GRAPH QUANTUM MECHANICS

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Abstract. We discuss the problem of counting paths going along the edges of a graph as a toy model for Feynman's path integral in quantum mechanics.

1. Paths on a graph

Let Γ be a graph.

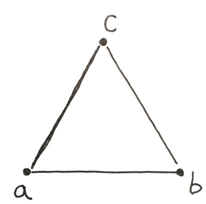

Figure 1

For simplicity we consider a finite *simple* graph, i.e. without multiple edges between vertices or loops – edges connecting a vertex to itself. Such a graph is defined by a combinatorial data: a set V of *vertices* and a set E of 2-element subsets of V – *edges*.

Example: The graph in Figure 1 has three vertices $V = \{a, b, c\}$ and three edges $E = \{\{a, b\}, \{b, c\}, \{c, a\}\}$.

The *adjacency* matrix of Γ is the square matrix of size $|V|$ – the number of vertices, with the following entries:

$$M_{uv} = \begin{cases} 1 & \text{if } \{u, v\} \in E \\ 0 & \text{otherwise} \end{cases} \qquad \text{for } u, v \in V$$

We view (M_{uv}) as the matrix of a linear operator $M : \mathbb{C}^V \to \mathbb{C}^V$ where

$$\mathbb{C}^V = \{\mathbb{C} - \text{valued functions on the set of vertices } V\}$$

is the complex vector space of dimension $|V|$ with basis $\{|v\rangle\}_{v\in V}$. Basis vector $|v\rangle$ corresponds to a function taking value 1 at the vertex v and vanishing at all other vertices. Thus, we have $M|v\rangle = \sum_{u\in V} M_{uv}|u\rangle$

Notation: for $A : \mathbb{C}^V \to \mathbb{C}^V$, we denote the matrix element A_{uv} as $\langle u|A|v\rangle$

The *graph Laplacian* of Γ is the operator Δ with matrix elements

$$\Delta_{uv} = \begin{cases} 1 & \text{if } \{u,v\} \in E \\ -\mathrm{val}(v) & \text{if } u = v \\ 0 & \text{otherwise} \end{cases} \qquad \text{for } u, v \in V$$

Here $\mathrm{val}(v)$ is the *valence* of the vertex, i.e. the number of edges containing it.

Example: For the graph in Figure 1, we have

$$M = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \qquad \Delta = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$$

We call a sequence $(v_0, v_1, \ldots, v_n)$ of vertices with the property that all $\{v_0, v_1\}, \{v_1, v_2\}, \ldots, \{v_{n-1}, v_n\}$ are edges, a *path* on Γ of length n, starting at v_0 and ending at v_n. For example, (a, b, c, a, c) is a path of length 4 on the graph of Figure 1 starting at a and ending at c.

For Γ a graph and $u, v \in V$ two vertices and t a real parameter, we have

$$\langle u|\exp(tM)|v\rangle = \sum_{n=0}^{\infty} \frac{t^n}{n!}\, p_n(u,v) \tag{1}$$

where $p_n(u,v)$ is the number of paths on Γ of length n from v to u.

Note that one can interpret the right hand side of (1) as the sum over all paths γ connecting v and u.

$$\langle u|\exp(tM)|v\rangle = \sum_{\text{paths } \gamma \text{ from } v \text{ to } u} \frac{t^{|\gamma|}}{|\gamma|!} \tag{2}$$

Here $|\gamma|$ is the length of a path.

To understand (1), consider the matrix element of n-th power of the adjacency matrix:

$$\langle u|M^n|v\rangle = \sum_{v_1,\ldots,v_{n-1}\in V} \langle u|M|v_{n-1}\rangle \cdot \langle v_{n-1}|M|v_{n-2}\rangle \cdots \langle v_1|M|v\rangle$$

– this is simply the matrix multiplication law for the n-fold product of the matrix M. The right had side is a sum, over $(n-1)$-tuples of vertices, of products of zeros and ones (since matrix elements of M are zeros and ones). The only tuples leading to products of ones, with no zeros, are those where $\{u, v_{n-1}\}, \ldots, \{v_1, u\}$ are edges, i.e. those where $(v, v_1, \ldots, v_{n-1}, u)$ is a path. Hence,

$$\langle u|M^n|v\rangle = p_n(u,v) \tag{3}$$

is simply the number of paths of length n. Now, if we expand the left hand side of the matrix element of the matrix exponential $\exp(tM)$ in Taylor series, we indeed obtain:

$$\langle u|\exp(tM)|v\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\langle u|t^n M^n|v\rangle = \sum_{n=0}^{\infty} \frac{t^n}{n!}\, p_n(u,v)$$

A graph Γ is called *regular* of valence k if *all* vertices have the same valence k. For instance, the graph in Figure 1 is regular of valence 2.

One consequence of (1) is the following: if Γ is regular of valence k, we have

$$\langle u|\exp(t\Delta)|v\rangle = \sum_{\text{paths } \gamma \text{ from } v \text{ to } u} \frac{t^{|\gamma|}}{|\gamma|!}\, e^{-kt} \tag{4}$$

This follows from the observation that, for Γ regular, Δ differs from M by a multiple of the identity matrix: $\Delta = M - k\cdot\mathrm{Id}$. Thus, $\exp(t\Delta) = e^{-kt}\cdot\exp(tM)$.

Remark. One can use (3) to count numbers of paths of arbitrary length on Γ if the eigenvalue spectrum of M is known. Indeed, let $\psi^{(i)} \in \mathbb{C}^V$ be the normalized eigenvectors of M with respective eigenvalues λ_i, for $i = 1, \ldots, |V|$. Then it follows from (3) that

$$p_n(u,v) = \sum_{i=1}^{|V|} \psi_u^{(i)} \lambda_i^n \bar{\psi}_v^{(i)} \tag{5}$$

Example. Consider the graph of Figure 1. Let us count the numbers of paths of given lengths from a to a.

n	paths	no. of paths
0	(a)	1
1	no paths	0
2	(aba), (aca)	2
3	(abca), (acba)	2
4	(abcba), (ababa), (abaca), (acbca), (acaca), (acaba)	6

Clearly the direct count becomes more and more cumbersome as n grows. On the other hand, we can explicitly diagonalize the adjacency matrix and apply (5), which gives the formula

$$p_n(a,a) = \frac{1}{3}(2^n + 2\cdot(-1)^n)$$

for the count of paths of arbitrary length.

Remark. One also has a version of formulae (2,4) for *closed* paths, i.e. paths which start and end at the same vertex:

$$\text{tr}\ \exp(t\Delta) = \sum_{\text{closed paths}\,\gamma} \frac{t^{|\gamma|}}{|\gamma|!}\, e^{-kt} \tag{6}$$

On the left hand side we now have the *trace* of the matrix exponential, rather than a matrix element.

2. Motivation: Feynman's approach to quantum mechanics

In quantum mechanics, one can consider a particle of mass m in $\mathbb{R}^N$ moving in a force field with potential $U(x)$ (a function on $\mathbb{R}^N$, such that minus its gradient is the force exerted on the particle). The state at a given time is given by a complex-valued function $\Psi(x)$ on $\mathbb{R}^N$ – the *wave function*. Evolution of the state in time is given by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(t,x) = \left(-\frac{\hbar^2}{2m}\Delta + U(x)\right)\Psi(t,x) \tag{7}$$

Here $\hbar$ is the Planck constant, $\Delta = \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator on $\mathbb{R}^N$. The differential operator in brackets in the right hand side of (7) is the *Schrödinger operator* $\widehat{H}$ on the *space of states* $\mathcal{H} = L^2(\mathbb{R}^N)$ – the space of square-integrable functions on $\mathbb{R}^N$, where Ψ lives. Starting with a state $\Psi(t_0,x)$ at time t_0, we can evolve it until time $t_1 > t_0$ using the equation (7). The resulting state has the form

$$\Psi(t_1,x) = \int_{\mathbb{R}^N\ni y} d^N y\, K(t_1-t_0;x,y)\,\Psi(t_0,y)$$

where K is certain function on $\mathbb{R}_{>0}\times\mathbb{R}^N\times\mathbb{R}^N$ obtained from solving the equation (7); it is known as the *Green's function* or the *propagator*. By definition, K is the integral kernel of the operator $\mathsf{K}(t_1-t_0) = \exp\left(-\frac{i(t_1-t_0)\widehat{H}}{\hbar}\right)$ on $\mathcal{H}$.

Feynman suggested the following presentation for the propagator as an integral over the space of parameterized paths in $\mathbb{R}^N$ connecting point y to point x:

$$K(t_1-t_0;x,y) = \int_{\text{paths in}\,\mathbb{R}^N\ x(\tau):[t_0,t_1]\to\mathbb{R}^N\ \text{with}\ x(t_0)=y,\,x(t_1)=x} \mathcal{D}[x(\tau)]\ e^{\frac{i}{\hbar}S[x(\tau)]} \tag{8}$$

where $S[x(\tau)] = \int_{t_0}^{t_1} d\tau\left(\frac{m\dot{x}^2}{2} - U(x(\tau))\right)$ is the *action functional* of the classical particle moving in the potential, evaluated on the path $x(\tau)$.

The "integral over paths" in the right hand side of (8) is very appealing (reducing the evolution of a quantum system to notions of classical mechanics – particle trajectories and the action functional from the classical action principle). However it is rather non-straightforward to define mathematically, in particular to define the measure $\mathcal{D}[x(\tau)]$ on paths. Here are some of the approaches to a mathematical definition of the integral over paths.

- A measure-theoretic definition from the theory of Brownian motion and Wiener integral; requires a subtle analytical continuation in $\hbar$.
- Feynman's approach (see [4]): understand the right hand side of (8) as a limit as $n \to \infty$ of finite-dimensional integrals over the space of continuous piecewise-linear paths in $\mathbb{R}^N$ which are linear for $\tau \in (t_0, t_0+\delta t), (t_0+\delta t, t_0+2\delta t), \ldots, (t_0+(n-1)\delta t, t_1)$ and are allowed to change direction at times $\tau = t_0 + j \cdot \delta t$. Here $\delta t = \frac{t_1 - t_0}{n}$ and $1 \leq j \leq n-1$. Under appropriate assumtions on the potential, the limit exists and formula (8) becomes a theorem.
- One can view the r.h.s. of (8), in the asymptotical regime $\hbar \to 0$, as a an integral of a fast oscillating function. Finite-dimensional integrals of fast oscillating integrals have asymptotics described by the *stationary phase formula*, as a sum over the points of stationary phase of certain algebraic (not measure-theoretic) contributions. Then one can *define* the integral over paths, as an asymptotic series at $\hbar \to 0$, by the stationary phase formula. Points of stationary phase in r.h.s. of (8) are the critical points of the action functional $S[x(\tau)]$, i.e. those paths that satisfy the classical equation of motion $m\ddot{x} = -\nabla U(x)$. Thus, from this perspective, the path integral in the asymptotical regime $\hbar \to 0$ explores a formal neighborhood of the classical trajectory of the system in the space of all trajectories.

2.1. **Combinatorial quantum mechanics on a graph.** On a regular graph Γ, a "state" Ψ is a complex-valued function on vertices. The "Schrödinger equation" $\frac{\partial}{\partial t}\Psi(t) = \Delta\Psi(t)$, with Δ the graph Laplacian,[1] has the solution $\Psi(t_1) = e^{(t_1-t_0)\Delta}\Psi(t_0)$. Here $\mathsf{K}(t_1 - t_0) = e^{(t_1-t_0)\Delta}$ is

[1]Our combinatorial quantum mechanics corresponds to the case of zero potential in (7). Also, for simplicity, physical normalization constants $i\hbar$, $-\hbar^2/(2m)$ appearing in (7) are set to 1.

the evolution operator and its matrix elements are given by (4):

$$\langle u|\exp(t\Delta)|v\rangle = \sum_{\text{paths}\,\gamma\,\text{from}\,v\,\text{to}\,u} \frac{t^{|\gamma|}}{|\gamma|!}\, e^{-kt}$$

which is very similar to Feynman's formula (8). Note however that here on the right hand side instead of the obscure path integral we have literally a sum over paths on the graph – an absolutely convergent infinite sum.

We have the following dictionary between quantum mechanics of and counting paths on a graph.

Quantum particle in $\mathbb{R}^N$	Combinatorial quantum mechanics on a graph
points in $\mathbb{R}^N$	vertices of Γ
Schrödinger operator $\widehat{H}$	graph Laplacian
wave-function	element of $\mathbb{C}^V$
space of states $L^2(\mathbb{R}^N)$	complex span of vertices $\mathbb{C}^V$
propagator $K(t;x,y)$	matrix elements of $e^{t\Delta}$
Feynman's path inegral	sum over paths on Γ

3. Beyond graph quantum mechanics

(i) Formula (6) can be improved to a formula where on the r.h.s. one sums over the elements of the fundamental group of the graph – "closed geodesics", rather than over all closed paths. This "trace formula for a regular graph" (see [5]) bears close resemblance to the Selberg's trace formula which connects the spectrum of the Laplacian on a hyperbolic surface with the length spectrum of closed geodesics.

(ii) One can take Γ to be a square grid graph (of some dimension N), wrapped around a torus. Considering the limit of the spacing of the grid going to zero and the size of the torus going to infinity, one can obtain true quantum mechanics on $\mathbb{R}^N$ as a "continuum limit" of the combinatorial quantum mechanics on a square grid graph (one has to rescale carefully the parameters of the combinatorial theory in order to have a well-defined continuum limit). One can see explicitly how the l.h.s. of (4) converges to the l.h.s. of (8) (for zero potential) and the sum over paths on a grid converges to the Feynman's integral.

(iii) One can consider a "supersymmetric version" of the combinatorial quantum mechanics. This requires one to replace the graph Γ by a cellular complex. Instead of counting paths, we will now be counting sequences of cells of dimensions alternating between j and $j+1$ for some j, weighed with a sign. The Hamiltonian now will be $dd^* + d^*d$ where d is the coboundary operator on cellular cochains, and d^* its Hodge dual. This gives a combinatorial version of (the Hodge limit of) Witten supersymmetric quantum mechanics [8].

4. From graph quantum mechanics to combinatorial quantum field theory on a graph

One can consider a combinatorial field theory with graph Γ playing the role of spacetime. In a particular example, this amounts to considering "partition functions" – integrals of form

$$Z = \int_{\mathrm{Fields}(\Gamma)\ni\phi} \mathcal{D}\phi \; e^{\frac{i}{\hbar}S(\phi)} \tag{9}$$

where

- $\mathrm{Fields}(\Gamma) = \mathbb{R}^V$ is the "space of fields", modelled here by real-valued functions on vertices of Γ.
- $S(\phi) = \frac{1}{2}\sum_{u,v\in V} \phi(u)(-\Delta + m^2 \cdot \mathrm{Id})_{uv}\phi(v) + \sum_{u\in V} F(\phi(u))$ is the "action functional"; a positive parameter m plays the role of the mass of the quantum of the field. $F(x) = \sum_{k=3}^{K} \frac{f_k}{k!}x^k$ is polynomial in a single real variable, defining the self-interaction of the theory.
- $D\phi = \prod_{u\in V} d\phi(u)$ is the integration measure on the space of fields.

Alongside partition functions (9), one can consider "n-point correlation functions", i.e. integrals of the form

$$\langle \phi(u_1)\cdot\phi(u_2)\cdots\phi(u_n)\rangle := \frac{1}{Z}\int_{\mathrm{Fields}(\Gamma)\ni\phi} \mathcal{D}\phi \; e^{\frac{i}{\hbar}S(\phi)}\phi(u_1)\cdot\phi(u_2)\cdots\phi(u_n) \tag{10}$$

with $u_1, \ldots, u_n$ an n-tuple of vertices of Γ.

4.1. Case of the free scalar field.

Considering the case $F = 0$ (free scalar theory on a graph), one can obtain out of (1) a presentation for the partition function as a sum over closed paths, and a presentation for $n = 2$ correlation function (also called the "propagator" of the field theory) as a sum over paths on Γ between two vertices.

Also, one can consider the case when the graph Γ is a union of two disjoint graphs, Γ_1 and Γ_2, over a set of edges $e_1, \ldots, e_N$, such that each e_j has one vertex in Γ_1 and the other in Γ_2. Here, one can recover the propagator and the partition function on Γ from respective entities on Γ_1 and Γ_2.

Sum over paths formulae for the partition function and the propagator of the combinatorial free scalar field theory were obtained in [3], together with the gluing formula in the sense above (recovering entities on Γ - the "glued graph" from $\Gamma_{1,2}$).

Furthermore, one can consider Γ to be a square grid graph, of some dimension, as in (ii) of Section 3, and pass to a continuum limit, recovering (the special case of) the gluing formulae for determinants of Laplacians and for Green's function for the Laplacian on Riemannian manifolds. This continuum limit is the subject of [3] and [7].

4.2. **Interacting theory.** Next, one can consider the case of nonzero interaction F in (9). Treating the integral (9) as a perturbed Gaussian integral, one expands Z as a sum over graphs γ ("Feynman diagrams") with valences ≥ 3 allowed, of certain contributions Φ_γ. The value of a Feynman diagram Φ_γ is constructed in terms of propagators of the free theory of Section 4.1. Using the path sum formula of [3], one can write Φ_γ itself as a sum over "combinatorial mappings" $\gamma \to \Gamma$ (i.e. sets of paths in Γ, corresponding to edges of γ; these paths are required to meet at a vertex of Γ whenever the respective edges of γ meet at a vertex of γ).

Moreover, this picture is compatible to gluing/cutting of graphs as in Section 4.1: one can recover the value of Φ_γ on spacetime graph $\Gamma = \Gamma_1 \cup \Gamma_2$ from values of Φ_{γ_1} on Γ_1 and Φ_{γ_2} on Γ_2. Where γ_1, γ_2 are all possible pairs of graphs such that $\gamma = \gamma_1 \cup \gamma_2$.

Developing the details of this model and some of its extensions is a project in progress by P. M. joint with S. Kandel.

This model gives a concrete combinatorial realization of Segal's formulation of quantum field theory [6]. In Segal's description (omitting many details), an n-dimensional quantum field theory associates a Hilbert space of states $\mathcal{H}_\Sigma$ to every closed compact $(n-1)$-dimensional manifold Σ and associates to an n-dimensional manifold M with boundary ∂M a vector $Z_M \in \mathcal{H}_{\partial M}$ (the "partition function"). This association should be multiplicative with respect to disjoint unions and should respect unions of n-manifolds over boundary components:

$$Z_{M_1 \cup_\Sigma M_2} = \langle Z_{M_1}, Z_{M_2} \rangle_\Sigma$$

where $\langle , \rangle_\Sigma$ is the inner product in the Hilbert space $\mathcal{H}_\Sigma$.

The program of perturbative quantization of gauge theories on manifolds with boundary by Cattaneo-P. M.-Reshetikhin [1, 2] produces as an output particular examples of Segal's quantum field theories, with partition functions given in terms of Feynman diagrams (their values, in turn, are given in terms of integrals over configuration spaces of points on the manifold, of the product of propagators). Feynman diagrams have a gluing property similar to the one described above in the combinatorial case. Thus, combinatorial quantum field theory on a graph also provides a combinatorial realization for the program of [1, 2].

Studying continuum limit (in the sense of passing to a limit of a dense grid for the partition function of the interacting theory) is quite nontrivial and requires appropriate rescaling of the coefficients of F simultaneous with decreasing the spacing of the grid, in order for the limit to exist. This rescaling is a model for renormalization in quantum field theory.

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