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.

8.1. **Hamilton's equations in classical mechanics.** We start with recalling the Lagrangian formalism of classical mechanics. For more details, we refer the reader to the excellent book of Arnold "Mathematical methods of classical mechanics".

Consider 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

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) = \frac{\partial L}{\partial q}.$$

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

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

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

Remark. 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.

Proposition 8.2. *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 ω. In fact, $\omega = d\alpha$, where α is a canonical 1-form on T^*M 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 $\alpha = \sum p_i dq_i$, and $\omega = \sum dp_i \wedge dq_i$.

Now let (M, ω) be a symplectic manifold (in our case $M = T^*X$). Since ω is nondegenerate, 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 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:

$$\frac{d}{dt} f(q(t),p(t)) = \{f,H\}(q(t),p(t)). \tag{21}$$

for any smooth function ("classical observable") $f \in C^\infty(T^*X)$. In other words, Hamilton's equations say that the rate of change of the observed value of f equals the observed value of $\{f,H\}$.

Note that for a given Lagrangian, the unique function H (up to adding a constant) for which equations (21) are equivalent to the equations of motion is the Hamiltonian. This provides another definition of the Hamiltonian, which does not use the notion of the Legendre transform.

8.2. **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. real functions $f \in C^\infty(T^*X)$, by quantum observables $\hat{f}$, which are (unbounded) self-adjoint operators on $\mathcal{H}$ (not commuting with each other, in general). Then the (expected) value of an observable A at a state $\psi \in H$ of unit norm is by definition $(\psi, A\psi)$.

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

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

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 $\hbar \to 0$.

We must immediately disappoint the reader by confessing that there is no canonical choice of the quantization map $f \to \hat{f}$. Nevertheless, there are some standard choices of $\hat{f}$ 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 there are the following standard conventions.

1. $\hat{f} = f(q)$ (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 $[\hat{q},\hat{p}] = i\hbar$, while $\{q,p\} = 1$.)

Example. For the classical Hamiltonian $H = p^2/2 + U(q)$ considered above, the quantization will be $\hat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + U(q)$.

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

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

where $(,)$ is the Hermitian form on $\mathcal{H}$ (antilinear on the first factor) and $\hat{H}$ is some quantization of the classical Hamiltonian H. Since this equation must hold for any A, it is equivalent to the Schrödinger equation

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

Thus, the quantum analog of the Hamilton equation is the Schrödinger equation.

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

The general solution of the Schrödinger equation has the form

$$\psi(t) = e^{-it\hat{H}/\hbar}\psi(0).$$

Therefore, for any quantum observable A it is reasonable to define a new observable $A(t) = e^{it\hat{H}/\hbar}A(0)e^{-it\hat{H}/\hbar}$ (such that to observe $A(t)$ is the same as to evolve for time t and then observe A). The observable $A(t)$ satisfies the equation

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

and we have

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

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

8.3. **Feynman-Kac formula.** Let us consider a 1-dimensional particle with potential $U(q) = m^2q^2 + \sum_{j\geq 3} g_j q^j/j!$. Let us assume that $U \geq 0$ and $U(q) \to \infty$ as $|q| \to \infty$. In this case, the operator $\hat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + U(q)$ is positive definite, and its spectrum is discrete. In particular, we have unique lowest eigenvector Ω, which is given by a positive function with norm 1. The correlation functions in the Hamiltonian setting are defined by the formula

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

Remark 1. The vector Ω is called the ground, 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).

Remark 2. Physicists usually write the inner product (v, Aw) as $< v|A|w >$. In particular, Ω is written as $< 0|$ or $|0 >$.

Theorem 8.3. *(Feynman-Kac formula) If $t_1 \geq \cdots \geq t_n$ 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 $\mathcal{G}_n^{\mathrm{Ham}}(-it_1, \ldots, -it_n)$ equals $\mathcal{G}_n^E$.*

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

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

and

$$\mathcal{G}_{n,L}(t_1, \ldots, t_n) = \frac{\mathrm{Tr}(q(-it_n)\cdots q(-it_1)e^{-L\hat{H}/\hbar})}{\mathrm{Tr}(e^{-L\hat{H}/\hbar})}$$

Theorem 8.4. *(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 8.3 is obtained from Theorem 8.4 by sending L to infinity. Thus, it is sufficient to prove Theorem 8.4.

Remark. As we mentioned before, the function $\mathcal{G}_n^E$ can be defined by means of Wiener integral, and the equality $\mathcal{G}_n^{\mathrm{Ham}}(-it_1, \ldots, -it_n) = \mathcal{G}_n^E(t_1, \ldots, t_n)$ actually holds for numerical values of $\hbar$, and not only 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 is technically more complicated and are beyond the scope of these notes.

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

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

The eigenvectors of this operator are well known: they are $H_k(x)e^{-x^2/2}$, where H_k are the Hermite polynomials ($k \geq 0$), and the eigenvalues are $k + 1/2$ (see Theorem 4.10). Hence,

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

as expected from the Feynman-Kac formula. (This shows the significance of the choice $C = 1/2$ in the normalization of Z_L).

8.4. **Proof of the Feynman-Kac formula in the free case.** Consider again the quadratic Hamiltonian $\hat{H} = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{q^2}{2}$. Note that it can be written in the form

$$\hat{H} = a^\dagger a + 1/2,$$

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 algebra on $\mathcal{H}$:

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

Thus the eigenvectors of $\hat{H}$ are $(a^\dagger)^n\Omega$ (where $\Omega = e^{-q^2/2}$) is the lowest eigenvector), and the eigenvalues $n + \frac{1}{2}$ (as we already saw before in Theorem 4.10).

Remark. The operators a and $a^\dagger$ are called the annihilation and creation operators, since $a\Omega = 0$, while all eigenvectors of $\hat{H}$ 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

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

Now we can easily prove Theorem 8.4. 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,

$$\mathcal{G}_{n,L}^{\mathrm{Ham}}(t_1, \ldots, t_n) = \sum_{j=2}^n \frac{1}{2}\mathcal{G}_{n-2,L}(t_2, \ldots, t_{j-1}, t_{j+1}, \ldots, t_n)(\frac{e^{t_1 - t_j}}{e^L - 1} - \frac{e^{t_j - t_1}}{e^{-L} - 1}) =$$

$$\sum_{j=2}^n \mathcal{G}_{n-2,L}(t_2, \ldots, t_{j-1}, t_{j+1}, \ldots, t_n)G_L(t_1 - t_j).$$

This implies the theorem by induction.

Note that in the quadratic case there is no formal expansions and the Feynman-Kac formula holds as an equality between usual functions.

8.5. **Proof of the Feynman-Kac formula (general case).** Now we consider an arbitrary potential $U = m^2q^2/2 + V(q)$, where $V(q) = \sum_{k\geq 3} g_k q^k/k!$. For simplicity we will assume that $\hbar = 1$ and coefficients g_j as formal parameters (this 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 $Z_L^{\mathrm{Ham}} = \mathrm{Tr}(e^{-L\hat{H}}) = \mathrm{Tr}(e^{-L(\hat{H}_0+V)})$, where $\hat{H}_0 = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{1}{2}m^2q^2$ is the free (=quadratic) part of the Hamiltonian. Since g_j are formal parameters, we have a series expansion

(22)

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

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

$$e^{A+B} = e^A + \sum_{N\geq 1} \int_{1\geq s_1\geq \cdots \geq s_N\geq 0} e^{(1-s_1)A} B e^{(s_1-s_2)A} B \cdots e^{(s_{N-1}-s_N)A} B e^{s_N A} d\mathbf{s} \tag{23}$$

(check this identity!).

Equation 22 shows that

$$Z_L^{\mathrm{Ham}} = \sum_{N\geq 0}(-1)^N \sum_{j_1,\ldots,j_N=3}^{\infty} \frac{g_{j_1}\cdots g_{j_N}}{j_1!\cdots j_N!} \mathrm{Tr}(q_0(-is_1)^{j_1}\cdots q_0(-is_N)^{j_N} e^{-L\hat{H}_0}),$$

where $q_0(t)$ is the operator $q(t)$ in the free theory, associated to the potential $m^2q^2/2$.

Since the Feynman-Kac formula for the free theory has been proved, the trace on the right hand side can be evaluated as a sum over pairings. 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 $i_3, i_4, \ldots$ of occurrences of $3, 4, \ldots$ among $j_1, \ldots, j_N$. 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

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

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

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

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

Expanding 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 $t_1, \ldots, t_n$. This implies that $\mathcal{G}_{n,L}^{\mathrm{Ham}} = \mathcal{G}_{n,L}$, and we are done.

8.6. **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 $\hat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dq^2}$. 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 $< \Omega, q(t_1)\ldots q(t_n)\Omega >$. (This is the reflection, in the Hamiltonian setting, of the difficulties related to the growth of the Green's function at infinity, 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 $e^{iNq/r}$, with eigenvalues $\hbar^2N^2/2r^2$. In particular, the lowest eigenvector is $\Omega = 1$. Thus the Hamiltonian correlation functions (in the Euclidean setting, for $t_1 \geq \ldots \geq t_n$) are

$$(\Omega, e^{t_1\hat{H}/\hbar} e^{ip_1q/r} e^{(t_2-t_1)\hat{H}/\hbar} \cdots e^{ip_nq/r} e^{-t_n\hat{H}/\hbar}\Omega) =$$

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

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

Now we pass to the case of quantum mechanics on the circle. First consider circle valued maps q. In this case, we have $\mathrm{Tr}(e^{-L\hat{H}/\hbar}) = \sum_N e^{-N^2 L\hbar/2r^2}$, and

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

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

$$e^{\frac{\hbar}{2r^2}\sum_j (t_j-t_{j+1})(p_1+\dots+p_j)^2}\sum_N e^{-\frac{\hbar}{2r^2}(LN^2+2\sum_{j=1}^n p_j t_j N)} =$$

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

Comparing with (20), we see that the Feynman-Kac formula holds, and follows from the modular invariance of the theta-function:

$$\theta(u,T) = e^{-2\pi^2 u^2/T}\theta(\frac{2\pi u}{iT}, \frac{4\pi^2}{T}).$$

(which follows from the Poisson summation formula).

Note that the Feynman-Kac formula would be 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. 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 $q_N(t) = 2\pi t N r/L$, so it is of the order $e^{-2\pi^2 N^2 r^2/L\hbar}$. 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".