QUANTUM PHYSICS AND FUNCTIONAL INTEGRATION

Methods based on integration in function space are a powerful tool in the understanding of quantum dynamics, especially in quantum field theory, where they not only give a useful formulation of perturbation theory but also provide one of the few tools that go beyond perturbation theory.

Since the time-dependent Schrödinger equation (in units with $\hbar = 1$)

$$i\dot{\psi}_t(x) = -(2m)^{-1}\Delta\psi_t(x) + V(x)\psi_t(x) \quad (1)$$

is similar to the diffusion equation

$$-\dot{\phi}_t = -\Delta\phi_t(x), \quad (2)$$

for which Wiener invented functional integration [11], it is not surprising that functional integration can be used to study (1). Of course, (1) is solved by $\psi_t = e^{-itH}\psi_0$; $H = -(2m)^{-1}\Delta + V$, while (2) is solved by $\phi_t = e^{-2tH_0}\phi_0$; $H_0 = -\frac{1}{2}\Delta$. Feynman's initial formal framework of "path integrals in quantum mechanics [3]" involved the study of e^{-itH}. Although there has been some partially successful rigorous study of Feynman "integrals" (one must extend the notion of measure in all these approaches) [1, 4, 5], most of the rigorous work and an increasing fraction of the heuristic literature has studied the semigroup e^{-tH} rather than e^{-itH}.

At first sight it seems surprising that the study of e^{-tH} would be a suitable substitute for the study of e^{-itH}, but the semigroup even has some real advantages. (1) If one wants to understand the lowest eigenvalue*, E (*ground state energy*), and corresponding eigenvector (*ground state*) of H, the operator e^{-tH} is often more useful than e^{-itH}; for example,

$$E = -t^{-1}\ln\|e^{-tH}\|.$$

(2) If one views the parameter t as $1/(kT)$, with k equal to Boltzmann's constant and T the temperature, then the semigroup is the basic object of quantum statistical mechanics. (3) In quantum field theory, the formal continuation from it to t should replace Lorentz invariance by invariance under a Euclidean group of rotations and various hyperbolic equations by better-behaved elliptic equations. This passage to Euclidean invariance is often called *analytic continuation to the Euclidean region* in the theoretical physics literature.

In units with $m = 1$, the basic formula for e^{-tH} is the *Feynman–Kac formula*, named after fundamental contributions by their authors [3, 6]:

$$(e^{-tH}f)(x) = E_x\left(e^{-\int_0^t V(b(s))\,ds}f(b(t))\right). \quad (3)$$

In this formula, b is Brownian motion* and E_x denotes expectation with respect to paths starting at x, that is, $b(s)$ is an R^ν-valued Gaussian process* with mean x and covariance:

$$E_x((b_i(s) - x_i)(b_j(t) - x_j)) = \delta_{ij}\min(t,s).$$

For detailed conditions on f, V for (3) to hold and several proofs, see ref. 8. An especially useful way of looking at (3) is in terms of the Lie–Trotter formula:

$$\exp(-tH) = \lim_{n\to\infty}\left[\exp(-tH_0/n)\exp(-tV/n)\right]^n$$

and Riemann sum approximations to $\int_0^t V(b(s))\,ds$.

While (3) is very useful to study H, it can also be turned around and used to study Brownian motion; for example [see ref. 8 (pp. 58–60)], one can compute the distribution of the Lebesgue measure of $\{s \leqslant t \mid b(s) > 0\}$ by using (3) with V the indicator function of $\{x \mid x > 0\}$.

The differential operator

$$H(a) \equiv \tfrac{1}{2}(-i\nabla - a)^2 + V \quad (4)$$

is the Hamiltonian operator for particles (with $\hbar = 1$, $m = 1$, $e/(mc) = 1$) moving in a magnetic field $B = \text{curl}\,(a)$ and potential V. There is an analog of (3) for $H(a)$, sometimes called the *Feynman–Kac–Ito formula*:

$$(e^{-tH}f)(x) = E_x\left(e^{-iF(b)}e^{-\int_0^t V(b(s))\,ds}f(b(t))\right) \quad (5)$$

with

$$F(b) = \int_0^t a(b(s)) \cdot db - \frac{1}{2}\int_0^t (\operatorname{div} a)(b(s))\,ds. \qquad (6)$$

In (6), $\int a \cdot db$ is an Ito stochastic integral* (*see also* BROWNIAN MOTION); if the Stratonovich integral is used instead, the second term in (6) will not be present. Since F is real-valued, (5) immediately implies the *diamagnetic inequality* of Nelson and Simon:

$$|(e^{-tH(a)}f)(x)| \leqslant (e^{-tH(a=0)}|f|)(x),$$

which has been very useful in the study of operators of the form (4).

As an intermediate situation to describing quantum field theory, one can consider $P(\phi)_1$-processes. Let $h = -\frac{1}{2}d^2/dx^2 + v(x)$ on $L^2(R, dx)$. Suppose that e is the ground-state energy and $\Omega(x)$ the ground state. Let $P_t(x, y)$ be the integral kernel of the operator $\Omega \exp[-t(h-e)]\Omega^{-1}$. $P_t(x, y)$ has the semigroup property; it is positive since $\Omega(x) \geqslant 0$, and $\int P_t(x, y)\,dx = 1$ since e^{-th} is symmetric and $e^{-th}\Omega = \Omega$. Thus $P_t(x, y)$ defines a Markov process* with invariant measure $\Omega^2 dx$. The Markov process $q(t)$ with this invariant measure as initial distribution and transition kernel $P_t(x, y)$ is called the $P(\phi)_1$-*process* [since V is often a polynomial $P(x)$]; we use E to denote the corresponding expectation. The expectations $E^{(v)}$ and $E^{(v+w)}$ associated to h and $h + w$ are related by

$$E^{(v+w)}(F) = \lim_{t\to\infty} Z_t^{-1} E^{(v)}\left\{ F \exp\left[-\int_{-t}^{t} w(q(s))\,ds \right] \right\} \qquad (7)$$

with

$$Z_t = E^{(v)} \exp\left[-\int_{-t}^{t} w(q(s)) \right] ds.$$

This sets up an analogy to statistical mechanics which is often useful.

The $P(\phi)_1$-process with $v(x) = \frac{1}{2}x^2$ is of particular interest since it is a Gaussian process. Its covariance is

$$E(q(s)q(t)) = \tfrac{1}{2}\exp(-|t-s|). \qquad (8)$$

Up to changes of scale of q and/or t, it is the unique stationary, Markov-Gaussian process, called the *Ornstein–Uhlenbeck* velocity process*, or occasionally the *oscillator process*, since $-\frac{1}{2}d^2/dx^2 + \frac{1}{2}x^2$ is the Hamiltonian of a harmonic oscillator.

Quantum field theories analytically continued to the Euclidean region are analogs of $P(\phi)_1$-processes with the time, s, now a multidimensional variable. In generalizing (8), it is important to realize that the right side of (8) is the integral kernel of the operator $(-d^2/dt^2 + 1)^{-1}$. Let $G_0(x - y)$ be the integral kernel of the operator $(-\Delta + 1)^{-1}$ on $L^2(R^\nu, d^\nu x)$. The generalized Gaussian process $\phi(x)$ with mean zero and covariance

$$E(\phi(x)\phi(y)) = G_0(x-y)$$

is called the *free Euclidean field* or occasionally the *free Markov field* (since it has a kind of multitime Markov property). If $(-\Delta + 1)^{-1}$ is replaced by $(-\Delta + m^2)^{-1}$, the phrase "of mass m" is added to "free Euclidean field." This process is the analytic continuation to the Euclidean region of quantum field theory describing noninteracting spinless particles.

The process above is only "generalized" [i.e., $\phi(x)$ must be smeared in (x), since G_0 is singular at $x = y$, if $\nu \geqslant 2$]. For $\nu = 2$, the singularity is only logarithmic, but it is a power singularity if $\nu \geqslant 3$. The natural analog of (7) is to try to construct an expectation by

$$\lim_{\Lambda\to R^\nu} Z(\Lambda)^{-1} \int F(\phi) \exp\left[-\int_\Lambda w(\phi(x))\,d^\nu x \right], \qquad (9)$$

where

$$Z(\Lambda) = \int \exp\left[-\int_\Lambda w(\phi(x))\,d^\nu x \right].$$

Such a construction would yield models of quantum fields. In $\nu = 2$ and 3 ($\nu = 4$ is the physical case), this program, called *constructive quantum field theory*, has been successful, due to the efforts of many mathematical physicists, most notably J. Glimm and A. Jaffe.

In (9), there are two general problems. The limit $\Lambda \to R^\nu$ is not trivial to control; it has been controlled by making an analogy to the corresponding limit in statistical mechanics and extending various ideas from that discipline.

The other problem is special to quantum field theory. When $\nu = 1$, the oscillator process is supported on continuous functions, but for $\nu \geqslant 2$, the corresponding free field is supported on distributions that are signed measures with probability zero! Thus the typical choice $w(\phi(x)) = \phi(x)^4$ is meaningless since $\phi(x)$ does not have powers. This is the celebrated problem of *ultraviolet divergences*, which occurred in all the earliest attempts to study quantum field theory. It is solved by *renormalization theory*. For example, let $\phi_f(x) = \int f(x-y)\phi(y)\,d^\nu y$, which yields a nice process if $f \in C_0^\infty$. We want to let $f \to \delta$. One lets w depend on f and in (9) lets $w(\phi)$ be replaced by $w_f(\phi_f)$ and then also takes a limit as $f \to \delta$. For example, in $\nu = 2$ dimensions, one can take

$$w_f(\phi(x)) = \phi_f(x)^4 - 6E(\phi^2(x))\phi_f^2(x) \quad (10)$$

and control the limit in (9) if first $f \to \delta$ and then $\Lambda \to \infty$. In (10), $E(-)$ denotes expectation with respect to the free Euclidean field, so

$$E(\phi_f^2(x)) = \int f(x) G_0(x-y) f(y)\,dx\,dy \to \infty$$

as $f \to \delta$. The resulting theory is often denoted as the ϕ_2^4 theory. There have been developed ϕ_3^4 theories and $P(\phi)_2$ for a large class of polynomials P. Fermion theories and certain gauge models have been constructed in two and three dimensions, but this goes beyond the scope of this article.

An especially useful device in the theory is the *lattice approximation*, where x is replaced by a discrete variable and $-\Delta$ by a finite difference* operator. One realizes that these models are lattice systems* with unbounded spins and one uses intuition from that subject. As the lattice spacing goes to zero, one can hope to recover the continuum theory.

Recently, steepest descent ideas have come into use in functional integration pictures of quantum theory. A major role is played by functions minimizing an exponent. The quantity in the exponent is usually called *Euclidean action* and the minimizing functions are *instantons*.

Glossary

Fermion Theories: Field theories describing particles that obey the Pauli exclusion principle (also called Fermi–Dirac* statistics, hence "fermions").

Gauge Models (also called "Yang–Mills" or "non-Abelian gauge" theories): These are the current popular quantum field models which describe both weak interactions (Weinberg–Salam theories) and strong interactions (quantum chromodynamics).

Perturbation Theory: Expansion in physical coupling constants of the basic quantities of a quantum field theory which is especially useful in quantum electrodynamics, where the natural coupling constant is small (about 1/137).

Quantum Field Theory: The only successful way of synthesizing quantum mechanics and special relativity.

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(LATTICE SYSTEMS
QUANTUM MECHANICS AND PROBABILITY
QUANTUM MECHANICS: STATISTICAL INTERPRETATION
STOCHASTIC INTEGRALS)

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QUARTIC EXPONENTIAL DISTRIBUTION

The quartic exponential distribution has a probability density function of the form

$$f(x) \propto \exp\left[-\left(\alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4\right)\right],$$
$$\alpha_4 > 0, \quad -\infty < x < \infty.$$

It belongs to the general exponential family*. Fisher [2] discussed a general "polynomial" exponential family, but the fourth-degree case seems to be first explicitly considered by O'Toole [4] and subsequently by Aroian [1].

Matz [3] studied the quartic exponential family in detail, with special emphasis on maximum likelihood* estimation of parameters. Application to bimodal data seems the principal use of this distribution.

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(EXPONENTIAL DISTRIBUTION
EXPONENTIAL FAMILIES)

QUARTILE *See* QUANTILES

QUARTILE DEVIATION

This is one-half of the interquartile* distance. It is also called the *semi-interquartile range*.

(PROBABLE ERROR
QUARTILE DEVIATION, COEFFICIENT OF)

QUARTILE DEVIATION, COEFFICIENT OF

The quartile deviation* is an appropriate measure of variation when the median is used as the measure of central tendency. It is defined as

$$Q = \tfrac{1}{2}(Q_3 - Q_1)$$

where Q_1 and Q_3 are the first and third quartiles*, respectively.

The *relative variation* is measured by expressing the quartile deviation as the percentage of the midpoint between Q_1 and Q_3. This percentage is denoted by

$$V_Q = \frac{(Q_3 - Q_1)/2}{(Q_3 + Q_1)/2} \times 100$$
$$= \frac{Q_3 - Q_1}{Q_3 + Q_1} \times 100$$

and is called the coefficient of quartile deviation. It is an analog of the coefficient of variation*.