8. Operator approach to quantum mechanics

In mechanics and field theory (both classical and quantum), there are two main languages – Lagrangian and Hamiltonian. In the classical setting, the Lagrangian language is the language of variational calculus (i.e. one studies extremals of the action functional), while the Hamiltonian language is that of symplectic geometry and Hamilton equations. Correspondingly, in the quantum setting, the Lagrangian language is the language of path integrals, while the Hamiltonian language is the language of operators and Schrödinger equation. We have now studied the first one (at least in perturbation expansion) and are passing to the second one.

8.1. **Hamilton's equations in classical mechanics.** We start with recalling the Hamiltonian formalism of classical mechanics. For more details, we refer the reader to the excellent book [A].

Recall first the Lagrangian description of the motion of a classical particle or system of particles. The position of a particle is described by a point q of the configuration space X, which we will assume to be a manifold. The Lagrangian of the system is a (smooth) function $\mathcal{L} : TX \to \mathbb{R}$ on the total space of the tangent bundle of X. Then the action functional is $S(q) = \int \mathcal{L}(q, \dot{q})dt$. The trajectories of the particle are the extremals of S. The condition for $q(t)$ to be an extremal of S is equivalent to the Euler-Lagrange equation (=the equation of motion), which in local coordinates has the form

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}}{\partial q_i}.$$

For example, if X is a Riemannian manifold and $\mathcal{L}(q, v) = \frac{v^2}{2} - U(q)$ where $U : X \to \mathbb{R}$ is a potential function, then the Euler-Lagrange equation is the Newton equation

$$\ddot{q} = -U'(q),$$

where $\ddot{q} = \nabla_{\dot{q}}\dot{q}$ is the covariant derivative with respect to the Levi-Civita connection.

Consider now a system with Lagrangian $\mathcal{L}(q, v)$, whose differential with respect to v (for fixed q) is a diffeomorphism $T_qX \to T_q^*X$. This is definitely true in the above special case of Riemannian X.

Definition 8.1. The *Hamiltonian (or energy function)* of the system with Lagrangian $\mathcal{L}$ is the function $H : T^*X \to \mathbb{R}$, which is the Legendre transform of $\mathcal{L}$ along fibers; that is, $H(q, p) = pv_0 - \mathcal{L}(q, v_0)$, where v_0 is the (unique) critical point of $pv - \mathcal{L}(q, v)$. The manifold T^*X is

called the *phase space (or space of states)*. The variable p is called the *momentum variable*.

For example, if $\mathcal{L} = \frac{v^2}{2} - U(q)$, then $H(q,p) = \frac{p^2}{2} + U(q)$.

Remark 8.2. Since Legendre transform is involutive, we also have that the Lagrangian is the fiberwise Legendre transform of the Hamiltonian.

Let q_i be local coordinates on X. This coordinate system defines a coordinate system (q_i, p_i) on T^*X. We obtain

Proposition 8.3. *The equations of motion are equivalent to the Hamilton equations*

$$\dot{q}_i = \frac{\partial H}{\partial p_i},\ \dot{p}_i = -\frac{\partial H}{\partial q_i},$$

in the sense that they are obtained from Hamilton's equations by elimination of p_i.

It is useful to write Hamilton's equations in terms of Poisson brackets. Recall that the manifold T^*X has a canonical symplectic structure $\omega = d\alpha$, where α is the canonical 1-form on T^*M (called the *Liouville form*) constructed as follows: for any $z \in T_{(q,p)}(T^*X)$,

$$\alpha(z) = (p, d\pi(q,p)z),$$

where $\pi : T^*X \to X$ is the projection. In local coordinates, we have

$$\alpha = \sum_i p_i dq_i,\ \omega = \sum_i dp_i \wedge dq_i.$$

Now let (M, ω) be a symplectic manifold (in our case $M = T^*X$). Since ω is non-degenerate, one can define the Poisson bivector ω^{-1}, which is a section of the bundle $\wedge^2 TM$. Now, given any two smooth functions f, g on M, one can define a third function – their *Poisson bracket*

$$\{f, g\} = (df \otimes dg, \omega^{-1}).$$

This operation is skew-symmetric and satisfies the Jacobi identity, i.e. it is a Lie bracket on $C^\infty(M)$. For $M = T^*X$, in local coordinates we have

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right).$$

This shows that Hamilton's equations can be written in the following manner in terms of Poisson brackets:

$$\frac{d}{dt} f(q(t), p(t)) = \{f, H\}(q(t), p(t)). \tag{8.1}$$

for any smooth function ("classical observable") $f \in C^\infty(T^*X)$, or, for shorthand

$$\frac{df}{dt} = \{f, H\}.$$

In other words, Hamilton's equations say that the rate of change of the observed value of f equals the observed value of $\{f, H\}$.

8.2. **Unbounded self-adjoint operators.** The rigorous mathematical treatment of quantum mechanics in the Hamiltonian setting is based on von Neumann's theory of unbounded self-adjoint operators in a Hilbert space. Let us recall the basics of this theory.

8.2.1. *Spectral theorem for bounded self-adjoint operators.* Let $\mathcal{H}$ be a separable complex Hilbert space with inner product $\langle\ ,\ \rangle$ (antilinear in the first argument, as is traditional in quantum physics). We first recall the *spectral theorem* for bounded self-adjoint operators $A : \mathcal{H} \to \mathcal{H}$, which generalizes the diagonalization theorem for a Hermitian matrix.

Theorem 8.4. *(von Neumann) Let A be a bounded self-adjoint operator. There exists a measure space (X, μ), an essentially bounded measurable function $h : X \to \mathbb{R}$, and an isometry $\mathcal{H} \to L^2(X, \mu)$ under which A maps to the operator of multiplication by h. Moreover, the spectrum $\sigma(A)$ is the set of $\lambda \in \mathbb{R}$ for which $h^{-1}(\lambda-\varepsilon, \lambda+\varepsilon)$ is positive for each $\varepsilon > 0$, and the eigenvalues of A (if they exist) are $\lambda \in \mathbb{R}$ such that $\mu(h^{-1}(\lambda)) > 0$, with eigenfunctions being indicator functions of subsets of $h^{-1}(\lambda)$ of positive measure.*

8.2.2. *Closable and closed operators.* Now we pass to not necessarily bounded operators. Let $\mathcal{H}'$ be another separable Hilbert space. A *densely defined linear operator* on $\mathcal{H}$ is a pair (A, V) where $V \subset \mathcal{H}$ is a dense subspace and A is a (possibly unbounded) linear operator $V \to \mathcal{H}'$. The space V is called the *domain* of A; in the notation, we will often suppress it and denote the operator just by A. Such an operator A has a graph $\Gamma_A \subset V \times \mathcal{H}' \subset \mathcal{H} \times \mathcal{H}'$. Let $\overline{\Gamma}_A$ be the closure of Γ_A in $\mathcal{H} \times \mathcal{H}'$. The operator A is said to be *closable* if $(0, u) \in \overline{\Gamma}_A$ for $u \in \mathcal{H}'$ implies $u = 0$, i.e., if the first projection $p_1 : \overline{\Gamma}_A \to \mathcal{H}$ is injective. In this case, setting $\overline{V} := p_1(\overline{\Gamma}_A) \subset \mathcal{H}$, we have $V \subset \overline{V}$ and obtain an extension of the operator $A : V \to \mathcal{H}'$ to a densely defined operator $\overline{A} : \overline{V} \to \mathcal{H}'$ which is called the *closure* of A. If A is closable and $\overline{A} = A$, we will say that A is *closed*; in other words, A is closed iff it has closed graph in $\mathcal{H} \times \mathcal{H}'$. Obviously, the closure $\overline{A}$ is closed for any closable A. Also, if A is bounded then it is closable, $\overline{V} = \mathcal{H}$, and $\overline{A} : \mathcal{H} \to \mathcal{H}'$ is just the continuous (=bounded) extension of A.

In general, however, a densely defined operator need not be closable. For example, if $\mathcal{H}'$ is finite dimensional and $A : V \to \mathcal{H}'$ is unbounded then there exists a sequence $v_n \in V$ such that $v_n \to 0$ but $||Av_n|| \geq 1$. Then the sequence $w_n := \frac{v_n}{||Av_n||}$ goes to 0, while $||Aw_n|| = 1$, so, as the unit sphere in $\mathcal{H}'$ is compact, passing to a subsequence if needed, we may assume that $Aw_n \to u$ for some $u \in \mathcal{H}'$ with $||u|| = 1$. Then $(0, u) \in \overline{\Gamma}_A$ and A is not closable. So we see that A is closable iff it is bounded.

On the other hand, if $\mathcal{H}'$ is infinite dimensional, then there are important classes of unbounded closable operators. For example, consider the case $\mathcal{H} = \mathcal{H}'$. Let us say that an operator $A : V \to \mathcal{H}$ is *symmetric* if $\langle v, Aw \rangle = \langle Av, w \rangle$ for all $v, w \in V$. We claim that every symmetric operator is closable and its closure is symmetric. Indeed, suppose $(v_n, Av_n) \to (0, u)$ for $u \in \mathcal{H}$. Fix a sequence $u_k \in V$ such that $u_k \to u$. Then

$$\langle Au_k, v_n \rangle = \langle u_k, Av_n \rangle \to \langle u_k, u \rangle, \ n \to \infty.$$

But the leftmost expression goes to zero, so $\langle u_k, u \rangle = 0$ for all k, hence $||u||^2 = 0$ which gives $u = 0$, i.e., A is closable. Moreover, given $v, w \in \overline{V}$, there exist sequences $v_n \to v, w_n \to w$ in V such that $Av_n \to \overline{A}v$, $Aw_n \to \overline{A}w$, thus

$$\langle v, \overline{A}w \rangle = \lim_{n\to\infty} \langle v_n, Aw_n \rangle = \lim_{n\to\infty} \langle Av_n, w_n \rangle = \langle \overline{A}v, w \rangle,$$

so $\overline{A}$ is symmetric.

8.2.3. *Adjoint operator.* Closed symmetric operators by themselves are not sufficient for quantum mechanics, however, since such operators cannot, in general, be diagonalized. Instead we need *self-adjoint* operators, which are closed symmetric operators satisfying an important additional property. To formulate this property, we first need to define the notion of an adjoint operator.

Let (A, V) be a closed symmetric operator. Denote by $V^\vee$ the space of $u \in \mathcal{H}$ such that the linear functional $v \mapsto \langle u, Av \rangle$ is bounded on V. In this case by the Riesz representation theorem there exists a unique vector $w \in \mathcal{H}$ such that $\langle u, Av \rangle = \langle w, v \rangle$, which depends linearly on u. Thus we obtain an operator $A^\dagger : V^\vee \to \mathcal{H}$. Note that $V^\vee \supset V$ and $A^\dagger$ is an extension of A to $V^\vee$, so $(A^\dagger, V^\vee)$ is a densely defined operator called the *adjoint operator* of (A, V). Furthermore, this operator is closed: if $(u_n, A^\dagger u_n) \to (u, w)$ then for $v \in V$,

$$\langle A^\dagger u_n, v \rangle = \langle u_n, Av \rangle \to \langle u, Av \rangle, \ n \to \infty,$$

and at the same time $\langle A^\dagger u_n, v \rangle \to \langle w, v \rangle$, so $\langle u, Av \rangle = \langle w, v \rangle$, hence $u \in V^\vee$ and $w = A^\dagger u$.

However, we will see that the operator $A^\dagger$ fails to be symmetric, in general. So we may consider the skew-Hermitian form

$$B(v,w) := (A^\dagger v, w) - (v, A^\dagger w)$$

on $V^\vee$ that measures its failure to be symmetric, called the *boundary form* (it is called this way because in examples it corresponds to boundary terms arising from integration by parts). By definition, $V \subset \mathrm{Ker}B$ (in fact, one can show that $V = \mathrm{Ker}B$, but we don't need this fact). It is easy to see that closed symmetric extensions of A correspond to isotropic closed subspaces $V \subset L \subset V^\vee$ with respect to the form B; namely, the extension of A to L is defined to be the restriction of $A^\dagger|_L$. Moreover, the adjoint operator to such an extension $(A^\dagger, L)$ is $(A^\dagger, L^\perp)$, where $L^\perp$ is the orthogonal complement of L in $V^\vee$ with respect to B.

8.2.4. *Self-adjoint operators.* Let us say that a closed symmetric operator (A, V) is *self-adjoint* if $V^\vee = V$, i.e., $A^\dagger = A$. We see that *self-adjoint extensions* of A correspond to *Lagrangian* subspaces L, i.e., those for which $L = L^\perp$. Note that such extensions/subspaces may or may not exist: the necessary and sufficient condition for existence of self-adjoint extensions (or Lagrangian subspaces) is that the signature (n_+, n_-) of the Hermitian form iB satisfies the equation $n_+ = n_-$ (i.e., the so-called *deficiency indices* $n_\pm \in \mathbb{Z}_{\geq 0} \cup \infty$ of A are equal). However, in quantum mechanical models they usually exist and correspond to various spatial boundary conditions.

We say that a symmetric operator (A, V) is *essentially self-adjoint* if the closure $(\overline{A}, \overline{V})$ is self-adjoint. Thus an essentially self-adjoint operator has a unique self-adjoint extension, so having such an operator is basically as good as having a self-adjoint one. This notion is convenient, for instance, when we do not want to describe explicitly the space $\overline{V}$.

The importance of unbounded self-adjoint operators consists in the fact that von Neumann's spectral theorem extends naturally to them. Namely, define the *spectrum* $\sigma(A, V)$ of a self-adjoint operator (A, V) to be the subset of $\lambda \in \mathbb{C}$ for which the operator $A - \lambda : V \to \mathcal{H}$ fails to be surjective. Then we have

Theorem 8.5. *Theorem 8.4 except for the statement that h is essentially bounded holds for not necessarily bounded self-adjoint operators. Moreover, the domain V of A in its spectral theorem realization is the space of $g \in L^2(X, \mu)$ such that $hg \in L^2(X, \mu)$.*

If the measure μ is concentrated on a countable set (i.e., we may take $X = \mathbb{N}$ with $\mu(j) = 1$ for $j \in \mathbb{N}$) then $\mathcal{H}$ has a basis consisting of

eigenfunctions, and vice versa; in this case one says that the spectrum of A is *purely point spectrum*. This happens, for example, when A is compact (the Hilbert-Schmidt theorem). The other extreme is *purely continuous spectrum*, when there are no eigenvalues (i.e., in the spectral theorem realization, all points of X have zero measure). The spectral theorem implies that any self-adjoint operator can be uniquely written as an orthogonal direct sum of two self-adjoint operators with purely point and purely continuous spectrum, respectively.

The spectral theorem also implies the following corollary.

Corollary 8.6. *Let (A, V) be a self-adjoint operator. Then there exists a unique 1-parameter group of unitary operators $U(t) = e^{iAt} : \mathcal{H} \to \mathcal{H}$ strongly continuous in t which preserve V and commute with A, such that for all $v \in V$ the function $t \mapsto U(t)v$ is differentiable and*

$$\frac{d}{dt}(U(t)v) = iAU(t)v.$$

Proof. Using the spectral theorem realization where A is the operator of multiplication by $h : X \to \mathbb{R}$, we may define $U(t)$ as the operator of multiplication by e^{ith}. □

In fact, the converse also holds: every strongly continuous 1-parameter group $U(t)$ (i.e., a unitary representation of the Lie group $\mathbb{R}$ on $\mathcal{H}$) arises uniquely (up to isometry) from a self-adjoint operator.

Remark 8.7. The spectral theorem implies that if (A, V) is a self-adjoint operator and $Av = \lambda v$ for some nonzero $v \in V$ then $\lambda \in \mathbb{R}$. On the contrary, if (A, V) is only symmetric and not self-adjoint, von Neumann showed that the set of eigenvalues of A on V is either the (open) upper-half plane $\mathbb{C}_+$ (if $n_+ > 0, n_- = 0$), or the lower half-plane $\mathbb{C}_-$, (if $n_- > 0, n_+ = 0$), or contains both (if $n_+, n_- > 0$).

8.2.5. *Examples.*

Example 8.8. Consider the symmetric operator $P := -i\frac{d}{dx}$ on $\mathcal{H} = L^2(S)$, where $S := \mathbb{R}/2\pi\mathbb{Z}$ (the momentum operator on the circle). This operator is symmetric on the space $V := C^\infty(S)$, and one can show that it is moreover essentially self-adjoint on this space (check it!). The corresponding space $\overline{V}$ is the *Sobolev space* $H^1(S)$ of functions $f \in L^2(S)$ with $f' \in L^2(S)$ in the sense of distributions (note that such functions are continuous). The spectrum of the corresponding self-adjoint operator is purely point and equals $\mathbb{Z}$, with eigenfunctions e^{inx}, i.e., $Pe^{inx} = ne^{inx}$. Thus the spectral realization of A is on $\ell_2(\mathbb{Z})$ with counting measure on which P acts by multiplication by the function n

(i.e., this realization reduces simply to the Fourier expansion of functions on S). Similarly, the energy operator $P^2 = -\frac{d^2}{dx^2}$ is essentially self-adjoint on the same space but with smaller domain of the closure - the Sobolev space $H^2(S)$ of functions $f \in L^2(S)$ such that $f'' \in L^2(S)$. Its spectrum in $\mathbb{Z}_{\geq 0}$ with the same eigenfunctions: $P^2 e^{inx} = n^2 e^{inx}$.

Example 8.9. The next example is more interesting, and prototypical for the theory of self-adjoint extensions. Namely consider the same momentum operator $P := -i\frac{d}{dx}$, but now acting on the dense subspace $V \subset L^2[0, 2\pi]$ of smooth functions with vanishing derivatives of all orders on both ends of the interval. In this case, P is **not** essentially self-adjoint: the space $\overline{V}$ is the space of functions $f \in H^1[0, 2\pi]$ with $f(0) = f(2\pi) = 0$, while $V^\vee = H^1[0, 2\pi]$ with

$$B(f, g) = i(\overline{f(2\pi)}g(2\pi) - \overline{f(0)}g(0)).$$

So on the quotient $V^\vee/\overline{V} = \mathbb{C}^2$ we have

$$B((a, b), (a, b)) = i(|b|^2 - |a|^2),$$

where $a = f(0)$, $b = f(2\pi)$. Thus a Lagrangian subspace of $V^\vee$ is given by points $b \in \mathbb{C}$ with $|b| = 1$; namely, it is the space L_b of functions $f \in H^1[0, 2\pi]$ with $f(2\pi) = bf(0)$. The spectrum of the corresponding self-adjoint operator is again purely point, so we should look for eigenfunctions in the space L_b. Thus we get eigenfunctions $e^{i(n+s)x}$ where $b = e^{2\pi i s}$. So the set of eigenvalues is $\mathbb{Z} + s$, and we see that the spectrum depends on the choice of the self-adjoint extension.

Observe also that any complex number λ is the eigenvalue of the symmetric (non-self-adjoint!) operator $P^\dagger$ on $V^\vee$, with eigenvector $e^{i\lambda x}$.

Example 8.10. Now consider the same momentum operator $P := -i\frac{d}{dx}$ but acting on the space $V = C_0^\infty(\mathbb{R})$ of compactly supported smooth functions, a subspace of $\mathcal{H} = L^2(\mathbb{R})$. In this case P is essentially self-adjoint, with $\overline{V} = V^\vee$ being the subspace of $H^1(\mathbb{R})$ of $f \in L^2(\mathbb{R})$ such that $f' \in L^2(\mathbb{R})$. The spectral theorem realization of P is on $L^2(\mathbb{R})$ as the operator of multiplication by x, which is given by the Fourier transform. Thus the spectrum of this operator is purely continuous and constitutes the whole real line $\mathbb{R}$. Similarly, the operator $P^2 = -\frac{d^2}{dx^2}$ is also essentially self-adjoint on V, and its self-adjoint extension has purely continuous spectrum $\mathbb{R}_{\geq 0}$.

Example 8.11. And yet again, take $P := -i\frac{d}{dx}$, but now on the subspace V of $\mathcal{H} = L^2(\mathbb{R}_{\geq 0})$ of compactly supported smooth functions with vanishing derivatives at 0. This operator is not essentially self-adjoint: the space $\overline{V}$ is the space of $f \in H^1(\mathbb{R}_{\geq 0})$ with $f(0) = 0$, while

$V^\vee$ is the whole $H^1(\mathbb{R}_{\geq 0})$. Thus the space $V^\vee/\overline{V}$ is 1-dimensional with form B given by $B(f,g) = -i\overline{f(0)}g(0)$, and so there are no self-adjoint extensions (the deficiency indices are not equal: $n_+ = 1, n_- = 0$).

Let us find the eigenvalues of P on V. The eigenvector with eigenvalue λ is $e^{i\lambda x}$, and it belongs to V iff $\lambda \in \mathbb{C}_+$. Thus the set of eigenvalues of P is $\mathbb{C}_+$.

Example 8.12. Let $A = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$ with $V = C_0^\infty(\mathbb{R})$ (quantum harmonic oscillator). Then A is essentially self-adjoint and $\overline{A}$ has pure point spectrum $n + \frac{1}{2}$, $n \in \mathbb{N}$, with eigenvectors $H_n(x)e^{\frac{x^2}{2}}$, where H_n are Hermite polynomials (Theorem 4.13).

Remark 8.13. More generally, it is known that if $U(x)$ is a piecewise continuous potential on $\mathbb{R}$ which tends to $+\infty$ at $\pm\infty$ then the operator $A := -\frac{1}{2}\frac{d^2}{dx^2} + U(x)$ is essentially self-adjoint on $V = C_0^\infty(\mathbb{R})$ and has pure point spectrum, with eigenvalues $E_0 < E_1 \leq E_2 \leq ...$ (it is shown in Lemma 8.19 below that E_0 is always a simple eigenvalue and the corresponding eigenvector is a positive function).

Example 8.14. Let M be a compact Riemannian manifold with boundary ∂M, $\mathcal{H} = L^2(M)$, and $A = \Delta$ be the Laplace operator on M acting on the space V of smooth functions on M vanishing with all derivatives on the boundary. In this case $\overline{V}$ is the space of functions in the Sobolev space $H^2(M)$ (functions $f \in L^2(M)$ such that $\Delta f \in L^2(M)$) which vanish with first normal derivative on ∂M, and $V^\vee = H^2(M)$. By Stokes' formula

$$\int_M (u\Delta v - v\Delta u)dx = \int_{\partial M} (u\partial_{\mathbf{n}} v - v\partial_{\mathbf{n}} u)d\sigma,$$

where $\mathbf{n}$ denotes the normal derivative to ∂M, so we have

$$B(f,g) = i\int_{\partial M} (\overline{f}\partial_{\mathbf{n}} g - g\partial_{\mathbf{n}}\overline{f})d\sigma.$$

So if $\partial M = 0$, the operator A is essentially self-adjoint and has a unique self-adjoint extension, while if $\partial M \neq 0$, it is not and there are many self-adjoint extensions corresponding to various boundary conditions on ∂M. The most common ones are the Dirichlet boundary condition $f = 0$ and Neumann boundary condition $\partial_{\mathbf{n}} f = 0$. Of course, the spectra associated to these conditions (which are always purely point) are completely different.

The simplest example with non-trivial boundary is $M = [0, \pi]$, in which case we have $\dim V^\vee/\overline{V} = 4$ and

$$B(f,g) = i(\overline{f}g' - \overline{f'}g)|_0^\pi.$$

For the Dirichlet boundary conditions $f(0) = f(\pi) = 0$ we get eigenbasis $\sin nx$ with eigenvalues $-n^2$, $n \in \mathbb{Z}_{\geq 1}$, while for the Neumann boundary conditions $f'(0) = f'(\pi) = 0$ we get eigenbasis $\cos nx$ also with eigenvalues $-n^2$ but now for $n \in \mathbb{Z}_{\geq 0}$.

Let us consider the mixed boundary condition:

$$f(0) = 0,\ f'(\pi) - af(\pi) = 0$$

for some real number a. Then the eigenfunctions are $\sin \lambda x$ where

$$\lambda \cos \pi\lambda = a \sin \pi\lambda.$$

Thus the eigenvalues are $-\lambda^2$ where λ runs over solutions of the equation

$$\lambda \operatorname{cotan} \pi\lambda = a.$$

For example, in the limit $a \to \infty$ we recover the answer for the Dirichlet boundary condition.

Exercise 8.15. *Let $H = -\frac{1}{2}\frac{d^2}{dx^2} + a\chi_{[-1,1]}(x)$ where χ is the indicator function and $a \in \mathbb{R}$, and let it be defined on $V = C_0^\infty(\mathbb{R}) \subset \mathcal{H} = L^2(\mathbb{R})$. Show that H is essentially self-adjoint and find the spectrum and eigenvalues of its self-adjoint extension (consider separately the cases $a \geq 0$ and $a < 0$).*

Hint. *As explained above, the spectrum consists of $E \in \mathbb{R}$ for which $H - E : \overline{V} \to \mathcal{H}$ is not surjective. So try to solve the equation*

$$(H - E)u = f$$

for $f \in \mathcal{H}$ as

$$f(x) = \int_{\mathbb{R}} G(x, y)dy,$$

where $G(x, y)$ is the fundamental solution of the equation

$$(H - E)f = \delta(x - y).$$

You should get that there are no eigenfunctions for $a \geq 0$ (purely continuous spectrum), while for $a < 0$ the spectrum is mixed: there is continuous spectrum and also some eigenfunctions with negative eigenvalues; they are called **bound states**.

8.3. **Hamiltonians in quantum mechanics.** The yoga of quantization says that to quantize classical mechanics on a manifold X, we need to replace the classical space of states T^*X by the quantum space of states – the Hilbert space $\mathcal{H} = L^2(X)$ on square integrable complex half-densities on X (or, more precisely, the corresponding projective space). Further, we need to replace classical observables, i.e. (sufficiently nice) real functions $f \in C^\infty(T^*X)$, by quantum observables

$\widehat{f}$, which are (unbounded, densely defined) operators on $\mathcal{H}$, not commuting with each other in general. Then the (expected) value of an observable A in a state $\psi \in \mathcal{H}$ of unit norm is, by definition, $\langle \psi, A\psi \rangle$ (provided that it is well defined).

The operators $\widehat{f}$ should linearly depend on f. Moreover, they should depend on a positive real parameter $\hbar$ called the *Planck constant*, and satisfy the following relation:

$$[\widehat{f}, \widehat{g}] = i\hbar\widehat{\{f, g\}} + O(\hbar^2),\ \hbar \to 0.$$

Since the role of Poisson brackets of functions is played in quantum mechanics by commutators of operators, this relation expresses the condition that classical mechanics should be the limit of quantum mechanics as $\hbar \to 0$.[13]

We must immediately disappoint the reader by confessing that there is no canonical choice of the quantization map $f \mapsto \widehat{f}$. Nevertheless, there are some standard choices of $\widehat{f}$ for particular f, which we will now discuss.

Let us restrict ourselves to the situation $X = \mathbb{R}$, so on the phase space we have coordinates q (position) and p (momentum). In this case we can naturally think of half-densities as functions and there are the following standard conventions.

1. $\widehat{f} = f(q)$ (multiplication operator by $f(q)$) when f is independent of p.

2. $\widehat{p^m} \to (-i\hbar\frac{d}{dq})^m$.

(Note that these conventions satisfy our condition, since $[\widehat{q}, \widehat{p}] = i\hbar$, while $\{q, p\} = 1$.)

Example 8.16. For the classical Hamiltonian $H = \frac{p^2}{2} + U(q)$ considered above, the quantization will be the *Schrödinger operator*

$$\widehat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + U(q).$$

Remark 8.17. The extension of these conventions to other functions is not unique. However, such an extension will not be used, so we will not specify it.

Now let us see what the quantum analog of Hamilton's equations should be. In accordance with the outlined quantization yoga, Poisson brackets should be replaced in quantum theory by commutators

[13]Note that the assignment $f \mapsto \widehat{f}$ cannot possibly satisfy the identity $\widehat{fg} = \widehat{f}\widehat{g}$ since the product of functions is commutative but the product of operators is not.

(with coefficient $(i\hbar)^{-1} = -i/\hbar$). Thus, Hamilton's equations should be replaced by the equation

$$\frac{d}{dt}\langle\psi(t), A\psi(t)\rangle = \langle\psi(t), \tfrac{[A,\widehat{H}]}{i\hbar}\psi(t)\rangle = -\tfrac{i}{\hbar}\langle\psi(t), [A,\widehat{H}]\psi(t)\rangle,$$

where $\langle,\rangle$ is the Hermitian form on $\mathcal{H}$ and $\widehat{H}$ is some quantization of the classical Hamiltonian H. Since this equation must hold for any A, it is equivalent to the *Schrödinger equation*

$$\dot{\psi} = -\frac{i}{\hbar}\widehat{H}\psi$$

up to changing ψ by a time-dependent phase factor (check it!). Thus, the quantum analog of the Hamilton equations is the Schrödinger equation.

Remark 8.18. This "derivation" of the Schrödinger equation is definitely not a mathematical argument. It is merely a reasoning aimed to motivate a definition.

To solve the initial value problem for the Schrödinger equation, we need to make sense of the Hamiltonian $\widehat{H}$ as an unbounded self-adjoint operator on $\mathcal{H}$ in the sense of von Neumann, which in practice boils down to giving spatial boundary conditions for ψ, in addition to the initial value. The general solution of the Schrödinger equation then has the form

$$\psi(t) = e^{-\frac{it\widehat{H}}{\hbar}}\psi(0),$$

where $e^{-\frac{it\widehat{H}}{\hbar}}$ is the 1-parameter group of unitary operators attached to the self-adjoint operator $\widehat{H}$, which exists thanks to von Neumann's spectral theorem. Therefore, for any quantum observable A it is reasonable to define a new observable

$$A(t) := e^{\frac{it\widehat{H}}{\hbar}}A(0)e^{-\frac{it\widehat{H}}{\hbar}}$$

(such that to observe $A(t)$ is the same as to evolve for time t and then observe $A = A(0)$). The observable $A(t)$ satisfies the equation

$$A'(t) = -\frac{i}{\hbar}[A(t), \widehat{H}]$$

called the *operator Schrödinger equation*, and we have

$$\langle\psi(t), A\psi(t)\rangle = \langle\psi(0), A(t)\psi(0)\rangle.$$

The two sides of this equation represent two pictures of quantum mechanics: Schrödinger's (states change in time, observables don't) and Heisenberg's (observables change in time, states don't). The equation expresses the equivalence of the two pictures.

8.4. **Feynman-Kac formula.** Let us consider a 1-dimensional particle with potential $U(q)$. Let us assume that $U \geq 0$ and $U(q) \to \infty$ as $|q| \to \infty$. In this case, the operator $\widehat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + U(q)$ is essentially self-adjoint on Schwartz functions, positive definite, and its spectrum is purely point.

Lemma 8.19. *There is a unique eigenvector Ω of $\widehat{H}$ with smallest eigenvalue given by a positive function with norm 1.*

Proof. An eigenvector Ω of $\widehat{H}$ with smallest eigenvalue λ minimizes the "energy" functional

$$E(\phi) := \langle \phi, \widehat{H}\phi \rangle = \int_{\mathbb{R}} (\tfrac{\hbar^2}{2}\phi'(q)^2 + U(q)\phi(q)^2)dq$$

on the space of real C^1-functions $\phi : \mathbb{R} \to \mathbb{R}$ with $\int_{\mathbb{R}} \phi(t)^2 dt = 1$. Suppose that $\Omega(a) = 0$, then the equation $\widehat{H}\Omega = \lambda\Omega$ implies $\Omega'(a) \neq 0$. But $E(\Omega) = E(|\Omega|)$, so, since $\Omega'(a) \neq 0$, this value can be reduced by smoothing out Ω in a small neighborhood of a and then normalizing it to have unit norm, a contradiction. This also implies that λ is a simple eigenvalue, hence Ω is unique. □

Remark 8.20. The vector Ω is called the *ground state*, or *vacuum state*, since it has lowest energy, and physicists often shift the Hamiltonian by a constant so that the energy of this state is zero (i.e. "there is no matter").

The correlation functions in the Hamiltonian setting are defined by the formula

$$\mathcal{G}_n^{\mathrm{Ham}}(t_1, ..., t_n) := \langle \Omega, q(t_1)...q(t_n)\Omega \rangle$$

where $q(t)$ is the operator quantizing the observable "coordinate of the particle at the time t".

Remark 8.21. Physicists usually write the inner product $\langle v, Aw \rangle$ as $\langle v|A|w\rangle$. In particular, Ω is written as $\langle 0|$ or $|0\rangle$ (the so-called Dirac *bra-ket notation*).

Theorem 8.22. *(Feynman-Kac formula) If $t_1 \geq ... \geq t_n$ then the function $\mathcal{G}_n^{\mathrm{Ham}}$ admits an asymptotic expansion in $\hbar$ (near $\hbar = 0$), which coincides with the path integral correlation function $\mathcal{G}_n^M$ constructed above. Equivalently, the Wick rotated function $\mathcal{G}_n^{\mathrm{Ham}}(-it_1, ..., -it_n)$ equals $\mathcal{G}_n^E(t_1, ..., t_n)$.*

This theorem plays a central role in quantum mechanics, and we will prove it below. Before we do so, let us formulate an analog of this theorem for "quantum mechanics on the circle".

Let $\mathcal{G}_{n,L}(t_1,...,t_n)$ denote the correlation function on the circle of length L (for $0 \leq t_n \leq ... \leq t_1 \leq L$), and let Z_L be the partition function on the circle of length L, defined from (Euclidean) path integrals. Also, let

$$Z_L^{\mathrm{Ham}} = \mathrm{Tr}(e^{-\frac{L\widehat{H}}{\hbar}}),$$

and

$$\mathcal{G}_{n,L}^{\mathrm{Ham}}(-it_1,...,-it_n) = \frac{\mathrm{Tr}(q(-it_n)...q(-it_1)e^{-\frac{L\widehat{H}}{\hbar}})}{\mathrm{Tr}(e^{-\frac{L\widehat{H}}{\hbar}})}.$$

Theorem 8.23. *(Feynman-Kac formula on the circle) The functions Z_L^{Ham}, $\mathcal{G}_{n,L}^{\mathrm{Ham}}$ admit asymptotic expansions in $\hbar$, which coincide with the functions Z_L and $\mathcal{G}_{n,L}$ computed from path integrals.*

Note that Theorem 8.22 is obtained from Theorem 8.23 by sending L to infinity. Thus, it is sufficient to prove Theorem 8.23.

Remark 8.24. As we mentioned before, the function $\mathcal{G}_n^E$ can be defined by means of the Wiener integral, and the equality

$$\mathcal{G}_n^{\mathrm{Ham}}(-it_1,...,-it_n) = \mathcal{G}_n^E(t_1,...,t_n)$$

actually holds for numerical values of $\hbar$, and not just in the sense of power series expansions. The same applies to the equalities $Z_L^{\mathrm{Ham}} = Z_L$, $\mathcal{G}_{n,L}^{\mathrm{Ham}} = \mathcal{G}_{n,L}$. However, these results are technically more complicated (as they require non-trivial analytic input) and thus are beyond the scope of these notes.

Example 8.25. Consider the case of the quadratic potential. By renormalizing variables, we can assume that $\hbar = m = 1$, so $U = \frac{q^2}{2}$. In this case we know that $Z_L = \frac{1}{2\sinh(\frac{L}{2})}$. On the other hand, $\widehat{H}$ is the Hamiltonian of the quantum harmonic oscillator:

$$\widehat{H} = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{q^2}{2}.$$

The eigenvectors of this operator are $H_n(x)e^{-\frac{x^2}{2}}$, where H_n are the Hermite polynomials ($k \geq 0$), and the eigenvalues are $n + \frac{1}{2}$ (see Theorem 4.13). Hence,

$$Z_L^{\mathrm{Ham}} = e^{-\frac{L}{2}} + e^{-\frac{3L}{2}} + ... = \frac{1}{e^{\frac{L}{2}} - e^{-\frac{L}{2}}} = Z_L,$$

as expected from the Feynman-Kac formula. (This shows the benefit of the choice $C = \frac{1}{2}$ in the normalization of Z_L).

8.5. **Proof of the Feynman-Kac formula in the free case (harmonic oscillator).** Consider again the quadratic Hamiltonian $\widehat{H} = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{q^2}{2}$ of the quantum Harmonic oscillator. Note that it can be written in the form

$$\widehat{H} = a^\dagger a + \tfrac{1}{2},$$

where $a = \frac{1}{\sqrt{2}}(\frac{d}{dq} + q)$, $a^\dagger = \frac{1}{\sqrt{2}}(-\frac{d}{dq} + q)$. The operators $a, a^\dagger$ define a representation of the Heisenberg Lie algebra on (a dense subspace of) the Hilbert space $\mathcal{H}$:

$$[a, a^\dagger] = 1.$$

Thus the eigenvectors of $\widehat{H}$ are $(a^\dagger)^n\Omega$ where $\Omega = e^{-\frac{q^2}{2}}$ is the lowest eigenvector and the corresponding eigenvalues are $n + \frac{1}{2}$, $n \in \mathbb{Z}_{\geq 0}$ (as we already saw before in Theorem 4.13).

Remark 8.26. The operators a and $a^\dagger$ are called the *annihilation and creation operators*, since $a\Omega = 0$, while all eigenvectors of $\widehat{H}$ can be "created" from Ω by action of powers of $a^\dagger$.

Now, we have

$$q(0) = q = \frac{1}{\sqrt{2}}(a + a^\dagger).$$

Since $[a^\dagger a, a] = -a$, $[a^\dagger a, a^\dagger] = a^\dagger$, we have

$$q(t) = \frac{1}{\sqrt{2}}e^{ita^\dagger a}(a + a^\dagger)e^{-ita^\dagger a} = \frac{1}{\sqrt{2}}(e^{-it}a + e^{it}a^\dagger)$$

This shows that

$$\mathcal{G}^{\mathrm{Ham}}_{n,L}(-it_1, ..., -it_n) = 2^{-\frac{n}{2}}\frac{\mathrm{Tr}(\prod_{j=1}^n (e^{t_j}a^\dagger + e^{-t_j}a)e^{-L(a^\dagger a + \frac{1}{2})})}{\mathrm{Tr}(e^{-L(a^\dagger a+\frac{1}{2})})}.$$

Now we can easily prove Theorem 8.23. Indeed, let us move the terms $e^{t_1}a^\dagger$ and $e^{-t_1}a$ around the trace (using the cyclic property of the trace). This will yield, after a short calculation, using (7.3) :

$$\mathcal{G}^{\mathrm{Ham}}_{n,L}(-it_1, ..., -it_n) =$$

$$\sum_{j=2}^n \tfrac{1}{2}\mathcal{G}^{\mathrm{Ham}}_{n-2,L}(-it_2, ..., -it_{j-1}, -it_{j+1}, ..., -it_n)\left(\frac{e^{t_1-t_j}}{e^L - 1} - \frac{e^{t_j-t_1}}{e^{-L}-1}\right) =$$

$$\sum_{j=2}^n \mathcal{G}^{\mathrm{Ham}}_{n-2,L}(-it_2, ..., -it_{j-1}, -it_{j+1}, ..., -it_n)G_L(t_1 - t_j).$$

This implies the theorem by induction in n.

Remark 8.27. 1. In the quadratic case there is no formal expansions and the Feynman-Kac formula holds as an equality between usual functions.

2. Note that the equality $\frac{e^{t-s}}{e^L-1} - \frac{e^{s-t}}{e^{-L}-1} = G_L(t-s)$ used above holds only if $t \geq s$. In fact, the matrix coefficient $\langle \Omega, q(t_1)...q(t_n)\Omega \rangle$ is not symmetric in t_j, as the operators $q(t_j)$ do not commute. Thus the Feynman-Kac formula only holds if $t_1 \geq ... \geq t_n$. For this reason the correlation function $\mathcal{G}_n^M$ is called time-ordered - it corresponds to the matrix coefficient where the operators $q(t_j)$ are ordered chronologically.

8.6. **Proof of the Feynman-Kac formula (general case).** Now we consider an arbitrary potential $U(q) := \frac{m^2q^2}{2} - V(q)$, where

$$V(q) = \sum_{k \geq 3} \frac{g_k q^k}{k!}.$$

For simplicity we will assume that the coefficients g_j are formal parameters and $\hbar = 1$ (the latter condition does not cause a loss of generality, as this situation can be achieved by rescaling). Let us first consider the case of partition function. We have

$$Z_L^{\mathrm{Ham}} = \mathrm{Tr}(e^{-L\widehat{H}}) = \mathrm{Tr}(e^{-L(\widehat{H}_0 - V)}),$$

where $\widehat{H}_0 = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{1}{2}m^2q^2$ is the free (=quadratic) part of the Hamiltonian. Since g_j are formal parameters, we have a series expansion

(8.2)
$$e^{-L(\widehat{H}_0 - V)} = e^{-L\widehat{H}_0} + \sum_{N \geq 1} \int_{L \geq s_1 \geq ... \geq s_N \geq 0} e^{-(L-s_1)\widehat{H}_0} V e^{-(s_1-s_2)\widehat{H}_0} V ... e^{-(s_{n-1}-s_n)\widehat{H}_0} V e^{-s_n \widehat{H}_0} d\mathbf{s}$$

This follows from the general fact that in the (completed) free algebra with generators A, B, one has

(8.3)
$$e^{A+B} = e^A + \sum_{N \geq 1} \int_{1 \geq s_1 \geq ... \geq s_N \geq 0} e^{(1-s_1)A} B e^{(s_1-s_2)A} B ... e^{(s_{N-1}-s_N)A} B e^{s_N A} d\mathbf{s}$$

(check this identity!).

Equation (8.2) shows that

$$Z_L^{\mathrm{Ham}} =$$

$$\sum_{N \geq 0} \sum_{j_1,...,j_N=3}^{\infty} \frac{g_{j_1}...g_{j_N}}{j_1!...j_N!} \int_{1 \geq s_1 \geq ... \geq s_N \geq 0} \mathrm{Tr}(q_0(-is_1)^{j_1}...q_0(-is_N)^{j_N} e^{-L\widehat{H}_0}) d\mathbf{s},$$

where $q_0(t)$ is the operator $q(t)$ in the free theory associated to the potential $\frac{m^2q^2}{2}$.

Since the Feynman-Kac formula for the free theory has already been proved, we know that the trace on the right hand side can be evaluated as a sum over matchings. To see what exactly is obtained, let us collect the terms corresponding to all permutations of $j_1, ..., j_N$ together. This means that the summation variables will be the numbers $i_3, i_4, ..$ of occurences of $3, 4, ..$ among $j_1, ..., j_N$. Further, to every factor $q_0(-is)^j$ will be assigned a j-valent vertex, with a variable s attached to it, and it is easy to see that Z_L^{Ham} equals the sum over all ways of connecting the vertices (i.e. Feynman diagrams Γ) of integrals

$$\int_{0\leq s_1,...,s_N\leq L} \prod_{v-w} G_L(s_v - s_w) d\mathbf{s},$$

multiplied by the coefficients $\frac{\prod_k g_k^{i_k}}{|\mathrm{Aut}\Gamma|}$. Thus, $Z_L^{\mathrm{Ham}} = Z_L$, as desired.

Now let us consider correlation functions. Thus we have to compute

$$\mathrm{Tr}(e^{-(L-t_1)\widehat{H}} q e^{-(t_1-t_2)\widehat{H}} q ... q e^{-t_n \widehat{H}}).$$

Explanding each exponential inside the trace as above, we will clearly get the same Feynman diagram sum, except that the Feynman diagrams will contain n external vertices marked by variables $t_1, ..., t_n$. This implies that $\mathcal{G}_{n,L}^{\mathrm{Ham}} = \mathcal{G}_{n,L}$, and we are done.

8.7. **The massless case.** Consider now the massless case, $m = 0$, in the Hamiltonian setting. For maps $q : \mathbb{R} \to \mathbb{R}$, we have $\mathcal{H} = L^2(\mathbb{R})$, and $\widehat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2}$. This operator has continuous spectrum, and there is no lowest eigenvector Ω (more precisely, there is a lowest eigenvector $\Omega = 1$, but it is not in L^2), which means that we cannot define the correlation functions in the usual way, i.e. as $\langle \Omega, q(t_1)...q(t_n)\Omega \rangle$. (This is the reflection, in the Hamiltonian setting, of the difficulties related to the growth of the Green's function at infinity, i.e., infrared divergences, which we encountered in the Lagrangian setting).

Consider now the case $q : \mathbb{R} \to S^1 = \mathbb{R}/2\pi r\mathbb{Z}$. In this case, we have the same Hamiltonian but acting in the space $\mathcal{H} := L^2(S^1)$. The eigenvectors of this operator are $e^{\frac{iNq}{r}}$, with eigenvalues $\hbar^2 \frac{N^2}{2r^2}$. In particular, the lowest eigenvector is $\Omega = 1$. Thus the Hamiltonian correlation functions (in the Euclidean setting, for $t_1 \geq ... \geq t_n$) are

$$\langle\, \Omega, e^{\frac{t_1\widehat{H}}{\hbar}} e^{\frac{ip_1 q}{r}} e^{\frac{(t_2-t_1)\widehat{H}}{\hbar}} ... e^{\frac{ip_n q}{r}} e^{-\frac{t_n\widehat{H}}{\hbar}} \Omega \,\rangle =$$

$$e^{\frac{\hbar}{2r^2}\sum_j (t_j - t_{j+1})(p_1+...+p_j)^2},$$

which is equal to the correlation function in the Lagrangian setting. Thus the Feynman-Kac formula holds.

Now we pass to the case of circle-valued quantum mechanics on the circle. In this case, we have

$$\mathrm{Tr}(e^{-\frac{L\widehat{H}}{\hbar}}) = \sum_{N\in\mathbb{Z}} e^{-\frac{N^2 L\hbar}{2r^2}}$$

and

$$\mathrm{Tr}(e^{\frac{t_1\widehat{H}}{\hbar}} e^{\frac{ip_1 q}{r}} e^{\frac{(t_2-t_1)\widehat{H}}{\hbar}} ... e^{\frac{ip_n q}{r}} e^{\frac{(L-t_n)\widehat{H}}{\hbar}}) = \sum_{N\in\mathbb{Z}} e^{\frac{\hbar}{2r^2}\sum_{j=0}^{n}(t_j-t_{j+1})(N-p_1-...-p_j)^2},$$

where $t_{n+1} := L$, $t_0 := 0$. Simplifying this expression, we obtain

$$e^{\frac{\hbar}{2r^2}\sum_j (t_j-t_{j+1})(p_1+...+p_j)^2} \sum_{N\in\mathbb{Z}} e^{-\frac{\hbar}{2r^2}(LN^2+2N\sum_j p_j t_j)} =$$

$$e^{\frac{\hbar}{2r^2}\sum_j (t_j-t_{j+1})(p_1+...+p_j)^2} \theta(\frac{\hbar}{2\pi i r^2}\sum_j p_j t_j, \frac{L\hbar}{2\pi r^2}).$$

Comparing with (7.7), we see that the Feynman-Kac formula reduces to the modular invariance of the theta-function:

$$\theta(\frac{u}{iT}, \frac{1}{T}) = \sqrt{T} e^{\frac{\pi u^2}{T}} \theta(u, T)$$

with $T = \frac{2\pi r^2}{\hbar L}$ (which follows from the Poisson summation formula applied to the Gaussian).

Note that the Feynman-Kac formula in this example would have been false if in the Lagrangian setting we had ignored the topologically nontrivial maps. Thus we may say that the Feynman-Kac formula "sees topology". This ability of the Feynman-Kac formula to "see topology" (in much more complex situations) lies at the foundation of many interrelations between geometry and quantum field theory.

Remark 8.28. It should be noted that the contributions of topologically nontrivial maps from the source circle to the target circle are, strictly speaking, beyond our usual setting of perturbation theory, since they are exponentially small in $\hbar$. To be specific, the contribution from maps of degree N mostly comes from those maps which are close to the minimal action map $q_N(t) = \frac{2\pi t N r}{L}$, so it is of the order $e^{-\frac{2\pi^2 N^2 r^2}{L\hbar}}$. The maps $q_N(t)$ are the simplest examples of "instantons" – nonconstant solutions of the classical equations of motion, which have finite action (and are nontrivial in the topological sense). Exponentially small contributions to the path integral coming from integration over neighborhoods of instantons are called "instanton corrections to the perturbation series".

Remark 8.29. This calculation allows us to give sense to the partition function $Z(L)$ of the line-valued massless quantum mechanics on the circle. To this end, we just need to look at the asymptotics $r \to \infty$ of the partition function

$$Z(r, L) = \theta(0, \tfrac{\hbar L}{2\pi r^2}) = r\sqrt{\tfrac{2\pi}{\hbar L}}\theta(0, \tfrac{2\pi r^2}{\hbar L}).$$

Since $\theta(0, T) \to 1$ as $T \to \infty$, for the leading coefficient of the asymptotics we have (up to numerical scaling, which we are free to choose):

$$Z(L) \sim \frac{1}{\sqrt{\hbar L}}.$$

Note however that in this case we cannot write $Z(L) = \mathrm{Tr}(e^{-\frac{L\widehat{H}}{\hbar}})$ since this operator is not trace class. Also the vector $\Omega = 1$ is not normalizable. Thus this theory is somewhat ill-defined, as already mentioned above.

8.8. **Spectrum of the Schrödinger operator for a piecewise constant periodic potential.** In this subsection we demonstrate the behavior of the spectrum of a 1-dimensional Schrödinger operator on the example of a piecewise constant periodic potential, when the eigenvalues and eigenfunctions can be computed fairly explicitly.

We consider the Schrödinger operator on the circle $\mathbb{R}/2\pi\mathbb{Z}$ given by $H := -\frac{\hbar^2}{2}\partial^2 + U(x)$, where U is a piecewise continuous 2π-periodic potential. Clearly, without loss of generality we may assume that $\int_0^{2\pi} U(x)dx = 0$, otherwise we can shift $U(x)$ by a constant. By a standard result in analysis (the theory of Sturm-Liouville operators), the operator H has discrete spectrum, i.e., eigenvalues $E_0 < E_1 \leq E_2 \leq ...$ going to $+\infty$ with the corresponding eigenfunctions $\Psi_0, \Psi_1, \Psi_2, ...$ For example, if $U = 0$ then $E_0 = 0$ and $E_{2m-1} = E_{2m} = \frac{\hbar^2 m^2}{2}$ for $m > 0$, with eigenfunctions $\Psi_0 = 1, \Psi_{2m-1} = \sin mx, \Psi_{2m} = \cos mx$.

Consider now the simplest non-trivial example – the piecewise constant potential

$$U(x) = \begin{cases} Mb, \ 0 \leq x < a \\ -Ma, a \leq x < 2\pi \end{cases} \tag{8.4}$$

where $a, b, M > 0$, $a + b = 2\pi$.

For every $p \in \mathbb{R}$, we have a basis f_p, g_p of solutions of the equation $H\Psi = E\Psi$ on $[p, \infty]$ such that $f_p(p) = g_p'(p) = 1, g_p(p) = f_p'(p) = 0$.

For example,

$$f_0(x) = \cos\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}x,\ g_0(x) = \frac{\sin\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}x}{\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}}$$

for $0 \le x < a$ and

$$f_a(x) = \cos\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}(x-a),\ g_a(x) = \frac{\sin\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}(x-a)}{\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}(x-a)}$$

for $a \le x < 2\pi$. Thus the monodromy matrices along the intervals $[0,a]$, $[a,2\pi]$ in these bases are

$$A := \begin{pmatrix} \cos\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a & \frac{\sin\sqrt{\frac{2}{\hbar^2}(E-Mb)}a}{\sqrt{\frac{2}{\hbar^2}(E-Mb)}} \\ -\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}\sin\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a & \cos\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a \end{pmatrix},$$

$$B := \begin{pmatrix} \cos\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b & \frac{\sin\sqrt{\frac{2}{\hbar^2}(E+Ma)}b}{\sqrt{\frac{2}{\hbar^2}(E+Ma)}} \\ -\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}\sin\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b & \cos\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b \end{pmatrix}.$$

The condition for a periodic solution is that the matrix AB (monodromy around the circle) has an eigenvalue 1. Since $\det A = \det B = 1$, in this case the second eigenvalue of AB is also 1 (generically this matrix is a unipotent Jordan block), so the condition is $\mathrm{Tr}(AB) = 2$, which gives

(8.5)
$$\cos\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a\cos\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b - \tfrac{E+M\frac{a-b}{2}}{\sqrt{(E-Mb)(E+Ma)}}\sin\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a\sin\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b = 1.$$

Thus the eigenvalues of H are the solutions E of (8.5).

If $a < E < b$ then $\sqrt{\frac{2}{\hbar^2}(E-Mb)}$ is imaginary, so (8.5) can be written in terms of real parameters as

(8.6)
$$\cosh\sqrt{\tfrac{2}{\hbar^2}(Mb-E)}a\cos\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b - \tfrac{E+M\frac{a-b}{2}}{\sqrt{(Mb-E)(E+Ma)}}\sinh\sqrt{\tfrac{2}{\hbar^2}(Mb-E)}a\sin\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b = 1.$$

As mentioned above, if $M = 0$, then for each $n \ge 1$ the operator H double eigenvalue $\frac{1}{2}\hbar^2 n^2$. We would like to see what happens to this eigenvalue for large n as we turn on M and keep the product $\hbar n$ in a bounded interval $[C^{-1}, C]$ (so $\hbar \to 0$).

Let us rewrite (8.5) in the form

$$1 - \cos\left(\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a + \sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b\right) =$$

$$\left(1-\frac{E+M\frac{a-b}{2}}{\sqrt{(E-Mb)(E+Ma)}}\right)\sin\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a\sin\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b$$

and look for solutions

$$E=\frac{1}{2}(\hbar^2n^2+\varepsilon),$$

where $|\varepsilon|\ll\frac{1}{n}$. We have

$$\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}=\sqrt{n^2+\tfrac{\varepsilon-2Mb}{\hbar^2}}=n\left(1+\tfrac{\varepsilon-2Mb}{2\hbar^2n^2}-\tfrac{(\varepsilon-2Mb)^2}{8\hbar^4n^4}...\right),$$

$$\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}=\sqrt{n^2+\tfrac{\varepsilon+2Ma}{\hbar^2}}=n\left(1+\tfrac{\varepsilon+2Ma}{2\hbar^2n^2}-\tfrac{(\varepsilon+2Ma)^2}{8\hbar^4n^4}...\right),$$

so

$$\sqrt{\tfrac{2}{\hbar^2}(E-Mb)}a+\sqrt{\tfrac{2}{\hbar^2}(E+Ma)}b=2\pi n\left(1+\tfrac{\varepsilon}{2\hbar^2n^2}-\tfrac{M^2ab}{2\hbar^4n^4}+...\right).$$

Thus the left hand side of the above equation has the form

$$LHS=\frac{\pi^2}{2}\left(\frac{\varepsilon}{\hbar^2n}-\frac{M^2ab}{2\hbar^4n^3}\right)^2+...$$

We also have

$$1-\frac{E+M\frac{a-b}{2}}{\sqrt{(E-Mb)(E+Ma)}}=-\frac{\pi^2M^2}{2\hbar^4n^4}+...$$

So we get

$$RHS=\frac{\pi^2M^2}{2\hbar^4n^4}\sin^2na+...$$

Thus we obtain

$$\frac{\varepsilon}{\hbar^2n}-\frac{M^2ab}{2\hbar^4n^3}=\pm\frac{M|\sin na|}{\hbar^2n^2},$$

which yields

$$\varepsilon=\frac{M^2ab}{2\hbar^2n^2}\pm\frac{M|\sin na|}{n},$$

We see that the double eigenvalue $\Lambda_n=\frac{\hbar^2n^2}{2}$, $n>0$ for $M=0$ bifurcates into two eigenvalues

(8.7)

$$\Lambda_n^{\pm}(M)=\Lambda_n+\frac{M^2a(2\pi-a)}{8\Lambda_n}\pm\frac{M|\sin na|}{2n}+o((M+\tfrac{1}{n})^2),\ M\to0,n\to\infty.$$

8.9. **WKB approximation and the Weyl law.** The goal of this subsection is to explain how to compute semiclassical asymptotics of eigenvalues and eigenfunctions of quantum hamiltonians. This method is called the **Wentzel-Kramers-Brillouin (WKB) approximation**, named after the authors of three separate papers which introduced it independently in 1926.

We start with a general discussion of WKB approximation for linear ODE. Suppose we have an equation

$$\hbar\frac{dF}{dx} = AF \tag{8.8}$$

for a vector-function of one variable $F(x) \in \mathbb{C}^n$, where $A(x) \in \mathrm{Mat}_n(\mathbb{C})$ is a matrix-valued function (smooth on a certain interval $I \subset \mathbb{R}$). We would like to understand the asymptotic behavior of solutions of this equation as $\hbar \to 0$. To this end, assume for simplicity that $A(x)$ has simple spectrum for generic x, and let $v_1(x), ..., v_n(x)$ be its column eigenvectors with eigenvalues $\lambda_1(x), ..., \lambda_n(x)$, and $v_1^*(x), ..., v_n^*(x)$ the dual basis of row eigenvectors. Let us now look for solutions of (8.8) in the form

$$F(x) = e^{\frac{\phi(x)}{\hbar}}(\psi_0(x) + \hbar\psi_1(x) + \hbar^2\psi_2(x)...),$$

where $\psi_0(x) \neq 0$ and the series in parentheses is formal. Substituting, we get

$$(\hbar\partial_x + \phi' - A)(\psi_0 + \hbar\psi_1 + \hbar^2\psi_2 + ...) = 0,$$

which in degree 0 with respect to $\hbar$ yields the equation

$$A\psi_0 = \phi'\psi_0.$$

Thus $\phi' = \lambda_j$ is an eigenvalue of A, so

$$\phi(x) = \int \lambda_j(x)dx,\ \psi_0(x) = f(x)v_j(x),$$

where f is a scalar function.

Further, in degree 1 in $\hbar$ we obtain the equation

$$\psi_0' = (A - \lambda)\psi_1,$$

i.e.,

$$f'v_j + fv_j' = (A - \lambda)\psi_1.$$

For this to have a solution ψ_1, we need $(v_j^*, f'v_j + fv_j') = 0$, i.e.,

$$f' = -(v_j^*, v_j')f.$$

Thus

$$f(x) = \exp\left(-\int (v_j^*, v_j')dx\right).$$

Now we can recursively solve for $\psi_1, \psi_2, \ldots$. This leads to the following result.

Theorem 8.30. *There is a unique, up to scaling, basis of formal solutions of equation* (8.8) *of the form*

$$F_j(x) = \exp\left(\frac{\int \lambda_j(x)dx}{\hbar}\right)\left(\exp\left(-\int (v_j^*(x), v_j'(x))dx\right) v_j(x) + O(\hbar)\right).$$

Let us now apply this theorem to the stationary Schrödinger equation

$$(-\tfrac{\hbar^2}{2}\partial_x^2 + U(x))\Psi = E\Psi. \tag{8.9}$$

Set $p(x) := \sqrt{2(E - U(x))}$, then (8.9) takes the form

$$\hbar^2\partial_x^2\Psi = -p^2\Psi.$$

This can be written as the system of equations

$$\hbar\partial_x\begin{pmatrix}\Psi\\ \hbar\Psi'\end{pmatrix} = \begin{pmatrix}0 & 1\\ -p^2 & 0\end{pmatrix}\begin{pmatrix}\Psi\\ \hbar\Psi'\end{pmatrix}.$$

Thus we have equation (8.8) with $A = \begin{pmatrix}0 & 1\\ -p^2 & 0\end{pmatrix}$. So we have

$$\lambda_1 = ip,\ \lambda_2 = -ip$$

and we may take

$$v_1 = \begin{pmatrix}1\\ ip\end{pmatrix},\ v_2 = \begin{pmatrix}1\\ -ip\end{pmatrix},$$

so that

$$v_1^* = \frac{1}{2}(1, -ip^{-1}),\ v_2^* = \frac{1}{2}(1, ip^{-1}).$$

Thus we obtain the following formal solutions of (8.9):

$$\Psi_\pm = \exp\left(\pm\frac{i\int pdx}{\hbar}\right)\left(\exp\left(-\frac{1}{2}\int p^{-1}p'dx\right) + O(\hbar)\right) =$$

$$p^{-\frac{1}{2}}\exp\left(\pm\frac{i\int pdx}{\hbar}\right)(1 + O(\hbar)).$$

We get

Theorem 8.31. *(local WKB approximation) Equation* (8.9) *has a basis of formal solutions*

$$\Psi_\pm(x) = (2(E - U(x))^{-\frac{1}{4}}\exp\left(\pm\frac{i\int\sqrt{2(E - U(x))}dx}{\hbar}\right)(1 + O(\hbar)).$$

The WKB approximation can also be used to find asymptotic distribution of eigenvalues of a Schrödinger operator when it has discrete spectrum. Let us explain, somewhat informally, how this works.

As an example, consider the stationary Schrödinger equation (8.9) on the circle $\mathbb{R}/2\pi\mathbb{Z}$ with piecewise continuous 2π-periodic potential $U(x)$. We would like to write an asymptotic formula for the n-th eigenvalue $E_n(\hbar)$ of the operator $H = -\frac{1}{2}\hbar^2\partial^2 + U(x)$ when $n \sim \frac{A}{\hbar}$ for a given constant A. This is equivalent to determining the number $\nu(E)$ of eigenvalues of H satisfying the inequality $\Lambda \leq E$ for a given constant E.

To this end, we will use Theorem 8.31. Assume first that

$$E > \sup U(x).$$

The periodicity condition for the solutions $\Psi_\pm$ in Theorem 8.31 (called the *quantization condition* in quantum mechanics) in the zeroth approximation is that

$$\int_0^{2\pi} \sqrt{2(E - U(x))}dx = 2\pi n\hbar,\ n \in \mathbb{Z}_{\geq 0}. \tag{8.10}$$

It follows that if 8.10 holds then the number of eigenvalues of H which are $\leq E$ is about $2n$. So we get

Proposition 8.32.

$$\nu(E) \sim \frac{A(E)}{\hbar},\ \hbar \to 0,\ \textit{where } A(E) := \frac{1}{\pi}\int_0^{2\pi} \sqrt{2(E - U(x))}dx.$$

Thus for sufficiently large A, we have

$$E_{[\frac{A}{\hbar}]}(\hbar) \sim E(A),$$

where $E(A)$ is the solution of the equation

$$A = \frac{1}{\pi}\int_0^{2\pi} \sqrt{2(E - U(x))}dx.$$

Note that $A(E)$ is the area of the region in the classical phase space $T^*S^1 = S^1 \times \mathbb{R}$ defined by the inequality

$$H_{\text{cl}} \leq E,$$

where $H_{\text{cl}} := \frac{1}{2}p^2 + U(x)$ is the corresponding classical hamiltonian. Moreover, one can show that with this definition of $A(E)$, the formula

$$\nu(E) \sim \frac{A(E)}{\hbar}$$

in fact holds in a much larger generality, whenever H has discrete spectrum (namely, for the operator $-\frac{1}{2}\hbar^2\Delta + U(x)$ on any compact

Riemannian manifold, or even on a non-compact one when one has $U(x) \to +\infty$ as $x \to \infty$). This formula is known as the *Weyl law*.

Exercise 8.33. *Prove the Weyl law on the circle for* $E \leq \sup U(x)$.

Finally, let $U(x) := MU_0(x)$ where U_0 is a fixed potential and consider the asymptotics of eigenvalues for small M, assuming that $\hbar \ll M$ (i.e., $\frac{1}{n} \ll M$). In this case we can write equation (8.10) as

$$\sqrt{2E} \int_0^{2\pi} \left(1 - \frac{MU_0(x)}{2E} - \frac{M^2 U_0(x)^2}{8E^2} + o(M^2)\right) dx = 2\pi n\hbar. \tag{8.11}$$

As before, we assume without loss of generality that $\int_0^{2\pi} U_0(x)dx = 0$. Let $I := \frac{1}{2\pi}\int_0^{2\pi} U_0(x)^2 dx$. Then we obtain

$$\sqrt{2E} = n\hbar + \tfrac{M^2 I}{2(2E)^{\frac{3}{2}}} + o(M^2) = n\hbar(1 + \tfrac{M^2 I}{2n^4\hbar^4} + ...) \tag{8.12}$$

It follows that

$$E = \tfrac{1}{2}n^2\hbar^2(1 + \tfrac{M^2 I}{n^4\hbar^4} + ...) = \Lambda_n + \frac{M^2 I}{8\Lambda_n} + ...$$

This gives the first correction of the eigenvalue $\Lambda_n := \frac{1}{2}n^2\hbar^2$ as we turn on M.

For example, if $U(x)$ is given by (8.4) then $I = a(2\pi - a)$ and we recover the asymptotics (8.7) without the last (bifurcation) term (which is negligible compared to $\frac{M^2 a(2\pi - a)}{8\Lambda_n}$ in the range $\frac{1}{n} \ll M$).

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18.238 Geometry and Quantum Field Theory

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