\ &= T^{-1}\big(\sum a_n \Lambda^n\big)T \\ &= T^{-1}\begin{pmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_n) \end{pmatrix} T \\ &= \sum_j f(\lambda_j)P_j. \end{aligned}$$

If $\Gamma$ is a contour enclosing $\sigma(A)$, we can also write this as

$$f(A) = \frac{1}{2\pi i}\sum_j \oint_\Gamma \mathrm{d}z\, \frac{f(z)}{\lambda_j - z}P_j,$$

or, if $f$ is analytic,

$$= \frac{1}{2\pi i}\oint_\Gamma \mathrm{d}z\, \frac{f(z)}{A - z}.$$

Now we generalize to infinite-dimensional Hilbert spaces.

**Theorem 8.3** (Spectral theorem for bounded Hermitian operators)**.** *Let $A$ be a bounded Hermitian operator on a Hilbert space $\mathcal{H}$, $\Omega$ be a complex domain containing $\sigma(A)$, and $f\colon \mathbb{C} \to \mathbb{C}$ be analytic in $\Omega$. If $\Gamma$is a contour in $\Omega$ encircling $\sigma(A)$, then*

$$f(A) = \frac{1}{2\pi i}\oint_\Gamma f(z)(A - z)^{-1}\,\mathrm{d}z.$$

Since $A = A^*$, $\sigma(A) \subset \mathbb{R}$; since $A$ is bounded, so is its spectrum, and therefore the picture makes sense.

This integral may be understood in the following way: the numbers $(\psi, f(A)\varphi)$ over all $\psi, \varphi \in \mathcal{H}$ determine $f(A)$ uniquely, and

$$(\psi, f(A)\varphi) = \frac{1}{2\pi i}\oint_\Gamma f(z)(\psi, (A - z)^{-1}\varphi),$$

and the inner product is analytic in $z$ in a neighborhood of $\Gamma$.

In quantum mechanics, we need to also understand unbounded operators. In this case, the spectrum is real, but may be unbounded, and the idea is to consider the contour that's the boundary of the rectangle $[-1/\varepsilon, 1/\varepsilon] \times [\varepsilon, \varepsilon]$, and let $\varepsilon \searrow 0$.

**Theorem 8.4** (Spectral theorem for unbounded, Hermitian operators)**.** *Let $A$ be an* unbounded *Hermitian operator on $\mathcal{H}$ and $f\colon \mathbb{R} \to \mathbb{R}$ be a Borel function.*[9] *Then,*

$$f(A) = \frac{1}{2\pi i}\lim_{\varepsilon \searrow 0} \operatorname{Im} \int_{-\infty}^{\infty} f(\lambda)(A - \lambda - i\varepsilon)^{-1}\,\mathrm{d}\lambda.$$

The proof is long and not terribly instructive, so we won't go into it. Instead, we'll focus specifically on Schrödinger operators.

**Theorem 8.5.** *Let $H = -\Delta + V$, where $V\colon \mathbb{R}^d \to \mathbb{R}$ is continuous, $V \geq 0$, and $V(x) \to \infty$ as $|x| \to \infty$. Then,*

(1) *$H$ is self-adjoint on $L^2(\mathbb{R}^d)$,*
(2) *$\sigma(H) = \sigma_d(H)$ is the set $\{\lambda_j\}$ of eigenvalues, and*

[9] This means for every $I \subset \mathbb{R}$ open, $f^{-1}(I)$ is a Borel set.

(3) $\lambda_j \to \infty$ *as* $j \to \infty$.

*Partial proof.* For self-adjointness, see Hislop-Segal. We next show there does not exist a spreading sequence for any $\lambda$: assume $\{\psi_n\}$ is such a sequence; then, for any $\lambda$ in the essential spectrum, $(\psi_n, (H-\lambda)\psi_n) \to 0$. And this is

$$\begin{aligned}(\psi_n, (H-\lambda)\psi_n) &= (\psi_n, (-\Delta)\psi_n) + (\psi_n, V\psi_n) - \lambda \\ &= \int |\nabla \psi_n|^2 + \int V|\psi_n|^2 - \lambda \\ &\geq \inf_{y \in \operatorname{supp}(\psi_n)} (V(y)) - \lambda,\end{aligned}$$

and this goes to $\infty$, since $\{\psi_n\}$ is a spreading sequence, providing a contradiction.

This means the essential spectrum is empty, so $\sigma(H) = \sigma_d(H)$, which is exactly the isolated eigenvalues.

To get at the limit of the eigenvalues, we'll use a variational characterization of the eigenvalues of an operator.

**Theorem 8.6.** *Let* $\mathcal{H}_h := \operatorname{span}\{\psi_1, \dots, \psi_n\}$, *where* $\psi_i$ *is an eigenvector for the* $i^{th}$ *lowest eigenvalue* $\lambda_i$ *(so* $\lambda_1 \leq \lambda_2 \leq \dots$*). Then,*

$$\inf_{\{\psi \in \mathcal{H}_n^\perp \cap D(H) \mid \|\psi\|=1\}} (\psi, H\psi) = \inf\{\sigma(H) \setminus \{\lambda_1, \dots, \lambda_n\}\}.$$

This is true because $H$ is unbounded and its eigenvalues do not accumulate (because there is no essential spectrum). Repeatedly invoking Theorem 8.6, one gets that there's always another eigenvalue $\lambda_{i+1}$, and it's at least as big as $\lambda_i$, but the eigenvalues cannot accumulate, so they go to $\infty$. ⊠

Not every Schrödinger operator meets the criteria of (8.5), though, including some famous ones.

**Example 8.7** (The hydrogen atom)**.** Consider the *Coulomb potential* $V(x) = 1/|x|$ on $\mathbb{R}^3$, which goes to 0 as $|x| \to \infty$, and the Hamiltonian

$$H = -\Delta - \frac{1}{|x|}.$$

Then, the essential spectrum of $H$ is $[0, \infty)$. There are infinitely many eigenvalues below 0, though, and we'll shw this by constructing a sequence $\{u_n\}_{n \geq 1}$ of linearly independent functions with $(u_n, Hu_n) < 0$ for all $n$.

Pick a $u \in C_0^\infty(\mathbb{R}^3)$ such that $\|u\|_{L^2} = 1$ and $\operatorname{supp} u \subset \{x \in \mathbb{R}^3 \mid 1 < |x| < 2\}$. Then, let

$$u_n := 2^{-3n/2} u(2^{-n}x),$$

for $n \in \mathbb{N}$. Since $(u_n, u_m) = \delta_{nm}$, these are linearly independent. Moreover, $(u_n, Hu_m) = 0$ when $n \neq m$:

$$(u_n, Hu_m) = \int \overline{\nabla u_n}(\nabla u_m)\, \mathrm{d}x + \int V(x)\overline{u_n(x)}u_m(x)\, \mathrm{d}x,$$

but $u_n$ and $u_m$ have disjoint domains, so these integrals are both 0. If $m = n$, then we get

$$(u_n, Hu_n) = \int |\nabla u_n|^2 - \int \frac{1}{|x|}|u_n|^2 < 0.$$ ◂

Lecture 9.

## The Birman-Schwinger principle: 9/28/17

We've been studying the Schrödinger operator

$$H = -\Delta - \frac{1}{|x|},$$

which corresponds to a hydrogen atom, a single electron bound to a nucleus. We're assuming the nucleus is static and its mass is so large as to make the mass of the hydrogen atom negligible. Last time, we saw that the essential spectrum of $H$ is $\mathbb{R}_+$, the eigenvalues are negative numbers, and there are infinitely many distinct eigenvalues. This implies there's an infinite-dimensional linear subspace on which $H$ is negative.

One might ask, what aspect of this operator leads $H$ to have infinitely many eigenvalues? For which values of $\alpha > 0$ does the operator

$$H = -\Delta - \frac{1}{|x|^\alpha}$$

have infinitely many eigenvalues?

Again we consider the function $u_n(x) := 2^{-3n/2}u(2^{-n}x)$, where $u \in C_0^\infty$ and $\operatorname{supp}(u) \subset \{|x| \mid 1 < |x| < 2\}$, so that $\|u_n\|_{L^2} = 1$.[10] Then,

$$\langle u_n, Hu_m\rangle = C\delta_{n,m},$$

because the support of the derivatives is also disjoint. Thus the kinetic term always vanishes. But the potential term may be nonzero, and is when $m = n$: we get

$$\begin{aligned}\langle u_n, Hu_n\rangle &= \int |\nabla u_n|^2 - \int \frac{1}{|x|^\alpha}|u_n|^2 \\ &= 2^{-2n}\int |\nabla u|^2 - 2^{-\alpha n}\int \frac{|u|^2}{|x|^\alpha}. \end{aligned} \tag{9.1}$$

If $\alpha < 2$, then for all $n$ large enough, this is less than 0, because the second term dominates. This implies there are infinitely many eigenvalues. If $\alpha > 2$, then (9.1) is positive for all $n$ sufficiently large. Does this mean we only have finitely many eigenvalues?

Another potential we might consider is $V(x) = 1/\langle x\rangle^\alpha$ (where $\langle x\rangle$ is the Japanese bracket). Then, $V \in L^{3/2}(\mathbb{R}^3)$. For $\alpha > 2$, do we only have finitely many eigenvalues?

The physical intuition comes from spectroscopic experiments: the hydrogen atom is in a state, and if it absorbs light of a certain energy (color), it can jump to a higher-energy state, and if it emits light of a certain energy (color), it falls to a lower-energy state. Every atom has a different potential and hence a different spectrum (of its Hamiltonian and observationally). The essential spectrum represents when the electron has been separated from the atom (ionization).

We'll use something called the *Birman-Schwinger principle* to solve this. Assume $H = -\Delta + V$, where $V < 0$, so $U(x) := -V(x) > 0$. For any $\lambda < 0$, $(-\Delta + V)\phi = \lambda\phi$ iff $(-\Delta - \lambda)\phi = U\phi$, so

$$\phi = (-\Delta - \lambda)^{-1}U\phi.$$

Since $U > 0$ then we can take a square root of it: let $v := U^{1/2}\phi$, so $v = K(\lambda)v$, where

$$K(\lambda) := U^{1/2}(-\Delta - \lambda)^{-1}U^{1/2}.$$

In particular, $\lambda$ is an eigenvalue of $H$ (for $\lambda < 0$) iff 1 is an eigenvalue of $K(\lambda)$. Therefore the number $n_H$ of $\lambda < 0$ that are eigenvalues of $H$ is the same as the number of $\lambda < 0$ such that 1 is an eigenvalue of $K(\lambda)$.

**Proposition 9.2.** *$n_H$ is also equal to the number of $\nu < 1$ such that $\nu$ is an eigenvalue of $K(0)$.*

We'll prove this in a series of lemmas.

**Lemma 9.3.** *For all $\lambda < 0$, $\partial_\lambda K(\lambda) > 0$.*

*Proof.* If $\phi \neq 0$,

$$\begin{aligned}\partial_\lambda(\phi, K(\lambda)\phi) &= \partial_\lambda\left(U^{1/2}\phi, (-\Delta - \lambda)^{-1}U^{1/2}\phi\right) \\ &= \left(U^{1/2}\phi, (-\Delta - \lambda)^{-2}U^{1/2}\phi\right) \\ &= \|(-\Delta - \lambda)^{-1}U^{1/2}\phi\|_{L^2}^2 > 0 \end{aligned}$$

⊠

**Lemma 9.4.** *As $\lambda \to \infty$, $K(\lambda) \to 0$.*

This proof is a nice application of a bunch of tools you learned in your functional analysis course.

[10] One might say that the $u_n$s are *supported in dyadic shells* and have mutually disjoint supports.

*Proof.* We'll prove this by calculating the integral kernel of $K(\lambda)$, using the integral kernel for $(-\Delta-\lambda)^{-1}$. First,

$$(-\Delta-\lambda)^{-1}(x,y) = \frac{1}{2\pi|x-y|}e^{\sqrt{|\lambda|}|x-y|}. \tag{9.5}$$

The integral kernel is one such that you get a convolution operator after the Fourier and inverse Fourier transforms, and is the infinite-dimensional generalization of matrix multiplication.

$$\begin{aligned}((-\Delta-\lambda)^{-1}f)(x) &= \left((\xi^2-\lambda)^{-1}\widehat{f}\right)^\vee(x)\\ &= \left(((|\cdot|^2-\lambda)^{-1})^\vee * f\right)(x),\end{aligned} \tag{9.6}$$

where inside the absolute value is

$$\int \frac{1}{\xi^2+|\lambda|}e^{i\xi z}\,\mathrm{d}\xi = C\frac{e^{-\sqrt{|\lambda|}|z|}}{2|z|},$$

where we integrated over the $\xi$ such that $|\xi| = \pm i|\lambda|^{1/2}$. Therefore (9.6) is

$$\int G_\lambda(x,y)f(y)\,\mathrm{d}y,$$

where $G_\lambda(x,y)$ is the Green's function, which in this case is either side of (9.5).

*Remark.* There are two norms one can put on a kernel: the usual operator norm and the *Hilbert-Schmidt norm*

$$\|K\|_{\mathrm{HS}} := \left(\int |K(x,y)|^2\,\mathrm{d}x\,\mathrm{d}y\right)^{1/2}.$$

It turns out this is always at least as big as the operator norm: for any $f \in L^2$,

$$\begin{aligned}\|Kf\|_{L^2}^2 &= (Kf, Kf)_{L^2}\\ &= \int \mathrm{d}x \left|\int K(x,y)f(y)\,\mathrm{d}y\right|^2.\end{aligned}$$

By Cauchy-Schwarz,

$$\begin{aligned}&\le \int \mathrm{d}x \left(|K(x,y)|^2\,\mathrm{d}y\right)\left(\int |f(y)^2|\,\mathrm{d}y\right)\\ &= \int |K(x,y)|^2\,\mathrm{d}x\,\mathrm{d}y\|f\|_{L^2}^2.\end{aligned}$$

Hence $\|K\|_{\mathrm{op}} \le \|K\|_{\mathrm{HS}}$.

It'll also be useful to recall the definition of the trace of an integral kernel: if $\{\phi_i\}$ is an orthonormal basis of $L^2(\mathbb{R}^3)$,

$$\operatorname{tr} K := \sum(\phi_j, K\phi_j).$$

Basis-independently, this is also

$$\operatorname{tr} K = \int K(x,x)\,\mathrm{d}x. \qquad \blacktriangleleft$$

Putting all this together,

$$K(\lambda) = U^{1/2}(x)\frac{1}{2\pi|x-y|}e^{-\sqrt{|\lambda|}|x-y|}U^{1/2}(y),$$

so

$$\|K(\lambda)\|_{\mathrm{op}} \le \left(\int \frac{U(x)U(y)}{4\pi^2|x-y|^2}e^{-2\sqrt{|\lambda|}|x-y|}\,\mathrm{d}x\,\mathrm{d}y\right)^{1/2},$$

and this tends to 0 as $\lambda \to -\infty$. $\boxtimes$

*Proof of Proposition 9.2.* Since $\|K(\lambda)\| \to 0$ as $\lambda \to -\infty$, all eigenvalues are less than 1 for $\lambda$ sufficiently negative. Since $\partial_\lambda K(\lambda) > 0$ for all $\lambda < 0$, then the eigenvalues of $K(\lambda)$ increase monotonically in $\lambda$. The idea is that there's this "eigenvalue flow" such that as $\lambda$ gets more negative, its eigenvalues get closer to 0.

Let $\nu_m(\lambda)$ be the $m^{\text{th}}$ eigenvalue of $\lambda$. Then, if $\nu_m(\lambda_m) = 1$ for some $\lambda_m < 0$, then $\nu_m(0) > 1$. This means there's a one-to-one correspondence between the eigenvalues $\nu_m(0) > 1$ of $K(0)$ and the points $\lambda_m$ at which some eigenvalue $\nu_m(\lambda)$ crosses 1, which is, as required, the number of $\lambda < 0$ which have 1 as an eigenvalue of $K(\lambda)$.

But then,

$$\begin{aligned}\{\nu > 1 \mid \nu \text{ is an eigenvalue for } K(0)\} &= \sum_{\substack{\nu_m > 1 \\ \text{eigenvalues of } K(0)}} 1 \\ &\le \sum_{\nu_m > 1} \nu_m^2 \\ &\le \sum_{\text{eigenvalues of } K(0)} \nu_m^2 \\ &= \operatorname{tr}|K(0)|^2 = \|K(0)\|_{\text{HS}}^2.\end{aligned}$$

This norm is also

$$\frac{1}{(2\pi)^2} \int \frac{U(x)U(y)}{|x-y|^2}\,dx\,dy = \frac{1}{(2\pi)^2} \frac{V(x)V(y)}{|x-y|^2}\,dx\,dy.$$

The right-hand side is sometimes called the *Rollwick norm* of $V$. Then, using the Hardy-Littlewood inequality,

$$\le \frac{1}{(2\pi)^2} C\|V\|_{L^{3/2}}^2. \tag{9.7}$$

The Hardy-Littlewood inequality here depends on the fact that the dimension is 3, and indeed, eigenvalues of Schrödinger operators behave differently in dimension 2.

But the point is, the number of eigenvalues is finite for $V \in L^{3/2}$, and there cannot be any if (9.7) is greater than 1. ⊠

Lecture 10.

## Lieb-Thirring inequalities: 10/3/17

Last lecture, we used the Birman-Schwinger principle to count eigenvalues of certain Hamiltonians in dimension 3 (specifically, on $L^2(\mathbb{R}^3)$). If $H = -\Delta + V$ and $V$ vanishes at infinity, then the eigenvalues of $H$ are in bijection with the eigenvalues of

$$K(\lambda) := U^{1/2}(-\Delta - \lambda)^{-1}U^{1/2},$$

i.e.

$$K(\lambda)(x,y) = U^{1/2}(x)\frac{e^{-\sqrt{|\lambda|}}}{2\pi}U^{1/2}(y).$$

This Green's function is why the theory is so nice in dimension 3: in higher dimensions, there are extra terms in powers of $|x-y|$, and they make the analysis considerably more complicated.

*Remark.* What if $V$ isn't positive definite? If $V = V_+ + V_-$, where $V_- \ge 0$, then $H \ge \widetilde{H} := -\Delta - V_-$, and by the minimax characterization of eigenvalues, the respective eigenvalues satisfy $E_j \ge \widetilde{E}_j$. This in particular tells us that it suffices to study $\widetilde{H}$, and $V_+$ is often just thrown out. ◂

Using the Birman-Schwinger principle, we obtain that the number of negative eigenvalues of $H$ is at most $\|H\|_{\text{HS}}$, the Hilbert-Schmidt norm. By Hardy-Littlewood-Sobolev, this is bounded by some scalar multiple $\|U\|_{L^{3/2}(\mathbb{R}^d)}^2$ (where $U = V_-$).

Today, we're going to bound eigenvalues in a different way, using the Lieb-Thirring inequalities. Specifically, let $E_j < 0$ be the $j^{\text{th}}$ eigenvalue of $H = -\Delta + V$, where $V = V_+ - V_-$. Let $e_j := |E_j|$; we want to bound

$$\sum_j e_j^\gamma.$$

**Lemma 10.1.**

$$\sum_j e_j^\gamma = \gamma \int_0^\infty e^{\gamma-1} N_e \, \mathrm{d}e,$$ [11]

*where $N_e$ is the number of eigenvalues of $H$ less than or equal to $-e$, which is a monotonically decreasing step function.*

*Proof.* Since $N_e$ is a step function,

$$\partial_e N_e = -\sum_j \delta_{E_j}(-e).$$

Therefore

$$\sum_j e_j^\gamma = -\int_0^\infty e^\gamma \partial_e N_e \, \mathrm{d}e,$$

and the result follows after integrating by parts. ⊠

If $B_e$ is the number of eigenvalues of $K(e)$ greater than or equal to 1 , where $K = V_-^{1/2}(-\Delta + e)V_-^{1/2}$, then as we saw

$$\begin{aligned} N_e &= B_e \\ &= \sum_{\substack{\nu \geq 1 \\ \nu \in \mathrm{Spec}(K(-e))}} 1 \\ &\leq \sum_{\substack{\nu \geq 1 \\ \nu \in \mathrm{Spec}(K(e))}} \nu^m \end{aligned} \tag{10.2}$$

for any $m > 0$.

The Green's function for $e$ is $G_e := -\Delta + e$. Hence we can bound (10.2):

$$(10.2) \leq \mathrm{tr}(K(-e))^m = \mathrm{tr}\Big(U^{1/2} G_e U^{1/2}\Big)^m. \tag{10.3}$$

This is a somewhat miraculous fact, which relies on the following lemma. We won't prove it, because that in itself would take the whole hour!

**Lemma 10.4.** *Let $A$ and $B$ be positive, self-adjoint operators. Then,*

$$\mathrm{tr}\Big(B^{1/2} A B^{1/2}\Big)^m \leq \mathrm{tr}\Big(B^{1/2} A^m B^{1/2}\Big).$$

For a proof, see Leib-Seiringer's book, or Bhatia's book on matrix analysis.

The Green's function here is

$$G_e(x,y) = \frac{\exp(-\sqrt{e}|x-y|)}{2\pi|x-y|}.$$

We'll let $\widetilde{G}_e(x-y) := G_e(x,y)$, as it only depends on their difference. Observe that

$$(G_e^m)(x,y) = \int \widetilde{G}_e(x-x_1)\widetilde{G}_e(x_1-x_2)\cdots\widetilde{G}_e(x_{m-1},y)\,\mathrm{d}x_1\cdots\mathrm{d}x_{m-1},$$

so $(G_e^m)(x,y)$ is a function of $x-y$ as well.

[11] This $e$ is a variable, not Euler's constant.

Now, applying Lemma 10.4 to (10.3), we have

$$\begin{aligned} N_E &\le \operatorname{tr}\left(U^{m/2} G_e^m U^{m/2}\right) \\ &= \operatorname{tr}(U^m(x) G_e^m(x,y)) \\ &= \widetilde{G}_e^m(0) \int U^m(x)\,\mathrm{d}x, \end{aligned}$$

using a Fourier estimate for $G_e(0)$ as an integral of its Fourier transform.

Therefore we conclude that

$$\sum_j e_j^\gamma \le C \int_0^\infty e^{\gamma - m + 3/2}\,\mathrm{d}e \int U^m(x)\,\mathrm{d}x. \tag{10.5}$$

This is never convergent: we need $\gamma - m + 3/2$ to be $< -1$ (so that it converges at $\infty$) and $> -1$ (so it converges at 0). So we need to do something smarter.

The trick is to instead of $U$, consider

$$W_e := \left(V + \frac{e}{2}\right)_- = \left(V_+ - \left(V_- - \frac{e}{2}\right)\right).$$

Then,

$$N_e(-V_-) = N_{e/2}\left(-V_- + \frac{e}{2}\right) \le N_{e/2}(W_e),$$

since $W_e \ge V_- - e/2$. Therefore we can replace $U$ by $W_e$ and $e$ by $e/2$ everywhere in (10.5), obtaining

$$\sum_j e_j^\gamma \le \gamma C_m \int_{\mathbb{R}^3} \mathrm{d}x \left( \int \mathrm{d}e\, e^{\gamma - 1 - m + d/2} \left(V_-(x) - \frac{e}{2}\right)^m \right).$$

Here $d$ is the dimension (in the end we care about $d = 3$, but being general will make it clearer where everything comes from). Since $W_e(x) = (V + e/2)_-$, then its support is contained within $\{x \mid V_-(x) - e/2 \ge 0\}$.

Let $a := 2V_-(x)$ and $\widetilde{e} := a \cdot e$. Then,

$$2^{-d/2} \int_0^a e^k (a-e)^m\,\mathrm{d}e = a^{k+m+1} 2^{-d/2} \int_0^1 \widetilde{e}^k (1-\widetilde{e})^m\,\mathrm{d}\widetilde{e}.$$

If we assume $k, m > -1$, though we already knew $m > 0$ anyways, then the above integral converges, and we can let

$$B_{m,d} := \int_0^1 \widetilde{e}^k (1-\widetilde{e})^m\,\mathrm{d}\widetilde{e}.$$

Moreover, we have

$$\gamma - 1 - m + \frac{d}{2} > -1,$$

and therefore that

$$m < \gamma + \frac{d}{2}.$$

Specializing to $d = 3$, and choosing $m < \gamma + d/2$ (a popular choice is $(\gamma + d)/2$), we get the Lieb-Thirring inequality.

**Theorem 10.6** (Lieb-Thirring inequality)**.**

$$\sum_j e_j^\gamma \le \gamma C_{d,m} \int \mathrm{d}x\, (V_-(x))^{\gamma + d/2},$$

*where $C_{d.m}$ is a constant depending on $d$ and $m$.*

This will be useful later, when we need to control the kinetic energy when analyzing the stability of matter.

A *bound state* of the Hamiltonian is a state $u_j$ that is an eigenvector for a negative eigenvalue $E_j$. Physically, these correspond to states where the electron is bound to the nucleus.

Later, we'll show that $|u_j(x)|$ is rapidly decaying (specifically, exponentially). If we consider the Schrödinger equation

$$i\partial_t u = Hu, \qquad u(0) = u_j \tag{10.7}$$

for these $u_j$, the solutions we obtain are periodic:

$$u(t) = e^{-itE_j} u_j(0).$$

If one imagines a gravitational potential, these correspond to circular, constant-height orbits around a gravitational source.

**Scattering states.** Let $H = -\Delta + V$. Let $\mathcal{H}_b$ denote the span of the eigenfunctions of $H$. We want to study solutions of the Schrödinger equation, as in (10.7), but where $u_0 \in \mathcal{H}_b^{\perp}$.

We should assume a bound on the potential: precisely, we require for every 3-tuple $\boldsymbol{\alpha}$,

$$|\partial_x^{\boldsymbol{\alpha}} V(x)| \leq (1 + |x|)^{-\mu - |\boldsymbol{\alpha}|}.$$

Here $|\boldsymbol{\alpha}| \coloneqq \alpha_1 + \alpha_2 + \alpha_3$, and

$$\partial_x^{\boldsymbol{\alpha}} \coloneqq \prod_{i=1}^{3} \partial_{x_j}^{\alpha_j}.$$

Scattering takes information at $t = -\infty$ to $t = \infty$. Wave operators bring information from the far past or far future to the current time.

**Definition 10.8.** The *wave operators* are the operators

$$\Omega^{\pm}\phi \coloneqq \lim_{t \to \pm\infty} e^{itH} e^{-it\Delta} \phi.$$

Sometimes, one also writes $H_0 \coloneqq -\Delta$. To precisely define $e^{-itH}$, one writes it as

$$e^{-itH} \coloneqq \frac{1}{2\pi i} \oint_{\Gamma} e^{itz} \frac{1}{z - H} \, \mathrm{d}z,$$

where $\Gamma$ is a contour enclosing $\sigma(H)$.[12]

Wave operators don't always exist, but we'll prove that they exist in the presence of *short-range interactions* (i.e. $\mu > 1$), and moreover they are $L^2$-isometries.

Thus

$$\begin{aligned} \left\| e^{-itH}\psi_0 - e^{-itH_0}\phi_0 \right\|_{L^2} &= \left\| \psi - e^{itH} e^{-itH_0} \phi_0 \right\|_{L^2} \\ &\xrightarrow{t \to \infty} \left\| \psi_0 - \Omega^{+}\phi_0 \right\|_{L^2} = 0. \end{aligned} \tag{10.9}$$

Thus $\psi_0 = \Omega^{+}\phi_0$ tells us that $\psi_0$ and $\phi_0$ have the same long-range physics. We'll investigate this further next time.

Lecture 11.

## Scattering states: 10/5/17

*"As you've all noticed, we're all stable, at least physically..."*

Recall that we've been studying Hamiltonians of the form $H = -\Delta + V$, where $H_0 = -\Delta$, and considering $\mathcal{H}_b$, the subspace spanned by bound states. Assume that the potential is rapidly decreasing, in that there's a $\mu > 1$ (corresponding to short-range behavior) such that

$$|\partial_x^{\boldsymbol{\alpha}} V(x)| \leq \left( \frac{1}{\langle x \rangle} \right)^{\mu + |\boldsymbol{\alpha}|}.$$

[12] Another way to define it is

$$e^{-itH} \coloneqq \frac{1}{2\pi} \lim_{\varepsilon \searrow 0} \operatorname{Im} \int_{\mathbb{R}} e^{-i\lambda t} \frac{1}{\lambda + i\varepsilon - H} \mathrm{d}\lambda.$$

We want to study the asymptotic behavior of $\psi(t) = e^{-itH}\psi_0$ as $t \to \infty$. Last time, we defined the wave operators

$$\Omega^{\pm} := \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}.$$

Then, we have (10.9), with the implication that

$$\left\| e^{-itH}\psi_0 - e^{-itH_0}\phi_0 \right\|_{L^2} \overset{t\to\pm\alpha}{\longrightarrow} 0 \tag{11.1a}$$

if and only if

$$\left\| \psi_0 - \Omega^{\pm}\phi_0 \right\|_{L^2} = 0, \tag{11.1b}$$

if and only if

$$\psi_0 = \Omega^{\pm}\phi_0. \tag{11.1c}$$

The existence of the operators $\Omega^{\pm}$ is equivaelent to the existence of *scattering states*

$$\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\phi_0.$$

Thus, one is led to ask, given a $\psi_0 \in \mathcal{H}_b^{\perp}$, does there exist a $\phi_0 \in L^2$ making (11.1c) true? This is called asymptotic completeness.

**Proposition 11.2.** $\operatorname{Im}(\Omega^+) \subset \mathcal{H}_b^{\perp}$.

*Proof.* Assume that $g \in \mathcal{H}_b$, $Hg = \lambda g$, and $\phi \in L^2 \cap L^1$. Since $g \in \mathcal{H}_b$, it's in both $L^2$ and $L^1$, and moreover has exponential decay. Then,

$$\begin{aligned}
\langle g, \Omega^+\phi_0\rangle &= \lim_{t\to\infty} \langle g, e^{itH}e^{-itH_0}\phi_0\rangle \\
&= \lim_{t\to\infty} \langle e^{-it\lambda}g, e^{-itH_0}\phi_0\rangle \\
&= \lim_{t\to\infty} e^{it\lambda}\langle g, e^{-itH_0}\phi_0\rangle.
\end{aligned}$$

We can write $e^{-itH_0}$ as a kernel:

$$\left(e^{-ih_0}\phi_0\right)(x) = \left(\frac{1}{2\pi it}\right)^{3/2} \int \exp\left(-i\frac{|x-y|^2}{4t}\right)\phi_0(y)\,\mathrm{d}y.$$

This implies

$$\begin{aligned}
\left|\langle g, e^{-itH_0}\phi_0\rangle\right| &\le \left(\frac{1}{2\pi t}\right)^{3/2} \iint \left|\overline{g(x)} \exp\left(-i\frac{|x-y|^2}{4t}\right)\phi_0(y)\right| \mathrm{d}x\,\mathrm{d}y \\
&\le \left(\frac{1}{2\pi t}\right)^{3/2} \|g\|_{L_1}\|\phi_0\|_{L_1}.
\end{aligned}$$

Since $g, \phi \in L^1$, this goes to 0 as $t \to \infty$. Finally, density implies the result for a general $\phi_0 \in L^2$. ⊠

**Definition 11.3.** If $\operatorname{Im}(\Omega^+) = \mathcal{H}_b^{\perp}$, one says the property of *asymptotic completeness* holds. There's a similar definition for $\Omega^-$.

Equivalently, $\mathcal{H}_b \oplus \operatorname{Im}(\Omega^+) = L^2$.

**Example 11.4.** Suppose $V \in L^1 \cap L^\infty$ with sufficiently small norm. Then, asymptotic completeness holds. ◂

To really do asymptotic completeness justice, we'll need some better tools, namely the Strichartz estimates from harmonic analysis. I haven't seen them before (and apparently I'm the only such person in the class), so we'll have to return to this later.

Given a $\psi_0$, we can define $\phi_\pm$ by $\psi_0 = \Omega^+\phi_+$ and $\psi_0 = \Omega^-\phi_-$. $\phi_-$ represents the $-\infty$-time state that flows to $\psi_0$, and $\psi_+$ denotes the $+\infty$-time state which has initial value $\psi_0$.

**Definition 11.5.** The *scattering operator* is $S := \Omega^{+*}\Omega^-$.

This operator sends $\phi_- \mapsto \phi_+$, and in this sense sees all of time for this theory.

*Remark.* In physics, this arises when one has waves or beams of particles which interact with each other. In this case, $t = \pm\infty$ is physically meaningful, as the interactions only exist for a few seconds, and therefore one minute in the past is an acceptable substitute for $t = -\infty$!

This is used in bubble chambers to learn more about the structure of atoms and subatomic particles. Feynman diagrams are needed to calculate matrix coefficients for $S$, i.e. coefficients of the form $\langle u_i, Su_j\rangle$ for an orthonormal basis $\{u_j\}$ of the Hilbert space, and these quantities are used to calculate expectations for measured quantities. ◁

Note also that

$$\Omega^+\phi_+ = \lim_{t\to\infty} e^{itH}e^{-itH_0}\phi_+.$$

Replacing $t \mapsto t + s$,

$$\begin{aligned} &= \lim_{t\to\infty} e^{isH}e^{itH}e^{-itH_0}e^{-isH_0}\phi_+ \\ &= e^{isH}\Omega^+e^{-isH_0}\phi_+. \end{aligned}$$

A similar statement for $\Omega^-$ means

$$e^{-isH}\Omega^\pm = \Omega^\pm e^{-isH_0},$$

and differentiating at $s = 0$,

$$H\Omega^\pm = \Omega^\pm H_0. \tag{11.6}$$

That is, the wave operators intertwine the full Hamiltonian and the free Hamiltonian.

If in addition we have asymptotic completeness, then $\Omega^{\pm *} = (\Omega^\pm)^{-1}$ on $\mathcal{H}_b^\perp$, so (11.6) means that on $\mathcal{H}_B^\perp$,

$$H = \Omega^\pm H_0 \omega^{\pm *}.$$

Thus the Hamiltonian is diagonalized by the wave operators.

In general, it seems like wave operators are really nice — so it would be good to know that they exist.

**Theorem 11.7.** *If $V \in L^2$, then the wave operators $\Omega^\pm$ exist.*

*Proof.* Let

$$\Omega_t := e^{itH}e^{-itH_0}.$$

Its operator norm is 1, so we'll prove the existence of $\lim_{t\to\infty}\Omega_t\phi$ when $\phi \in L^1 \cap L^2$, then invoke the density of $L^1$ in $L^2$.

Let $t > t'$. Then,

$$\begin{aligned} \Omega_t\phi - \Omega_{t'}\phi &= \int_t^{t'} \partial_s\Omega_s\phi \, ds \\ &= i\int_t^{t'} e^{isH}\underbrace{(H - H_0)}_{V}e^{-isH_0}\phi \, ds. \end{aligned}$$

Therefore

$$\begin{aligned} \|\Omega_t\phi - \Omega_{t'}\phi\|_{L^2} &\le \int_t^{t'} \|Ve^{-isH_0}\phi\|_{L^2} \, ds \\ &\le \|V\|_{L^2}\int_t^{t'} \|e^{-isH_0}\phi\|_{L^\infty} \, ds, \end{aligned}$$

and since $\|e^{-isH_0}\phi\|_{L^\infty} \le (1/2\pi s)^{3/2}\|\phi\|_{L^1}$, this simplifies to

$$\le C\|V\|_{L^2}\|\phi\|_{L^1}\left(\left(\frac{1}{t'}\right)^{1/2} - \left(\frac{1}{t}\right)^{1/2}\right). \tag{11.8}$$

For all $\varepsilon > 0$, there's a $T = T(\varepsilon)$ such that (11.8) is less than $\varepsilon$ for $t, t' > T$, and therefore this is Cauchy in $L^2$. ⊠

**Stability of matter.** If electrons were described by Newton's laws of mechanics, then eventually, energy would get lost and the electron would spiral into the nucleus, ultimately causing matter to implode. Obviously this doesn't happen, and one of the reasons is Heisenberg's uncertainty principle — which is not quite a physical law, but a theorem about Fourier transforms, and it applies to stability of matter, and another application in information transfer via radio waves, and plenty of other physical phenomena.

Let $H = -\Delta + V$. Then, $H$ is bounded below iff $\inf \operatorname{Spec} H > -\infty$. The eigenstates for negative eigenvalues correspond to systems where the electron is bound. Asking for stability imposes some more conditions, e.g. that the infimum is linearly proportional to the number of particles present in the system.

The *ground state* of the system is $E_0 := \inf \operatorname{Spec} H$; we want to make sure this is finite.

**Example 11.9.** Let $H = -\Delta - 1/|x|$, corresponding to a hydrogen atom. Is hydrogen stable?

The energy of the system is

$$\begin{aligned}\mathcal{E}[\psi] = (\psi, H\psi) &= \int |\nabla\psi|^2 - \int \frac{1}{|x|}\psi^2 \\ &= \|\nabla\psi\|_{L^2}^2 - \left\| \frac{1}{|x|^{1/2}}\psi \right\|_{L^2}^2 \\ &\geq \|\nabla\psi\|_{L^2}^2 - \||\nabla|^{1/2}\psi\|_{L^2}, \end{aligned} \tag{11.10}$$

using the *Hardy inequality*

$$\left\| \frac{1}{|x|^s}\psi \right\|_{L^2} \leq \||\nabla|^s\psi\|_{L^2}.$$

We can proceed further with a form of the *Gagliardo-Nirenberg inequality*

$$\begin{aligned}\||\nabla|^{1/2}\psi\|_{L^2}^2 = \int \overline{\hat{\psi}}|\xi|\hat{\psi}\,\mathrm{d}\xi \\ \leq \|\hat{\psi}\|_{L^2}\||\xi|\hat{\psi}\|_{L^2}.\end{aligned}$$

Therefore

$$(11.10) \geq \|\nabla\psi\|_{L^2}^2 - \|\psi\|_{L^2}\|\nabla\psi\|_{L^2},$$

and one can show that no matter which of these is large, it's still bounded below. ◂

Lecture 12.

## Stability of the First Kind: 10/10/17

*"At the beginning of one's education, one imagines 'if I could solve the equation, I would know everything.' Unfortunately, solving equations is hard."*

Last time, we discussed three inequalities that arose in our analysis of the stability of matter: the Hardy inequality, a Gagliano-Nirenberg inequality, and the Sobolev inequality. Today, we're going to play more with these inequalities.

Recall that the hydrogen operator has Schrödinger operator

$$H = -\Delta - \frac{1}{|x|}.$$

Then, the expectation of $u$ is

$$(u, Hu) = \int |\nabla u|^2 - \int \frac{1}{|x|}|u|^2.$$

The second piece is also $\|u/|x|^{1/2}\|_{L^2}$, and the Hardy inequality says there's a $C$ such that

$$\left\| \frac{1}{|x|^{1/2}}u \right\|_{L^2} \leq C_H \left\| |\nabla|^s u \right\|_{L^2}.$$

Using this, we concluded that

$$(u, Hu) \geq \|\nabla u\|_{L^2}^2 - C_H\|u\|_{L^2}\|\nabla u\|_{L^2} > -\infty.$$

One might ask whether the cusp in the potential at 0 leads the ground state to concentrate at 0 (in the ground state, the particle is in expectation near the origin). Concretely, one asks whether $(u, x^2 u) \to 0$. The answer is no.

$$1 = \|u\|_{L^2}^2 = \left(u, \frac{1}{|x|}|x|u\right)_{L^2} \tag{12.1a}$$

$$= \left(\frac{1}{|x|}u, |x|u\right)_{L^2}. \tag{12.1b}$$

By Cauchy-Schwarz,

$$\leq \left\|\frac{1}{|x|}u\right\|_{L^2} \||x|u\|_{L^2}, \tag{12.1c}$$

and by the Hardy inequality,

$$\leq C_H \|\nabla u\|_{L^2} \||x|u\|_{L^2}. \tag{12.1d}$$

Therefore

$$\|\nabla u\|_{L^2} \geq C \frac{1}{(u, x^2 u)^{1/2}}.$$

Thus the ground state cannot concentrate at 0 or even anywhere, because the kinetic energy would diverge.

Collecting equations (12.1a) to (12.1d), one has the inequality

$$1 \leq C_H \|\nabla u\|_{L^2} \||x|u\|_{L^2}, \tag{12.2}$$

which is called the *Heisenberg uncertainty principle*. Heisenberg originally formulated this as a physical law, but it's really a mathematical theorem which happens to apply to physics. It comes out of Fourier analysis, and appears in Fourier-theoretic contexts that have nothing to do with physics.

*Remark.* There's a rich and classic literature about actually constructing the ground state of the hydrogen atom, which uses spherical harmonics. We won't go into this, though. ◁

**Definition 12.3.** We say that a physical system $H = -\Delta + V$ (where $V \to 0$ as $|x| \to \infty$) has *stability of the* $1^{\text{st}}$ *kind* if $E_0 := \inf \operatorname{Spec} H > -\infty$.

**Theorem 12.4.** *Assuming that*

$$V \in \begin{cases} L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), & d \geq 3 \\ L^{1+\varepsilon}(\mathbb{R}^2) + L^\infty(\mathbb{R}^2), & d = 2 \\ L^1(\mathbb{R}) + L^\infty(\mathbb{R}), & d = 1, \end{cases}$$

*then* $E_0 > -\infty$ *and the system has stability of the* $1^{\text{st}}$ *kind. Moreover,*

$$\|\nabla u\|_{L^2}^2 \leq C_1 \mathcal{E}(u) + C_2 \|u\|_{L^2}^2,$$

*where* $\mathcal{E}(u) := (u, H)$.

*Proof for* $d \geq 3$. We have

$$\mathcal{E}(u) = \int |\nabla u|^2 + \int V|u|^2.$$

When $d = 3$, we want to write $V = V_1 + V_\infty$ where $V_1 \in L^{3/2}$ and $V_\infty \in L^\infty$. Assuming this,

$$\mathcal{E}(u) \geq \frac{1}{2}\|\nabla u\|_{L^2}^2 - \underbrace{\int |V_1||u|^2}_{(I)} - \underbrace{\int |V_\infty||u|^2}_{(II)}.$$

Since $V_\infty$ is $L^\infty$, we know that for some $C_\infty \in \mathbb{R}$,

$$(II) \leq C_\infty \|u\|_{L^2}^2. \tag{12.5}$$

Next, we use the Hölder inequality to dispatch $(I)$.

$$(I) \leq \|V_1\|_{L^{3/2}} \||u|^2\|_{L^r},$$

where $1/r + 2/3 = 1$, so $r = 6$. Now, using the Sobolev inequality,

$$\leq \|V_1\|_{L^{3/2}} \|\nabla u\|_{L^2}^2. \tag{12.6}$$

*Remark.* The Sobolev inequality might not be familiar to everyone in the audience.[13] The idea is that differentiability of a function, measured in the $L^p$-norm, also controls its $L^q$-norm. The way to remember the precise exponents is to remember that it's invariant under scaling $x \mapsto \lambda x$, so if you want there to be a $C$ such that

$$\left(\int |u|^p \, dx\right)^{1/p} \leq C\left(\int ||\nabla|^s u|^2 \, dx\right)^{1/2},$$

scaling by $\lambda$ on the left-hand side produces a factor of $\lambda^{d/p}$, and scaling by $\lambda$ on the right-hand side produces a factor of $\lambda^{d/2}$ (from the $|u|^2$) and a factor of $\lambda^{-s}$ (from the derivative). Thus we'd better have that

$$\frac{d}{p} = \frac{d}{2} - s,$$

or $s = d(1/2 - 1/p)$, and indeed this was true for $p = 6$, $d = 3$, and $s = 1$ as we used it above. ◂

Using (12.5) and (12.6), we obtain what looks like a lower bound.

$$\mathcal{E}(x) \geq \underbrace{\left(\frac{1}{2} - C\|V_1\|_{L^{3/2}}\right)}_{(III)} \|\nabla u\|_{L^2}^2 - C_\infty \|u\|_{L^2}^2. \tag{12.7}$$

However, if $\|V_1\|_{L^{3/2}}$ is large, $(III) < 0$, and this lower bound is not helpful. So we need to make sure that $V_1$ is small, or $(III) > 0$. For this we use the Chebyshev inequality. Let $A_>(\lambda) := \{x \in \mathbb{R}^d \mid |V(x)| > \lambda\}$ and $A_<(\lambda) := (A_>(\lambda))^c$.

**Lemma 12.8** (Chebyshev inequality)**.** *For any $p$,*

$$|A_>(\lambda)| \leq \frac{\|V\|_{L^p}^p}{\lambda^p}.$$

*Proof.*

$$\int_{A_>(\lambda)} |V|^p \geq \lambda^p \int_{A_>(\lambda)} 1 = \lambda^p |A_>(\lambda)|. \qquad \boxtimes$$

For any $\lambda$, $u|_{A_<(\lambda)}$ is $L^\infty$, and

$$\int_{A_>(\lambda)} |V|^p \leq \|V\|_{L^p}^p,$$

and the left-hand side is monotonically decreasing to 0 as $\lambda \to \infty$. Therefore there's a $\lambda_*$ such that for all $\lambda > \lambda_+$, $\|V\|_{L^p(A_>(\lambda)} < 1/4$. Thus, for $\lambda$ sufficiently large, we can define $V_1 := V|_{A_>(\lambda)}$, which implies that $V_\infty := V - V_1 \in L^\infty$, and that $(III) > 0$, so $\mathcal{E}(u)$ is bounded below.

We had assumed $d = 3$, and used this only in (12.6) when invoking the Sobolev inequality. In the general $d$-dimensional case, Hölder tells us that

$$\int |V_1||u|^2 \leq \|V_1\|_{L^{d/2}} \||u|^2\|_{L^r},$$

where $2/d + 1/r = 1$, i.e. $r = 2d/(d-2)$, so

$$\leq \|V_1\|_{L^{d/2}} \|u\|_{L^{2d/(d-2)}}^2.$$

The Sobolev inequality says that $s = d(1/2 - 1/p)$, so with $p = 2d/(d-2)$, $s = 1$, so

$$\leq \|V_1\|_{L^{d/2}} \|\nabla u\|_{L^2}^2.$$

Thus again

$$\mathcal{E}(u) \geq \left(\frac{1}{2} - C_2\|V_1\|_{L^{d/2}}\right) \|\nabla u\|_{L^2}^2 - \|V_\infty\|_{L^\infty} \|u\|_{L^2}^2.$$

[13] Certainly, I am only weakly familiar with it.

For a suitable choice of $V_1$, which can be produced by Chebyshev's inequality, the first term is positive, and we win. ⊠

After studying one-particle systems, we naturally move to many-particle systems, which will have a second-order stability condition. "Many" could mean different things in different contexts: for atoms other than hydrogen, it might be in the dozens, but if you're analyzing something like a neutron star, it might be $10^{10}$ or something in that ballpark. You can set up the Schródinger equation in this context, but if you solve it, obtaining some explicit function of $10^{10}$ variables, it's not going to give you any great insights.

Let's consider a quantum-mechanical system with $N$ variables, so its wavefunctions $\psi$ live in $L^2(\mathbb{R}^{dN})$, and we write $\psi = \psi(x_1, \dots, x_N)$, with $x_j \in \mathbb{R}^d$, and

$$\|\psi\|_{L^2} = \int |\psi(x_1, \dots, x_N)|^2 \, \mathrm{d}x_1 \cdots \mathrm{d}x_N = 1.$$

The probability density of finding a particle at $x$ (which becomes a probability after normalization) is

$$C_\psi(x) \coloneqq \sum_{j=1}^{N} \int_{\mathbb{R}^{d(N-1)}} |\psi(x_1, \dots, x_{j-1}, x, x_{j+1}, \dots, x_N)| \, \mathrm{d}x_1 \cdots \widehat{\mathrm{d}x_j} \cdots \mathrm{d}x_N.$$

That is, let $x$ stand in for $x_j$, and don't integrate out over $x_j$.

Now it's time to say something important in life, and talk about fermions. We've been studying non-relativistic quantum mechanics, but everything is relativistic, and almost everything is Lorentz invariant. Therefore we want the kinds of particles in our theories to match this description, and according to quantum field theory there are only two kinds of elementary particles, bosons and fermions.

This can be deduced from mathematics! Specifically, relativistic quantum field theory tells us that particles are given by representations of the group preserving the Lorentz metric on $\mathbb{R}^4$, which is $\mathrm{SL}(2, \mathbb{C})$ (containing $\mathrm{SU}(2)$, the maximal compact subgroup). There are three pieces:

- One-dimensional representations $\phi(t, x)$.
- Two-dimensional representations $(\psi_1, \psi_2)(t, x) \in \mathbb{C}^2$, called *spinors*.
- Three-dimensional representations $(A_1, A_2, A_3)(t, x) \in \mathbb{C}^3$, called *vectors*.

The *spin* of such a $k$-dimensional representation is $(k-1)/2$. If $s \in \mathbb{N}$, then the particle is called a *boson*; if $s \in \mathbb{N} + 1/2$, it's called a *fermion*. The reason for this dichotomy is which kind of equation they satisfy.

- Spin-0 particles satisfy the *Klein-Gordon equation*

$$\left(\partial_t^2 - \Delta\right)\phi = m^2\phi.$$

- Spin-1/2 particles satisfy the *Dirac equation*[14]

$$m\gamma_0 \Psi + \sum_j \gamma^j i \nabla_j \Psi = 0.$$

  Here $\Psi \coloneqq (\psi_1, \psi_2, \psi_3, \psi_4)$.
- For spin-1 particles, one has a *Maxwell equation*.

The difference is that the Dirac equation is indefinite: its spectrum is not bounded below, and therefore the theory is unstable. This causes problems that will be solved by quantization, but that introduces its own weirdness — if you assume that spacelike separated particles in Minkowski space have commuting operators and that the quantized Dirac operators have bounded-below spectrum, one obtains that the particle creation and annihilation operators for bosons must anticommute! And in fact the function itself is antisymmetric. This is encoded in the spin-statistics theorem of Pauli-Fierz.

Photons are bosons, and electrons are fermions. We'll say more about this next time.

[14] TODO: The heuristic is right, but there's something wrong with the equation.

Lecture 13.

## Density matrices and stability of matter: 10/12/17

Today we're going to discuss stability of matter in earnest. To truly understand this, one has to make some hardcore estimates, which we're not going to get into. However, we will mention where the estimates are, and provide estimates.

Last time, we mentioned that there are only two kinds of elementary particles, bosons and fermions, a classification of particles by their mutual statistics. Bosons are described by a Schrödinger wavefunction $\psi(x_1, \dots, x_N) \in L^2(\mathbb{R}^{dN})$ which is symmetric under arbitrary permutations of the particles $x_1, \dots, x_N$. That is, if $S_N$ denotes the symmetric group on $N$ letters, this wavefunction lives in

$$L^2_{\text{sym}}(\mathbb{R}^{dN}) \coloneqq L^2(\mathbb{R}^{dN})^{S_N}.$$

Fermions are again described by Schrödinger wavefunctions, but are completely antisymmetric under permutations:

$$\psi(x_1, \dots, x_N) = (-1)^{\text{sign}(\sigma)} \psi(x_{\sigma(1)}, \dots, \sigma(n))$$

for any $\sigma \in S_N$. Here $\text{sign}(\sigma)$ is its *signature*: a permutation can be written as a composition of transpositions, and the signature is the number of transpositions mod 2, which is well-defined. The subspace of antisymmetryc functions is denoted $L^2_{\text{anti}}(\mathbb{R}^{dN})$.

Matter is fermionic, so we're going to study stability of matter for fermions.

**Density matrices.** Let $\psi \in L^2(\mathbb{R}^{dN})$ with $\|\psi\| = 1$, and then define

$$\Gamma_\psi(\mathbf{x}, \mathbf{x}') \coloneqq \psi(\mathbf{x})\overline{\psi(\mathbf{x}')},$$

where $\mathbf{x} \coloneqq (x_1, \dots, x_N)$. This defines an integral operator with kernel $\Gamma_\psi(\mathbf{x}, \mathbf{x}')$:

$$(\Gamma_\psi \phi)(\mathbf{x}) = (\psi, \phi)\psi(\mathbf{x}),$$

because

$$\begin{aligned}\Gamma_\psi \phi &= \int \Gamma_\psi(\mathbf{x}, \mathbf{x}')\phi(\mathbf{x}')\, d\mathbf{x}' \\ &= \psi(\mathbf{x}) \underbrace{\int \overline{\psi(\mathbf{x}')}\phi(\mathbf{x}')\, d\mathbf{x}'}_{(\psi,\phi)}.\end{aligned}$$

In bra-ket notation, $|\psi\rangle$ refers to $\psi$ as a column vector, and $\langle\psi|$ refers to it as a row vector (its adjoint in the dual space). Then, $\Gamma_\psi = |\psi\rangle\langle\psi|$, and it's a projection, because

$$\Gamma_\psi \Gamma_\psi = |\psi\rangle \underbrace{\langle \psi \mid \psi\rangle}_{=1} \langle\psi| = |\psi\rangle\langle\psi| = 1.$$

This shows off the reason people like bra-ket notation: $\langle \psi \mid \phi\rangle$ is exactly their inner product.

$\Gamma$ is an example of a density matrix.

**Definition 13.1.** A *density matrix* is a linear, self-adjoint, positive semidefinite operator $\Gamma$ with unit trace: $0 \le \Gamma \le \mathbf{1}$ and $\operatorname{tr}\Gamma = 1$.

Let $(\phi_j)$ be an orthonormal basis for $L^2$. Then

$$\operatorname{tr}\Gamma = \sum_j (\phi_j, \Gamma\phi_j);$$

since this is finite, $\Gamma$ has a pure point spectrum: there are eigenvectors $\phi_j$ with corresponding eigenvalues $\lambda_j$ such that $\|\phi_j\|_{L^2} = 1$ and

$$\Gamma = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|.$$

Thus

$$\operatorname{tr}\Gamma = \sum_j \lambda_j = 1.$$

A density matrix which is not a rank-1 projection is called a *mixed state*; otherwise it is a *pure state*.

**Quantum mechanics and ground state energy.** Let $\psi \in L^2(\mathbb{R}^{dN})$ have unit norm. Then, $\mathcal{E}[\psi] = (\psi, H\psi)$, where $H$ is the Hamiltonian (an $N$-body Schrödinger operator). More generally, the *energy functional* for a density matrix $\Gamma$ is

$$\mathcal{E}[\Gamma] = \operatorname{tr}(H\Gamma).$$

We can simplify this somewhat:

$$\operatorname{tr}(H\Gamma) = \sum_{\lambda_j} \operatorname{tr}(H|\psi_i\rangle\langle\psi_j|) \tag{13.2}$$

$$= \sum_j \lambda_j (\phi_j, H\phi_j) \tag{13.3}$$

$$= \sum_j \lambda_j \mathcal{E}[\Gamma_{\phi_j}].$$

Here's why we can get from (13.2) to (13.3): let

$$K_j(x,\widetilde{x}) := \overline{\phi_j(\widetilde{x})}(H\phi_j)(x) = \underbrace{\int H(x,x')\phi(x)\,\mathrm{d}x'}_{H|\phi_j\rangle\langle\phi_j|}\overline{\phi_j(\widetilde{x})}.$$

Then,

$$\operatorname{tr} K = \int \overline{\phi_j} H \phi_j.^{15}$$

It will also be helpful to know about reduced density matrices, or marginals.

**Definition 13.4.** Let $\Gamma$ be a density matrix, fermionic or bosonic. Its *$k$-particle marginal* is

$$\gamma^{(k)}(\mathbf{x}_k, \mathbf{x}_k') = \frac{N!}{(N-k)!}\int \Gamma(\mathbf{x}_k, \mathbf{y}_{N-k}; \mathbf{x}_x, \mathbf{y}_{N-k})\,\mathrm{d}\mathbf{y}_{N-k},$$

where $\mathbf{x}_k := (x_1, \dots, x_k)$.

These arise as iterated partial traces, e.g. $\gamma^{(1)}$ is $1/(N-1)$ times a partial trace of $\gamma^{(2)}$.

The Hamiltonian for $N$ particles has to take into account particle-particle interactions, e.g. if $W_{ij} = w(x_i - x_j)$ for some $w \in \mathbb{R}$, we could set

$$H = -\sum_{j=1}^N \underbrace{\left(\Delta_{x_j} + V(x_j)\right)}_{=h^{(j)}} + \sum_{1\le i<j\le N} W_{ij}. \tag{13.5}$$

Here $h^{(j)}$ is the Hamiltonian for one particle (hence cannot see interactions) acting on $x_j$. Then,

$$\mathcal{E}[\Gamma] = \operatorname{tr}(H\Gamma) = \operatorname{tr}(h^{(1)}\gamma^{(1)}) + \frac{1}{2}\operatorname{tr}(W_{12})\gamma^{(2)}.$$

This is something very nice: the expectation only depends on $\gamma^{(1)}$ and $\gamma^{(2)}$, but since $\gamma^{(1)}$ is a partial trace of $\gamma^{(2)}$, it actually only requires $\gamma^{(2)}$. This is a consequence of the fact that we started with $\Gamma$ either bosonic or fermionic.

Now we're going to estimate the kinetic energy piece of (13.5). Recall the Lieb-Thirring estimate for $H = -\Delta + V$:

$$\sum_{j\ge 0}|E_j| \le L\int (V_-(x))^p\,\mathrm{d}x,$$

where $p = 1 + d/2$. Let

$$T_{\psi_N} := \left(\psi_N, \left(-\sum_{j=1}^N \Delta_{x_j}\right)\psi_N\right).$$

[15] TODO: Then something happened that I didn't get down in time.

**Theorem 13.6.**

$$T_{\psi_N} \geq \frac{K}{\|\gamma^{(1)}_{\psi_N}\|_\infty^{p'/p}} \int (\rho_{\psi_n}(x))^{p'} \,\mathrm{d}x,$$

*where $p'$ is the Hölder conjugate to $p$ ($1/p' + 1/p = 1$), $\rho_{\psi_N}(x) \coloneqq \gamma^{(1)}_{\psi_N}(x,x)$, and $K$ is a constant independent of $N$ and such that*

$$(pL)^{p'}(p'K)^p = 1.$$

*Proof.* Let $H \coloneqq -\Delta + V$ be the *one-particle operator*, and $K_N$ be a sum of one copy of $H$ acting on each particle $i$, which is called the *$N$-particle operator*. Then,

$$(\psi_N, K_N\psi_N) = \operatorname{tr} H\gamma^{(1)}_{\psi_N}.$$

This is because

$$(\psi_N, H_i\psi_N) = \int \overline{\psi}_N(x_1,\dots,x_n)(H_i\psi_N)(x_1,\dots,x_N)\,\mathrm{d}x_1\cdots\mathrm{d}x_N.$$

Integrating out everything except $x_i$, which is the only particle affected by $H_i$, we get

$$= \frac{1}{N}\int \left(H_i\gamma^{(1)}(x_i,x_i')\right)\Big|_{x_i=x_i'} \mathrm{d}x_i.$$

**Lemma 13.7.**

$$(\psi_N, K_N\psi_N) \geq \textit{TODO}.$$

*Proof.* Let $E_j$ be the $j^{\text{th}}$ eigenvalue of $H$, which is necessarily negative.
(a few lines missing)
Then,

$$\begin{aligned}
\operatorname{tr} H\gamma^{(1)}_{\psi_N} &\geq \sum_{i,j} E_i\lambda_j \operatorname{tr}\left(|\psi_i\rangle\langle\psi_i \mid \phi_j\rangle\langle\phi_j|\right) \\
&= \sum_{i,j} E_i\lambda_j |(\psi_i,\phi_j)|^2 \\
&\geq \left(\sum_j \lambda_j\right)\sum_i E_i \underbrace{\sum_j |(\psi_+{}_i,\phi_j)|^2}_{(\psi_i,\psi_i)=1}.
\end{aligned}$$

Since $\|\gamma^{(1)}\|_{\text{op}} = \|(\lambda_j)\|_\infty$, then

$$\geq \textit{TODO}.$$

Therefore

$$\begin{aligned}
(\psi_N, J_K\psi_N) &= T_{\psi_N} + \int V(x)\rho_{\psi_N}(x)\,\mathrm{d}x \\
&\geq \|\gamma^{(1)}_{\psi_N}\|_\infty \sum_{j\geq 0} E_j,
\end{aligned}$$

and by the Lieb-Thirring inequality,

$$\geq -\|\gamma^{(1)}_{\psi_N}\|_\infty L \int_{\mathbb{R}^d} (V_-(x))^p \,\mathrm{d}x,$$

where $p = 1 + d/2$ and $L$ is the Lieb-Thirring constant. And this holds for general $V$. ⊠

So let's choose

$$V(x) = -C\rho_{\psi_N}(x)^{1/(p-1)},$$

where $1/p + 1/p] = 1$, so $1/(p-1) = p/(p-1) - 1$. Then,

$$T_\psi \geq C\int (\rho_{\psi_N}(x))^{p'}\,\mathrm{d}x - \|\gamma^{(1)}_{\psi_N}\|_\infty LC^p \int (\rho_{\psi_N}(x))^{p'}\,\mathrm{d}x.$$

The optimal value of $C$ is

$$C = \left(p\|\gamma_{\psi_N}^{(1)}\|_\infty L\right)^{-p'/p},$$

so

$$T_{\psi_N} \geq \frac{K}{\|\gamma_{\psi_N}^{(1)}\|_\infty^{p'/p}} \int \left(\rho_\psi(x)\right)^{p'} \mathrm{d}x.$$

⊠

Lecture 14.

## Multi-nucleus systems and electrostatic inequalities: 10/17/17

Today we'll discuss the proofs for stability of matter in the fermionic case. We won't give the complete proofs, since they depend on some difficult estimates, but we will sketch them.

Let $\psi_N$, as last time, be an antisymmetric wave function for $N$ fermions, so that as we discussed last time,

$$T_{\psi_N} := \left(\psi_N, \left(-\sum_{j=1}^N \Delta_{x_j}\right)\psi_N\right) \geq \frac{K}{\|\gamma_{\psi_N}^{(1)}\|_\infty^{p'/p}} \int_{\mathbb{R}^d} \left(\rho_{\psi_N}(x)\right)^{p'} \mathrm{d}x, \tag{14.1}$$

where $p = 1 + d/2$ and $p'$ is the Hölder conjugate of $p$. For fermions, $\|\gamma_\psi^{(1)}\|_\infty \leq 1$, i.e. it's $O(1)$ in $N$. For $d = 3$, $p' = 5/3$ and $p = 5/2$, so since $\rho_\psi \sim O(N)$, the integral in (14.1) is $O(N^{5/3})$.

One way to see this explicitly is to consider $x \in T^3$. Under the Fourier transform we get $\xi \in \mathbb{Z}^3$, and the fermions can live at the lattice points. The Pauli exclusion principle tells us that at most one fermion can live at each lattice point, and fermions will prefer the lower-energy states which are closer to the origin. Therefore the electron furthest away from the origin will be $O(N^{1/3})$ away from the origin, and have energy asymptotically varying as $\xi^2 = O(N^{2/3})$. Therefore the total kinetic energy varies as $N \cdot N^{2/3}$, hence is $O(N^{5/3})$. This system is called the *Fermi sea*.

**Many-body Hamiltonians.** We assume there are multiple atomic nuclei of the same atomic number $Z$ at fixed positions $\mathbf{R} := (R_1, \ldots, R_M)$ together with electrons at varying positions $\mathbf{x} := (x_1, \ldots, x_N)$.

In this case,[16] the Hamiltonian is

$$H := -\frac{1}{2}\sum_{i=1}^N \Delta_{x_i} + V_C(\mathbf{x}, \mathbf{R}), \tag{14.2}$$

where

$$V_C(\mathbf{x}, \mathbf{R}) := W(\mathbf{x}, \mathbf{R}) + I(\mathbf{x}) + U(\mathbf{R}).$$

Here

$$W(\mathbf{x}, \mathbf{R}) := -\sum_{i=1}^N \sum_{j=1}^M \frac{Z}{|x_i - R_j|}$$

is the piece of the potential coming from electron-nucleus interactions,

$$I(\mathbf{x}) := \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}$$

is the piece coming from electron-electron interactions, and

$$U(\mathbf{R}) := \sum_{1 \leq i < j \leq M} \frac{1}{|R_i - R_J|}$$

is the piece coming from the nucleus-nucleus interactions. The ground state energy of this system is

$$E_N(Z, \mathbf{R}) = \inf\{\mathcal{E}(\psi) \mid \psi \text{ fermionic and } \|\psi\|_{L^2} = 1\}.$$

[16] This is a simplified version of the full model, which includes Laplacians for the $R_j$ terms weighted by the electron mass divided by the nuclear mass. This is a very small number, so we have neglected it by pretending electrons have zero mass.

**Definition 14.3.** We say the system has *stability of the first kind* if $E_N(Z, \underline{R}) > -\infty$. In this case, we can define the *absolute ground state*

$$E_{N,M}(Z) := \inf\{E_N(Z, \underline{R}) \mid \underline{R}\}.$$

If in addition

$$E_{N,M}(Z) > -C_0(Z)(N+M),$$

the system has *stability of the second kind*.

**Electrostatic inequalities.** These inequalities appear as ingredients in the proofs of statements we care about, but are interesting and beautiful on their own.

Let $\mu$ be a Borel measure, which physically represents the charge distribution. It has an associated *potential function*

$$\Phi(x) := \int_{\mathbb{R}^3} \frac{1}{|x-y|}\, \mathrm{d}\mu_y.$$

The *Coulomb energy* of $\mu$ is

$$D(\mu,\mu) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{1}{|x-y|}\, \mathrm{d}\mu_x\, \mathrm{d}\mu_y.$$

More generally, one can compute the Coulomb energy $D(\mu,\nu)$ of two different Borel measures.

**Theorem 14.4** (Newton's theorem)**.** *Assume that $\mu$ is rotationally symmetric around the origin. Then,*

$$\Phi(x) = \frac{1}{|x|}\int\limits_{|y|\le|x|} \mathrm{d}\mu_y + \int\limits_{|y|>|x|} \frac{1}{|y|}\, \mathrm{d}\mu_y.$$

*Proof.* Since $\mu$ is rotationally symmetric, $\Phi$ is too, so $\Phi(x) = \Phi(x')$ whenever $|x| = |x|'$. Thus

$$\Phi(x) = \int \frac{1}{|x-y|}\, \mathrm{d}\mu_y = \underbrace{\fint\!\!\!\fint_{S^2} \frac{1}{||x|\omega - y|}\, \mathrm{d}\omega\, \mathrm{d}\mu_y}_{(I)}.$$

Let's expand the inner integral in spherical coordinates, where $y$ is the direction of the north pole:

$$\begin{aligned}(I) &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\varphi \frac{1}{2}\int \mathrm{d}\theta\, \frac{1}{\left(|x|^2+|y|^2-2|x||y|\cos\theta\right)^{1/2}} \sin\theta \\ &= \frac{1}{2}\int_{-1}^{1} \frac{\mathrm{d}s}{\left(|x|^2+|y|^2-2|x||y|s\right)^{1/2}} \\ &= \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right).\end{aligned}$$

⊠

It's also possible to extend Coulomb energy from measures to signed measures (differences of two measures) without changing its definition.

**Theorem 14.5.** *Let $V$ be the vector space of signed Borel measures $\mu$ on which the Coulomb energy $D(\mu,\mu)$ is finite. As a quadratic form on $V$, the Coulomb energy is positive definite: if $\mu$ and $\nu$ are signed measures,*

- $D(\mu,\mu) \ge 0$, *and*
- $D(\mu,\nu)^2 \le D(\mu,\mu)D(\nu,\nu)$.

*Proof.* We will use the identity

$$'\frac{1}{|x-y|} = \frac{1}{\pi^3}\int_{\mathbb{R}^3} \frac{1}{|x-z|^2}\frac{1}{|y-z|^2}\, \mathrm{d}z. \tag{14.6}$$

*Remark.* The reason this is true is due to Fourier analysis (in this remark, we ignore factors of $2\pi$):

$$\mathcal{F}\left(\frac{1}{|\cdot|^\alpha}\right)(x) = \frac{1}{|\xi|^{d-\alpha}},$$

so the right-hand side of (14.6) is, after sending $z \mapsto z + y$,

$$\begin{aligned}(RHS) &= \int \frac{1}{|x-y-z|^2}\frac{1}{|z|^2}\,\mathrm{d}z \\ &= \left(\frac{1}{|\cdot|^2} * \frac{1}{|\cdot|^2}\right)(x-y).\end{aligned}$$

If we take this and apply $\mathcal{F}$, then $\mathcal{F}^{-1}$, we get

$$\mathcal{F}^{-1}\left(\frac{1}{|\xi|}\cdot\frac{1}{|\xi|}\right)(x-y) = \mathcal{F}^{-1}\left(\frac{1}{|\xi|^2}\right)(x-y) = \frac{1}{|x-y|},$$

which proves (14.6), at least up to a constant. ◂

To prove $D(\mu,\mu) \geq 0$, one can apply (14.6) to the definition of $D(\mu,\mu)$ and see that it's a positive number times a square. Details are TODO. The second part follows from Cauchy-Schwarz in the $z$-variable. ⊠

Now we want to make some estimates on $(\psi, W\psi)$. For this we'll need at least a little geometry.

**Definition 14.7.** Let $R_1, \ldots, R_M \in \mathbb{R}^3$ be distinct points, and

$$\Gamma_j := \{x \in \mathbb{R}^3 \mid |x-R_j| < |x-R_i|, i \neq j\}.$$

This $\Gamma_j$ is the set of points closer to $R_j$ than any other $R_i$, and is open and convex. It's called the *Voronoi cell* associated to $R_j$. $\partial\Gamma_j$ is a finite collection of segments and planes, and possibly the point at infinity.

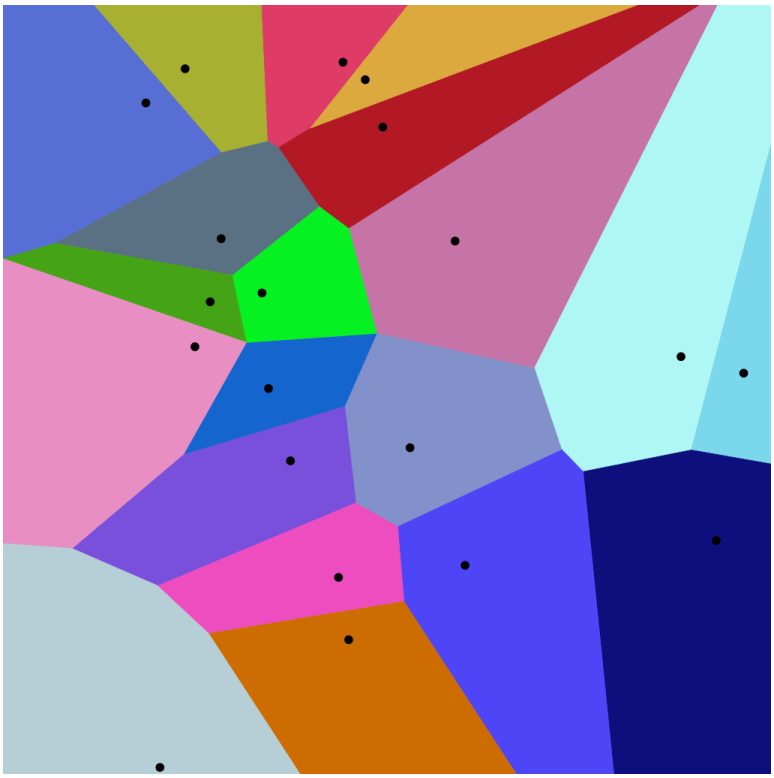

FIGURE 2. Voronoi cells for a collection of points in $\mathbb{R}^2$. Source: https://en.wikipedia.org/wiki/Voronoi_diagram.

Let

$$D_j := \frac{1}{2}\min_{\ell \neq j}|R_j - R_\ell|$$

denote the distance to the nearest neighboring $R_\ell$,

$$\mathcal{D}(x) := \min\{|x - R_i| \mid 1 \le i \le M\}$$

be the distance of $x$ to the closest nucleus, and

$$\widetilde{W}(x) := -W(x) = Z \sum_{j=1}^{M} \frac{1}{|x - R_j|}.$$

Then, we define

$$\Phi(x) := \widetilde{W}(x) - \frac{Z}{\mathcal{D}(x)},$$

which (the rest of this board was erased before I could get to it. TODO). Notice that $\Phi$ is continuous, but not differentiable on boundaries of Voronoi cells.

**Theorem 14.8** (Basic electrostatic inequality)**.** *Let $\mu = \mu_+ - \mu_-$ be a signed measure such that $D(\mu_\pm, \mu_\pm)$ is finite, and suppose that $R_1, \dots, R_M \in \mathbb{R}^3$ are distinct. Then,*

$$D(\mu, \mu) - \int \Phi(x) \mathrm{d}\mu_x + \sum \frac{Z^2}{|R_k - R_\ell|} \ge \frac{1}{8} \sum_j \frac{Z^2}{D_j}.$$

We'll prove this next time, using an auxiliary proposition.

**Proposition 14.9.**

$$\Phi(x) = \int_{\mathbb{R}^3} \frac{1}{|x - y|} \, \mathrm{d}\nu_y, \tag{14.10}$$

*where $\nu$ is some measure supported only on the boundaries of the Voronoi cells.*

*Proof.* To see this, let $f$ be a test function (Schwarz class); then,

$$\begin{aligned} \int \Delta\Phi(x) \, \mathrm{d}x &= \int \Phi(x) \Delta f(x) \, \mathrm{d}x \\ &= \sum_j \int_{\Gamma_j} \Phi(x) \Delta f(x) \, \mathrm{d}x. \end{aligned}$$

Integrating by parts,

$$= \underbrace{\sum_j \int_{\Gamma_j} \operatorname{div}(\Phi \nabla f) \, \mathrm{d}x}_{(I)} - \underbrace{\sum_j \int_{\Gamma_j} \nabla\Phi \cdot \nabla f \, \mathrm{d}x}_{(II)}.$$

Let $\mathbf{n}$ denote the outward-pointing unit normal vector on $\partial\Gamma_j$ and $\mathrm{d}S$ denote the surface measure on $\partial\Gamma_j$. Then,

$$\begin{aligned} (I) &= \sum_j \int_{\partial\Gamma_j} \Phi(x) \nabla f \cdot \mathbf{n}_j \, \mathrm{d}S \\ &= 0, \end{aligned}$$

because both $\Phi$ and $\nabla f$ are continuous on $\partial\Gamma_j$, so the opposite signs of $\mathbf{n}_j$ cancel out, as each piece of $\partial\Gamma_j$ is also the boundary of some other Voronoi cell with the opposite outward unit normal. The second piece is a little harder:

$$(II) = -\sum_j \int_{\Gamma_j} \operatorname{div}(f \nabla\Phi) \, \mathrm{d}x + \sum_j \int_{\Gamma_j} f \Delta\Phi \, \mathrm{d}x.$$

But inside $\Delta\Phi = 0$, because $-\Delta(1/|x|) = \delta(x)$, so the Fourier transform of its second derivative is $\xi^2/|\xi|^2 = 1$.

$$= -\sum_j \int_{\partial\Gamma_j} f \nabla\Phi \cdot \mathbf{n}_j \, \mathrm{d}S, \tag{14.11}$$

like before, but this time $\nabla\Phi$ is not continuous across $\partial\Gamma_j$. Here we need to think more carefully about the definition of $\Phi = \widetilde{W} - Z/\mathcal{D}$. Since $\widetilde{W}$ is differentiable away from the nuclei $R_j$, and in particular on $\partial\Gamma_j$,

$$\sum_j \int_{\partial\Gamma_j} f \nabla \widetilde{W} \mathbf{n}_j \, \mathrm{d}S = 0.$$

Therefore, returning to (14.11),

$$(II) = -\sum_j \int_{\partial\Gamma_j} f \nabla \frac{Z}{\mathcal{D}(x)} \mathbf{n}_j \, \mathrm{d}S.$$

Suppose $\Gamma_j$ and $\Gamma_k$ are neighboring cells, and let $B_{jk} := \partial\Gamma_j \cap \partial\Gamma_k$. Then, $\nabla(Z/\mathcal{D}(x))$ has opposite signs depending on from which side one approaches when tending to a point in $B_{jk}$, but the magnitude is the same. Therefore

$$\mathbf{n}_j \nabla \frac{Z}{\mathcal{D}(x)} = \mathbf{n}_k \nabla \frac{Z}{\mathcal{D}(x)},$$

where the left side comes from $\Gamma_j$ and the right side comes from $\Gamma_k$. Therefore

$$\begin{aligned}\int \Delta\Phi(x) f(x) \, \mathrm{d}x &= 2Z \int_{\bigcup_j \partial\Gamma_j} f(x) \underbrace{\mathbf{n}_j \nabla \frac{1}{|x - R_j|} \, \mathrm{d}S}_{\nu} \\ &= -4\pi \int f(x) \mathrm{d}\nu_x,\end{aligned}$$

as desired. ⊠

Lecture 15.

## Stability of matter for many-body systems: 10/19/17

Recall that we're in the middle of proving stability of matter for many-body systems with fixed nuclei. This system has Hamiltonian given in (14.2), with terms for the electron-electron interactions, electron-nucleus interactions, and nucleus-nucleus interactions. We then proved the basic electrostatic inequality, Theorem 14.8; the proof uses Voronoi cells to understand where $\Phi$ is continuous but not differentiable. We will continue to use notation from last lecture.

Last time, we proved Proposition 14.9, that

$$\Phi(x) := Z \sum_{k=1}^{M} \frac{1}{|x - R_k|} - \frac{Z}{\mathcal{D}(x)}$$

is actually $\int 1/|x-y| \mathrm{d}\nu_y$, where $\nu$ is a measure supported only on the boundaries of the Voronoi cells. Today, we'll use that to prove the basic electrostatic inequality.

*Proof of Theorem 14.8.* By Proposition 14.9, $\int \Phi(x) \mathrm{d}\mu_x = 2D(\mu, \nu)$, so

$$\begin{aligned}D(\mu,\mu) - \int \Phi(x) \mathrm{d}\mu_x + \sum_{i<j} \frac{Z^2}{|R_i - R_j|} &= \underbrace{D(\mu - \nu, \mu - \nu)}_{\geq 0} - D(\nu,\nu) + \sum_{i<j} \frac{Z^2}{|R_i - R_j|} \\ &\geq -D(\nu,\nu) + \sum_{i<j} \frac{Z^2}{|R_i - R_j|}.\end{aligned}$$

Let's look at $D(\nu,\nu)$.

$$\begin{aligned}D(\nu,\nu) &= \frac{1}{2} \int \Phi(x) \mathrm{d}\mu_x \\ &= \frac{Z}{2} \int \sum_k \int \delta(y - R_k) \frac{1}{|x-y|} \, \mathrm{d}y \, \mathrm{d}\nu_x - \frac{1}{2} \int \frac{Z}{\mathcal{D}(x)} \mathrm{d}\nu_x.\end{aligned}$$

Since everything is positive, we can switch the order of integration in the first term:

$$= \frac{Z}{2}\sum_k \int \delta(y-R_k)\Phi(y)\,dy - \frac{1}{2}\int \frac{Z}{\mathcal{D}(x)}\,d\nu_x$$
$$= \underbrace{\frac{Z}{2}\sum_k \Phi(R_k)}_{(I)} - \underbrace{\frac{1}{2}\int \frac{Z}{\mathcal{D}(x)}d\nu_x}_{(II)}.$$

We have that

$$(I) = \sum_{k<\ell}\frac{Z^2}{|R_k - R_\ell|}$$

and

$$(II) = \sum_j \frac{Z^2}{8\pi}\int_{\partial\Gamma_j}\frac{1}{|x-R_j|}\mathbf{n}_j\cdot\nabla\frac{1}{|x-R_j|}\,dS$$
$$= -\sum_j \frac{Z^2}{16\pi}\int_{\partial\Gamma_j}\mathbf{n}_j\cdot\nabla\frac{1}{|x-R_j|^2}\,dS$$
$$= \sum_j \frac{Z^2}{16\pi}\int_{\Gamma_j^c}\Delta\frac{1}{|x-R_j|^2}\,dx$$
$$= \sum_j \frac{Z^2}{8\pi}\int_{\Gamma_j^c}\frac{1}{|x-R_j|^4}\,dx.$$

We can break this into pieces: for any $x \in \Gamma_j^c$, let $D_j$ be the coordinate of the intersection point of $\partial\Gamma_j$ and line segment from $x$ to $R_j$. Then,

$$\geq \sum_j \frac{Z^2}{8\pi}\int_{\mathbb{R}}dz\int_{\mathbb{R}}dy\int_{D_j}^{\infty}dx\,\frac{1}{|x^2+y^2+z^2|},$$

and this is certainly bounded below:

$$\geq \sum_j \frac{Z^2}{8}\frac{1}{D_j}. \qquad \boxtimes$$

The real reason we care about Theorem 14.8 is to prove stability of matter. First, let's analyze the electron-electron repulsion. Suppose $\psi_N \in \Lambda^N L^2(\mathbb{R}^3)$ is a fermionic (i.e. antisymmetric) wavefunction. Then

$$I_{\psi_N} = \sum_{1\leq i<j\leq N}\int \frac{|\psi_N(x_1,\dots,x_N)|^2}{|x_i-x_j|}\,dx_1\cdots dx_N. \tag{15.1}$$

The integrand is $O(1)$, so $I_{\psi_N}$ is $O(N^2)$. We can write $I_{\psi_N}$ as a sum of two pieces:

$$I_{\psi_N} = \mathcal{D}(\rho_{\psi_N},\rho_{\psi_N}) + \mathrm{ind}_{\psi_N}.$$

The second term ("everything else") is called the *indirect term*. Here recall that

$$\rho_{\psi_N} :- \sum_{j=1}^N \int |\psi_N(x_1,\dots,x_{j-1},x,x_{j+1},\dots,x_N)|\,dx_1\cdots\widehat{dx_j}\cdots dx_N.$$

The bound on the indirect term is quite hard, so we won't prove it.

**Theorem 15.2.**

$$\mathrm{ind}_{\psi_N} \geq -C\int \rho_{\psi_N}^{4/3}.$$

For a proof, see Lieb-Seininger. Thus we have an $O(N^{4/3})$ lower bound for the indirect term, but $O(N)$ for the direct term.

Now we'll derive stability of matter (recall $N$ is the number of electrons, and $M$ is the number of nuclei).

**Theorem 15.3** (Stability of matter for many-body systems with fixed nuclei)**.** *The ground state energy for many-body systems is linearly proportional to the number of particles.*

*Proof.* The idea of the proof is to show

$$(\psi_N, H\psi_N) \geq -CN\left(1+\left(\frac{M}{N}\right)^{1/3}\right)^2.$$

Then, using the Cauchy-Schwarz inequality $ab \leq a^2/2 + b^2/2$,

$$\begin{aligned} &\geq -CN\left(1+M^{2/3}N^{-2/3}\right) \\ &= -C(N+M^{2/3}N^{1/3}). \end{aligned}$$

Using Young's inequality $ab \leq a^p/p + b^{p'}/p'$, where $p$ and $p'$ are Hölder conjugates, $M^{2/3}N^{1/2} \leq M+N$, so

$$\geq -\widetilde{C}(N+M),$$

where $\widetilde{C}$ is some other constant (to absorb the factor of 2).

Now let's look at the pieces, in order to get to that derivation. First, the kinetic term, which the Lieb-Thirring inequality shows is

$$\left(\psi_N, \left(-\sum \Delta_{x_j}\right)\psi_N\right) \geq \frac{K}{\|\gamma^{(1)}_{\psi_N}\|^{p/p'}} \int \rho^{5/3}_{\psi_N}\,\mathrm{d}x,$$

where $p = 1+3/2$ and $p'$ is its Hölder conjugate. Moreover, using creation and annihilation operators, one gets that $\|\gamma^{(1)}_{\psi_N}\| \leq 1$, so

$$\left(\psi_N, \left(-\sum \Delta_{x_j}\right)\psi_N\right) \geq C\int \rho^{5/3}_{\psi_N}\,\mathrm{d}x.$$

The electron-electron term: TODO.

The electron-nucleus term:

$$\left(\psi_N, -\sum_{\substack{1\leq i\leq N\\ 1\leq j\leq M}} \frac{Z}{|x_i - R_j|}, \psi_N\right) = -\sum_{k=1}^{M}\int \frac{Z}{|x-R_k|}\rho_{\psi_N}(x)\,\mathrm{d}x.$$

The total Coulomb energy:

$$\begin{aligned} (\psi_N, V_C\psi_N) &\geq \mathcal{D}(\rho_{\psi_N},\rho_{\psi_N}) - \sum_{k=1}^{M}\int \frac{Z}{|x-R_k|}\rho_{\psi_N}(x)\,\mathrm{d}x + U(\mathbf{R}) - C\int \rho^{4/3}_{\psi_N} \\ &\geq -\int \frac{Z}{\mathcal{D}(x)}\rho_{\psi_N}(x)\,\mathrm{d}x - C\int \rho^{4/3}_{\psi_N} \\ &\geq -\int \frac{Z}{\mathcal{D}(x)}\rho_{\psi_N}(x)\,\mathrm{d}x - C\left(\int \rho^{5/3}_{\psi_N}\right)^{1/2}\left(\int \rho_{\psi_N}\right)^{1/2}. \end{aligned} \tag{15.4}$$

We'll use a generalized Cauchy-Schwarz inequality

$$ab \leq \frac{\varepsilon}{2}a^2 + \frac{1}{2\varepsilon}b^2 \tag{15.5}$$

to infer that

$$-C\left(\int \rho^{5/3}_{\psi_N}\right)^{1/2}\left(\int \rho_{\psi_N}\right)^{1/2} \geq -C\varepsilon\int \rho^{5/3}_{\psi_N} - \frac{C}{\varepsilon}\underbrace{\int \rho_{\psi_N}}_{N}$$

and therefore improve (15.4) to

$$-\int \frac{Z}{\mathcal{D}(x)}\rho_{\psi_N}(x)\,\mathrm{d}x + C(1-\varepsilon)\int \rho^{5/3}_{\psi_N} - \frac{CN}{\varepsilon}. \tag{15.6}$$

We still don't know what $\rho_{\psi_N}$ is, but now everything is stated in terms of it, so we can minimize over it. For $b > 0$, write

$$\frac{1}{\mathcal{D}(x)} = \left(\frac{1}{\mathcal{D}(x)} - b\right) + b.$$

From minimizing over $\rho$ (set $\frac{\delta}{\delta\rho(x)} = 0\ldots$), one has that

$$C(1-\varepsilon)\frac{5}{3}\rho(x)^{2/3} = Z\left(\frac{1}{\mathcal{D}(x)} - b\right),$$

and therefore that our minimum is

$$\rho(x) = \frac{C}{(1-\varepsilon)^{3/2}} Z^{3/2}\left(\frac{1}{\mathcal{D}(x)} - b\right)_+^{3/2},$$

so

$$\begin{aligned}(\psi_N, H\psi_N) &\geq (15.6)\\ &\geq -\frac{CN}{\varepsilon} + C(1-\varepsilon)\int \rho^{5/3} - Z\int\left(\frac{1}{\mathcal{D}(x)} - b\right)\rho\\ &\geq -\frac{CN}{\varepsilon} - \frac{CZ^{5/3}}{(1-\varepsilon)^{3/2}}\int\left[\frac{1}{\mathcal{D}(x)} - b\right]_+^{5/2} \mathrm{d}x. \qquad (15.7)\end{aligned}$$

Next, observe

$$\begin{aligned}[\mathcal{D}(x) - b]_+^{5/2} &= \max_j \left[\frac{1}{|x-R_j|} - b\right]_+^{5/2}\\ &\leq \sum_{j=1}^M \left[\frac{1}{|x-R_j|} - b\right]_+^{5/2}.\end{aligned}$$

Therefore

$$\int_{\mathbb{R}^3}\left[\frac{1}{\mathcal{D}(x)} - b\right]_+^{5/2}\mathrm{d}x \leq M\int_{|x|\leq 1/b}\left(\frac{1}{|x|} - b\right)^{5/2}\mathrm{d}x = CMb^{-1/2}.$$

To see this, for each $j$, set $R_j = 0$, so $1/|x| - b \geq 0$, and therefore $|x| \leq 1/b$.

Next, optimize over $b$. The optimal value will satisfy

$$bN \sim \frac{M}{(1-\varepsilon)^{3/2}} b^{-1/2},$$

i.e.

$$b \sim \frac{1}{1-\varepsilon}\left(\frac{M}{N}\right)^{2/3}.$$

We've now reduced to

$$\begin{aligned}(\psi_N, H\psi_N) &\geq (15.7)\\ &\geq -\frac{1}{\varepsilon}CN - \frac{C}{1-\varepsilon}N\left(\frac{M}{N}\right)^{2/3}. \qquad (15.8)\end{aligned}$$

Now we optimize for $\varepsilon$, ending up with

$$\frac{1}{\varepsilon}N \sim \frac{1}{1-\varepsilon}N\left(\frac{M}{N}\right)^{2/3},$$

i.e.

$$\frac{1}{\varepsilon} \sim 1 + \left(\frac{M}{N}\right)^{2/3}.$$

Now, we can finally conclude stability of matter:

$$(\psi_N, H\psi_N) \geq (15.8) \geq -CN\left(1 + \left(\frac{M}{N}\right)^{2/3}\right) \geq -C(N+M)$$

by Young's inequality, as we discussed earlier. ⊠

This is typical of the kinds of analysis proofs in this kind of mathematical physics: the arguments don't use extremely fancy math *per se*, but physics intuition is essential in showing us the way. For example, in this case, it led us to Voronoi cells.

Lecture 16.

## Introduction to quantum field theory and Fock space: 10/24/17

Today, we move into quantum field theory: we'll start with tensor products, then move into Fock space and creation and annihilation operators, and use them to restate many-body quantum mechanics (second quantization). From there we move to other simple examples and further topics.

**Fock spaces** The quantum-mechanical systems we've so far considered have Hilbert spaces which depend on the number of particles present in the system. Particles can be created and annihilated (though this requires, resp. produces energy), so it would be useful to have a Hilbert space of states which does not fix the number of particles. This is what Fock spaces accomplish.

In order to understand Fock spaces, one must understand tensor products. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces, say corresponding to two particles in a quantum-mechanical system. We want a Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ which encodes the states of both particles.

**Definition 16.1.** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. For any $\varphi_1 \in \mathcal{H}_1$ and $\varphi_2 \in \mathcal{H}_2$, let $\varphi_1 \otimes \varphi_2 \colon \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ denote the conjugate bilinear form

$$\varphi_1 \otimes \varphi_2(f_1, f_2) = (\varphi_1, f_1)_{\mathcal{H}_1}(\varphi_2, f_2)_{\mathcal{H}_2}.$$

Bilinearity means that

$$(\varphi_1 \otimes \varphi_2)(f_1 + g, f_2) = (\varphi_1 \otimes \varphi_2)(f_1, f_2) + (\varphi_1 \otimes \varphi_2)(g, f_2),$$

and similarly for arguments of the form $(f_1, f_2 + g)$.

Let $\mathcal{E}$ denote the space of finite linear combinations of the forms $\varphi_1 \otimes \varphi_2$ for $\varphi_i \in \mathcal{H}_i$. It has an inner product, defined as the linear extension of the form

$$(\varphi_1 \otimes \varphi_2, \psi_1 \otimes \psi_2)_{\mathcal{E}} \coloneqq (\varphi_1, \psi_1)_{\mathcal{H}_1}(\varphi_2, \psi_2)_{\mathcal{H}_2} \tag{16.2}$$

(one must check it is well-defined and positive-definite). Then, the *tensor product* of $\mathcal{H}_1$ and $\mathcal{H}_2$, denoted $\mathcal{H}_1 \otimes \mathcal{H}_2$, is the completion of $\mathcal{E}$ with respect to its inner product.

**Proposition 16.3.** *If $\{\varphi_j\}$ is an orthonormal basis for $\mathcal{H}_1$ and $\{\psi_i\}$ is an orthonormal basis for $\mathcal{H}_2$, then $\{\varphi_j \otimes \psi_i\}_{i,j}$ is an orthonormal basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$.*

**Example 16.4.** Let $\mathcal{H}_1 = \mathbb{R}^2$, with coordinates $(a_1, a_2)$, and $\mathcal{H}_2 = \mathbb{R}^3$, with coordinates $(b_1, b_2, b_3)$. Then, $\mathcal{H}_1 \otimes \mathcal{H}_2 \cong \mathbb{R}^6$, with coordinates $(a_1b_1, a_1b_2, a_1b_3, a_2b_1, a_2b_2, a_2b_3)$. ◂

If $\mathcal{H}_1$ and $\mathcal{H}_2$ are $L^2$-spaces, we can identify $\mathcal{H}_1 \otimes \mathcal{H}_2$ as something somewhat more concrete. Let $(M_1, \mathrm{d}\mu_1)$ and $(M_2, \mathrm{d}\mu_2)$ be measure spaces such that $L^2(M_1, \mathrm{d}\mu_1)$ and $L^2(M_2, \mathrm{d}\mu_2)$ are both separable, with orthonormal bases $\{\varphi_i(x)\}$, resp. $\{\psi_j(y)\}$. By Proposition 16.3, $\{\varphi_i(x)\psi_\ell(y)\}$ is an orthonormal basis for $L^2(M_1 \times M_2, \mathrm{d}\mu_1 \otimes \mathrm{d}\mu_2)$ (the product measure).

**Theorem 16.5.** *Let $U \colon L^2(M_1, \mathrm{d}\mu_1) \otimes L^2(M_2, \mathrm{d}\mu_2) \to L^2(M_1 \times M_2, \mathrm{d}\mu_1 \otimes \mathrm{d}\mu_2)$ denote the map extending linearly from*

$$\varphi_1 \otimes \varphi_2 \longmapsto \varphi_1(x)\varphi_2(y).$$

*Then, $U$ is a unitary isomorphism.*

That is, up to isomorphism of complex Hilbert spaces, the tensor product of $L^2(M_1, \mathrm{d}\mu_1)$ and $L^2(M_2, \mathrm{d}\mu_2)$ is the space of $L^2$ functions on the product measure space (assuming separability).

One can prove that the tensor product is associative up to unitary isomorphism, and therefore uniquely define higher-order tensor products, such as $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. We will let $\mathcal{H}^{\otimes n}$ denote the *n-fold tensor product* of $\mathcal{H}$:

$$\mathcal{H}^{\otimes n} := \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{n \text{ times}}.$$

The notation $\otimes$ for tensor product reflects that its inner product (16.2) is the product of the two individual inner products. There is a corresponding notion for adding inner products, which is denoted $\oplus$.

**Definition 16.6.** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. Its *direct sum* $\mathcal{H}_1 \oplus \mathcal{H}_2$ is the space of pairs $(\varphi_1, \varphi_2)$ with $\varphi_i \in \mathcal{H}_i$, together with the inner product

$$((\varphi_1, \varphi_2), (\psi_1, \psi_2)) = (\varphi_1, \psi_1)_{\mathcal{H}_1} + (\varphi_2, \psi_2)_{\mathcal{H}_2}.$$

Unlike for the tensor product, there is no need to complete. As with tensor product, this is associative up to isomorphism, so we may define triple and higher-order direct sums.

We now have the ingredients we need to define Fock spaces.

**Definition 16.7.** Let $\mathcal{H}$ be a Hilbert space. Then, *Fock space* over $\mathcal{H}$ is

$$\mathcal{F}(\mathcal{H}) := \bigoplus_{n=1}^{\infty} \mathcal{H}^{\otimes n},$$

where we set $\mathcal{H}^0 := \mathbb{C}$.

We'll place an inner product on this space in just a moment.

**Example 16.8.** Suppose $\mathcal{H} = L^2(\mathbb{R}^m)$, so if $\varphi \in \mathcal{H}^{\otimes n}$, we may regard $\varphi$ as an $L^2$ function of $n$ arguments, with each argument in $\mathbb{R}^n$. Therefore $\mathcal{F}(\mathcal{H})$ is the space of functions

$$\Phi = (\lambda, \varphi_1(x), \varphi_2(x_1, x_2), \varphi_3(x_1, x_2, x_3), \dots). \tag{16.9}$$

◁

The inner product on $\mathcal{F}(\mathcal{H})$ is defined as follows: suppose $\Phi$ and $\Psi$ are defined as in (16.9). Then,

$$(\Phi, \Psi)_{\mathcal{F}(\mathcal{H})} := \overline{\varphi}_0 \psi_0 + \sum_{n=1}^{\infty} (\varphi_n, \psi_n)_{\mathcal{H}^{\otimes n}}.$$

*Remark.* TODO: in algebra, the infinite direct sum consists of tuples for which only finitely many are nonzero, but this space isn't complete under the above inner product. Do we take the completion of that space under the inner product, or consider tuples with potentially infinite nonzero elements such that the inner product converges?[17] ◁

**Lemma 16.10.** *If $\mathcal{H}$ is separable, so is $\mathcal{F}(\mathcal{H})$.*

In physics, there are two particularly relevant subspaces: the symmetric tensors (for bosons) and the antisymmetric operators (for fermions). Let $S_n$ denote the symmetric group on $n$ letters, i.e. the group of automorphisms of the set $\{1, \dots, n\}$. This acts on $\mathcal{H}^{\otimes n}$: if $\sigma \in S_n$, let

$$\sigma(\varphi_1 \otimes \cdots \otimes \varphi_n) := \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(n)}.$$

Define

$$\mathrm{Sym}_n := \frac{1}{n!} \sum_{\sigma \in S_n} \sigma,$$

e.g.

$$\mathrm{Sym}_2((\varphi_1 \otimes \varphi_2))(x, y) = \frac{1}{2}(\varphi_1(x)\varphi_2(y) + \varphi_2(x)\varphi_1(y)).$$

One can check that $\mathrm{Sym}^n$ is an orthonormal projection by verifying that

$$(\mathrm{Sym}_n \varphi, \psi)_{\mathcal{H}^{\otimes n}} = (\varphi_n, \mathrm{Sym}^n \psi_n)_{\mathcal{H}^{\otimes n}}$$

and $\mathrm{Sym}_n \circ \mathrm{Sym}_n = \mathrm{Sym}_n$; its range is called the *n-fold symmetric tensor product* of $\mathcal{H}$, denoted $\mathcal{H}^{\otimes_s n} := \mathrm{Sym}_n \mathcal{H}_n$.

[17] Less concerning but still interesting: $\mathcal{F}(\mathcal{H})$ has an algebra structure. Is this used at all in physics?

**Definition 16.11.** The *symmetric Fock space* or *bosonic Fock space* is

$$\mathcal{F}_s(\mathcal{H}) := \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes_s n}.$$

The fermionic story is the same: there is an *antisymmetrization operator*

$$\mathrm{Alt}_n := \frac{1}{n!} \sum_{\sigma \in S_n} (-1)^{\mathrm{sign}(\sigma)} \sigma,$$

which is again an orthonormal projection. Its range is called the *alternating tensor product* of $\mathcal{H}$ and denoted $\mathcal{H}^{\otimes_a n}$.

**Definition 16.12.** The *antisymmetric Fock space* or *fermionic Fock space* is

$$\mathcal{F}_a(\mathcal{H}) := \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes_a n}.$$

*Remark.* Suppose $\mathcal{H} = L^2(\mathbb{R}^d)$, corresponding to particles moving in $\mathbb{R}^d$. Then, $\mathcal{H}^{\otimes_s n}$ is isomorphic to the space of $L^2$ functions $f(x_1, \dots, x_n)$ in $n$ variables on $\mathbb{R}^d$ that are symmetric, i.e. $f(x_{\sigma(1)}, \dots, f_{\sigma(n)}) = f(x_1, \dots, x_n)$ for all $\sigma \in S_n$. We previously studied this space, and called it $L^2_{\mathrm{sym}}(\mathbb{R}^d)$, exactly the Hilbert space for a system of $n$ bosons. In this way, the bosonic Fock space is the direct sum of the $n$-boson Hilbert spaces for all $n$. The same analysis applies to fermionic Fock space and $n$-fermion systems. ◁

The physical interpretation of a $\Psi \in \mathcal{F}_s(\mathcal{H})$ is a generalized wavefunction: if $\Psi = (\varphi_n)_{n=0}^{\infty}$ and $\|\Psi\|_{\mathcal{F}_s(\mathcal{H})}$ is normalized to 1, then

$$\|\psi\|^2_{\mathcal{F}_s(\mathcal{H})} = \sum_{n \geq 0} \|\varphi_n\|_{L^2_{\mathrm{sym}}(\mathbb{R}^{nd})} = 1,$$

so we interpret $\Psi$ as a state of the quantum system where the probability that there are $n$ particles is $\|\varphi_n\|^2$, and the probability density function for particles being in positions $x_1, \dots, x_n$, given that the particle number is $n$, is $|\varphi_n(x_1, \dots, x_n)|^2$. The analogous description applies for fermionic wavefunctions.

To study the dynamics of such a system, we introduce a Hamiltonian $H$, a self-adjoint, bounded-below operator, and the Schrödinger equation

$$i\partial_t \Psi = H\Psi, \tag{16.13}$$

and initial data of a $\Psi(t = 0) \in \mathcal{F}_s(L^2(\mathbb{R}^d))$.

Suppose that $H$ preserves the particle number (maps $\mathcal{H}^{\otimes_s n}$ to itself). This physically means particles are neither created nor destroyed, and to understand the dynamics of the system, there's no need to introduce Fock space at all. However, there are interesting theories in which the particle number is not preserved over time, corresponding to maps on $\mathcal{F}_s(\mathcal{H})$ or $\mathcal{F}_a(\mathcal{H})$ which don't preserve the grading. There's an extremely elegant description of the algebra of these maps in terms of creation and annihilation operators, which we will use.

*Remark.* The zeroth graded piece $\mathcal{H}^0 = \mathbb{C}$ is called the *vacuum sector*. Its states are all in phase, so there's just one equivalence class of states $\Omega = (1, 0, 0, \dots)$, called the *Fock vacuum*.

We're used to thinking of the vacuum as the absence of particles, and indeed this vacuum state is for the zero-particle system. But just because there is nothing does not mean there isn't something else. For example, in the Fermi sea, all fermions are close together, and adding energy can pop one fermion out into the rest of the world. It leaves behind a hole — regarded as an antiparticle — and one can envision the Fermi sea as the Fock vacuum, and the popped-out fermion as producing a one-particle state. In this way there can be more than one way to think about the vacuum. ◁

**Definition 16.14.** Let $f \in \mathcal{S}(\mathbb{R}^d)$ (i.e. a Schwartz class operator).

- Define the *creation operator* $a^*(f) \colon \mathcal{F}_s(L^2(\mathbb{R}^d)) \to \mathcal{F}_s(L^2(\mathbb{R}^d))$ to send

$$\varphi_n \longmapsto \mathrm{Sym}_{n+1}(f \otimes \varphi_n).$$

  This increases the grading by 1, in that it maps $\mathcal{H}^{\otimes_s n}$ to $\mathcal{H}^{\otimes_s (n+1)}$.

- Define the *annihilation operator* $a(f)\colon \mathcal{F}_s(L^2(\mathbb{R}^d)) \to \mathcal{F}_s(L^2(\mathbb{R}^d))$ to send[18]

$$\varphi_n(x_1, \dots, x_n) \longmapsto \sqrt{n} \int_{\mathbb{R}^d} \overline{f}(x_n)\varphi_n(x_1, \dots, x_{n-1}, x_n)\, \mathrm{d}x_n.$$

  This decreases the grading by 1, in that for $n \geq 1$ it sends $\mathcal{H}^{\otimes_s n} \to \mathcal{H}^{\otimes_s (n-1)}$, and the Fock vacuum is destroyed: any $\lambda \in \mathcal{H}^0$ is sent to 0.

Another way to say this is: $a(f)\Omega = 0$ for all $f \in \mathcal{S}(\mathbb{R}^d)$.
Next time, we'll talk more about these operators and how to use them to express dynamics.

[18] Since $\varphi$ is symmetric, the choice of $n$ in $\overline{f(x_n)}$ is not important.