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Integration in Function Spaces and Some of Its Applications

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PREFACE

These notes based on a series of lectures delivered at the Scuola Normale Superiore in May 1980 are meant to provide an introduction to the subject of functional integration. Although integration in function spaces owes its origins to Probability Theory on the one hand, and to Quantum Mechanics on the other, I assumed only most rudimentary familiarity with either of these disciplines. Also I did not attempt to write a minitextbook on the subject of integration in function spaces. I was much more concerned in exhibiting the spirit of the subject than in teaching it in an organized and systematic way. Consequently I stressed the formal and eschewed, perhaps even above and beyond the call of duty, technicalities. To borrow a famous saying, I came to Pisa to praise functional integration not to bury it.

I hope the reader will keep this in mind and be willing to forgive me for being sketchy, incomplete and moving in too many directions at once. I also hope that the reader will understand that constraints the written word imposes on a speaker prevent him from including numerous side remarks of scientific and anecdotal nature which he could use freely to (hopefully!) edify (and perhaps even amuse) his live audience.

There remains the pleasant duty to thank Accademia Nazionale dei Lincei and the Scuola Normale Superiore for inviting me to deliver this year's Lezioni Fermiane and to all my friends for their wonderful hospitality for which Italy, in general, and Pisa, in particular, are justly famous.

It was a great honor to join a long line of distinguished colleagues in paying tribute to the memory of one of this century's greatest scientists.

Pisa, May 1980.

CONTENTS

SECTION 1

Introduction

The subject of integration in function spaces was first introduced by Norbert Wiener in a series of papers written in the early twenties. He later summarized certain aspects of his work in a chapter on *Random functions* in the book « *Fourier Transforms in the Complex Domain* » written jointly with R. E. A. C. Paley (the book was completed after Paley's premature and tragic death in a skiing accident).

Wiener has always been interested in problems of Physics (and Engineering) and he was familiar with the work of Einstein and Smoluchowski on the theory of Brownian motion. He has read Jean Perrin's beautiful book « *Les Atomes* » and it was a remark in this book that, according to Wiener's own account, provided the inspiration for his work in this area.

What made such an impression on Wiener was a passage in « *Les Atomes* » in which Perrin said in effect « that the very irregular curves followed by particles in Brownian motion led one to think of the supposed continuous nondifferentiable curves of the mathematicians » (quoted from Wiener's autobiography « *I am a mathematician. The later life of a prodigy* »).

It should be recalled that the fundamental result of the theory of Brownian motion is that the mean square displacement of a free particle during a time interval t is proportional to t

$$\langle x_t^2 \rangle = 2Dt \tag{1.1}$$

and that the « diffusion coefficient » D for spherical particles of radius a in a liquid with viscosity coefficient η is given by the formula

$$D = \frac{kT}{3a\eta} \tag{1.2}$$

where T is the absolute temperature and k the Boltzmann constant.

Since

$$k = \frac{R}{N} \tag{1.3}$$

where R is the well known gas constant and N the Avogadro number, experimental determination of D would provide a novel way of determining the Avogadro number. This in fact was done by Perrin, and for this (and a number of closely related experiments) he was awarded the Nobel Prize in Physics in 1926.

To determine D experimentally one can observe a large number n of (independent) Brownian particles for the same time interval t and measure their displacements

$$x_t(1),\ x_t(2),\ \ldots,\ x_t(n)\ ;$$

an estimate for D is then given by the obvious formula

$$2D \sim \frac{1}{t}\,\frac{\sum_{k=1}^{n} x_t^2(k)}{n}\ . \tag{1.4}$$

As can be noted this involves *statistics of particles* as indeed do all *experimentally* testable statements about Brownian Motion.

Wiener wanted to justify Perrin's remark about non-differentiability of Brownian paths and for this he needed a deeper theory based on what one might call the *statistics of the paths*, or, to use more conventional terminology, an appropriate measure in the space of paths. Since Wiener took continuity of paths for granted he proceeded to construct a measure in the space of continuous functions.

SECTION 2

Construction of the Wiener Measure and Integration of Some Simple Functionals

How does one construct a measure in a space? One begins with a collection of sets (called elementary) whose measure is somehow given and one uses the axioms of additivity and complementarity to extend the measure to a wider collection.

The axiom of (complete or denumerable) additivity states that if $A_1, A_2, \ldots$ are measurable and non-overlapping then the union $\bigcup_{n=1}^{\infty} A_n$ is measurable and

$$m\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{k=1}^{\infty} m(A_k) \tag{2.1}$$

where $m(\ldots)$ denotes the measure of the set in parenthesis. « Measurable » means that the set can be assigned a measure.

The axiom of complementarity merely says that if A is measurable then so is its complement $\tilde{A}$.

The whole space is assumed measurable (and hence so is the empty set), and in probability theory it is customarily assigned measure 1.

Lebesgue also added an axiom (which was at the center of a vigorous priority polemic with Borel who stopped with the first two axioms) that a subset of a set of measure zero is measurable (and hence also of measure zero).

The familiar Lebesgue measure on a line starts with open intervals as elementary sets assigning to each interval its *length* as its measure; one then extends this measure to the « Borel field » generated by the

open intervals by taking unions and complements. One then adds the Lebesgue axiom and one is done.

One can prove that the measure obtained in this way is equivalent to the measure as actually introduced by Lebesgue in terms of coverings and outer and inner measures.

Two points should be made:

1) The assignment of measures to elementary sets must be *consistent* with the axioms of additivity and complementarity.

2) The assignment of measures to elementary sets is often dictated by considerations which are *not* measure theoretic. E.g. assigning the length of an open interval as its measure is a response to a *geometric* desideratum that the measure be translationally invariant.

With this cursory review of the elementary facts about measure theory as background let me sketch Wiener's construction.

The space in question is the set $C_0(0, 1)$ of all *continuous* functions $x(t)$, $x(0) = 0$, $0 \leqslant t \leqslant 1$ (the extension to the time interval $0 \leqslant t < \infty$ is routine as will be indicated a little later).

The elementary sets are sets of functions $x(t)$ which at prescribed times

$$0 < t_1 < t_2 < \ldots < t_n \leqslant 1$$

assume values in prescribed intervals $(\alpha_1, \beta_1), \ldots, (\alpha_n, \beta_n)$ (« slalom gates » as the late Lars Onsager liked to call them).

The measure (or probability) assigned to the set of continuous functions

$$\{\alpha_1 < x(t_1) < \beta_1,\ \alpha_2 < x(t_2) < \beta_2,\ \ldots,\ \alpha_n < x(t_n) < \beta_n\} \tag{2.2}$$

is by the Einstein-Smoluchowski theory

$$\int_{\alpha_1}^{\beta_1} \int_{\alpha_2}^{\beta_2} \ldots \int_{\alpha_n}^{\beta_n} P(0|x_1;\, t_1)\, P(x_1|x_2;\, t_2 - t_1) \ldots P(x_{n-1}|x_n;\, t_n - t_{n-1})\, dx_1\, dx_2 \ldots dx_n \tag{2.3}$$

where

$$P(x|y;\, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{(y-x)^2}{2t}\right) \tag{2.4}$$

(choosing units so that $D = 1$).

Wiener then proved that if $G_0, G_1, G_2, \ldots$ are independent, Gaussian random variables each with mean 0 and variance 1 then

(a) The series

$$G_0 t + \sum_{n=1}^{\infty} \sum_{k=2^{n-1}}^{2^n-1} G_k \sqrt{2}\, \frac{\sin \pi k t}{\pi k} \tag{2.5}$$

converges *uniformly* with probability 1.

(b) Denoting by $x(t)$ the sum of the series in (a) one has

$$P\{\alpha_1 < x(t_1) < \beta_1, \ldots, \alpha_n < x(t_n) < \beta_n\} = \tag{2.6}$$

$$= \int_{\alpha_1}^{\beta_1} \cdots \int_{\alpha_n}^{\beta_n} P(0|x_1; t_1) \ldots P(x_{n-1}|x_n; t_n - t_{n-1})\, dx_1 \ldots dx_n ,$$

with P as given above.

Thus a measure in the space $C_0(0, 1)$ of continuous function $x(t)$, $(x(0) = 0)$, $0 < t < 1$, consistent with the *physical* theory of Brownian motion, is established by the mapping given by

$$x(t) = G_0 t + \sum_{n=1}^{\infty} \sum_{k=2^{n-1}}^{2^n-1} G_k \sqrt{2}\, \frac{\sin \pi k t}{\pi k} \tag{2.7}$$

of $C_0(0, 1)$ into the infinite product space $R \times R \times \ldots$ ($R \equiv$ the set of real numbers) with the Gaussian product measure.

The mapping is not quite one-to-one because while to each $x(t)$ in $C_0(0, 1)$ there corresponds a *unique* sequence $G_0, G_1, G_2, \ldots$ — the converse is only true if one allows a set of measure zero of exceptional sequences. In other words, only to *almost* every sequence $G_0, G_1, G_2, \ldots$ there corresponds a continuous function (recall that the series in (a) converges uniformly with *probability one* allowing for an exceptional event of probability zero when the series either doesn't converge at all or if it does converge its sum is not a continuous function).

Once the Lebesgue measure is constructed it is a matter of routine to define the Lebesgue integral with respect to the measure. The integral in probabilistic terminology is the mathematical expectation, and we shall throughtout these lectures use the symbol E for the integral.

Having established a Lebesgue measure (in $C_0(0, 1)$) Wiener then proved that almost every $x(t)$ is *nowhere* differentiable.

Let me conclude this part of the historical introduction with a number of remarks.

(*a*) To extend the construction of the measure to the space of continuous functions on the infinite interval $0 \leqslant t < \infty$ it is sufficient to construct infinitely many *independent* copies

$$x^{(k)}(t)\,, \qquad 0 \leqslant t \leqslant 1\,, \qquad x^{(k)}(0) = 0$$

(by simply taking many independent collections

$$(G_0^{(k)}, G_1^{(k)}, G_2^{(k)}, \ldots) \qquad k = 1, 2, \ldots)$$

and setting

$$x(t) = x^{(1)}(t) \qquad \text{for } 0 \leqslant t \leqslant 1$$

and

$$x(t) = x^{(1)}(1) + \ldots + x^{(k-1)}(1) + x^{(k)}\big(t - (k-1)\big)$$

for

$$k \leqslant t \leqslant k+1 \qquad (k > 1)\,.$$

(*b*) An alternative construction of the Wiener measure can be accomplished by means of a different representation which goes back to Paul Lévy and which I sketch here in a version devised by Z. Ciesielski [1].

We start with the orthonormal complete system of Haar, whose functions

$$h_0(t)\,, \qquad h_{2^n}^{(k)}(t)\,, \qquad 0 \leqslant k \leqslant 2^n - 1\,, \qquad 0 \leqslant t \leqslant 1$$

are defined as follows

$$h_0(t) \equiv 1\,,$$

$$h_n^{(k)}(t) = \begin{cases} +\sqrt{2^n} & \dfrac{k}{2^n} < t < \dfrac{k+\frac{1}{2}}{2^n}\,, \\ -\sqrt{2^n} & \dfrac{k+\frac{1}{2}}{2^n} < t < \dfrac{k+1}{2^n}\,, \\ 0 & \text{otherwise}\,, \end{cases}$$

for $n = 0, 1, \ldots$.

The integrals of the Haar functions

$$S_0(t) \equiv t\,,$$

$$S_{2^n}^{(k)}(t) = \int_0^t h_{2^n}^{(k)}(\tau)\,d\tau\,, \qquad n = 0, 1, 2, \ldots$$

are known as Schauder functions and they form a basis in the space of continuous functions

$$x(t)\,, \qquad x(0) = 0\,, \qquad 0 \leqslant t \leqslant i\,,$$

in the sense that every such $x(t)$ is *uniquely* representable as a *uniformly convergent* series of Schauder functions

$$x(t) = x_0 S_0(t) + \sum_{n=0}^{\infty} \sum_{k=0}^{2^n-1} x_{2^n}^{(k)} S_{2^n}^{(k)}(t)$$

(it is not necessary to partition the series into dyadic blocks).

To construct the measure we replace the x's by independent Gaussian random variables G_0, $G_{2^n}^{(k)}$ each with mean 0 and variance 1.

The proof that the series

$$G_0 t + \sum_{n=0}^{\infty} \sum_{k=0}^{2^n-1} G_{2^n}^{(k)} S_{2^n}^{(k)}(t)$$

converges uniformly with probability one and provides us with a suitable mapping to establish a Lebesgue measure in the space of continuous functions in $(0, 1)$ which vanish at the origin is much easier than for the Wiener representation and it remains equally easy (unlike in the Wiener case) if one abandons the dyadic partitioning.

(*c*) Neither the Wiener representation nor the one of Ciesielski are « natural » in the following sense:

Suppose we wish to calculate

$$E\left\{\exp\left(i\xi \int_0^1 x^2(\tau)\,d\tau\right)\right\}, \qquad \xi \text{ real}\,,$$

which is the characteristic function of the distribution of the functional

$$\int_0^1 x^2(\tau)\, d\tau\,.$$

Either the Wiener or the Lévy-Ciesielski representation gives

$$\int_0^1 x^2(\tau)\, d\tau = \sum_{i,j=0}^{\infty} a_{ij} G_i G_j$$

and upon diagonalizing the quadratic form on the right hand side we would get

$$\int_0^1 x^2(\tau)\, d\tau = \sum_{k=1}^{\infty} \lambda_k H_k^2\,,$$

where the H_k being *orthogonal* linear combinations of the G's are again independent, Gaussian random variables each with mean zero and variance 1.

It is now obvious that

$$E\left\{\exp\left(i\xi\int_0^1 x^2(\tau)\, d\tau\right)\right\} = \prod_{k=1}^{\infty} E\{\exp\,(i\xi\lambda_k H_k^2)\} = \prod_{k=1}^{\infty} \frac{1}{\sqrt{1-2i\xi\lambda_k}}\,.$$

But how does one find the λ's?

Here is a way to proceed. Let

$$\varphi_1(t),\ \varphi_2(t),\ \ldots,\ 0<t<1$$

be a *complete* orthonormal set and expand $x(t)$ in this system

$$x(t) \sim \sum_{n=1}^{\infty} L_n \varphi_n(t)\,,$$

$$L_n = \int_0^1 x(\tau)\varphi_n(\tau)\, d\tau\,.$$

Since $x(t)$ (either by the Wiener or the Ciesielski representation) is a linear combination of independent Gaussian variables (each with mean zero and variance 1) then clearly the L_n's are linear combinations of the same Gaussian variables. It is a well known and quite elementary fact that linear combination of independent Gaussian variables are themselves independent if and only if their correlations vanish. Thus for the L_n's to be independent it is necessary and sufficient that

$$E\left\{\int_0^1 x(t)\varphi_n(t)\,dt\int_0^1 x(t)\varphi_m(t)\,dt\right\} = 0$$

for $m \neq n$.

This condition is clearly equivalent to

$$\int_0^1\int_0^1 E\{x(t)x(s)\}\varphi_n(t)\varphi_m(s)\,dt\,ds = 0$$

(the interchange of the orders of integration being easily justified) and since

$$E\{x(t)x(s)\} = \text{Min}\,(t, s)$$

our condition is equivalent to

$$\int_0^1\int_0^1 \text{Min}\,(t, s)\varphi_n(t)\varphi_m(s)\,dt\,ds = 0\,, \qquad m \neq n\,.$$

It is obvious that if the φ_n's are eigenfunctions of the kernel Min (s, t) the condition above is satisfied and since Min (s, t) being a covariance (i.e. of the form $E\{x(t)x(s)\}$) is a positive definite kernel the φ's form a complete set. By Mercer's theorem we also have

$$\text{Min}\,(t, s) = \sum_{n=1}^{\infty} \lambda_n\varphi_n(t)\varphi_n(s)$$

the series being absolutely and uniformly convergent and the eigenvalues $\lambda_1, \lambda_2, \ldots$ positive.

We also have

$$E\{L_n^2\} = \int_0^1 \int_0^1 \text{Min}\,(t, s)\,\varphi_n(t)\,\varphi_n(s)\,dt\,ds = \lambda_n$$

and clearly

$$E\{L_n\} = 0\,.$$

Setting

$$L_n = \frac{H_n}{\sqrt{\lambda_n}}$$

we can write

$$x(t) \sim \sum_{n=1}^{\infty} \sqrt{\lambda_n}\, H_n \varphi_n(t)$$

where the H_n's are independent Gaussian variables each with mean zero and variance 1.

We now see that the λ_k's in the formula

$$E\left\{\exp\left(i\xi \int_0^1 x^2(\tau)\,d\tau\right)\right\} = \prod_{k=1}^{\infty} \frac{1}{\sqrt{1 - 2i\xi\lambda_k}}$$

are the eigenvalues of the kernel

$$\text{Min}\,(s, t)\,, \qquad 0 < s\,, \qquad t < 1\,.$$

It is an elementary exercise to verify that the integral equation

$$\int_0^1 \text{Min}\,(s, t)\,\varphi(t)\,dt = \lambda\varphi(s)$$

is equivalent to the differential equation

$$\varphi'' + \frac{1}{\lambda}\varphi = 0$$

with the boundary conditions

$$\varphi(0) = 0\,, \qquad \varphi'(1) = 0\,.$$

Thus

$$\varphi_n(t) = \sqrt{2}\sin\left(n + \frac{1}{2}\right)\pi t\,,$$

$$\lambda_n = \frac{1}{(n+\frac{1}{2})^2\pi^2}$$

and

$$E\left\{\exp\left(i\xi\int_0^1 x^2(\tau)\,d\tau\right)\right\} = \frac{1}{\sqrt{\cos\sqrt{2i\xi}}}\,.$$

This result was first derived in 1944 by Cameron and Martin [2] by a different method.

The « natural » reppresentation

$$x(t) \sim \sum_{n=1}^{\infty} \frac{H_n}{2(n+\frac{1}{2})\pi}\sqrt{2}\sin\left(n+\frac{1}{2}\right)\pi t$$

is a special case of a representation introduced by Kac and Siegert [3] (and suggested by a problem in the theory of noise in radio receivers [4]) and independently by Karhunen [5] and Loève [5*a*].

Cameron and Martin [6] also calculated

$$E\left\{\exp\left(i\xi\int_0^1 x^2(\tau)p(\tau)\,d\tau\right)\right\}$$

for $p(\tau) > 0$ and sufficiently regular (e.g. continuous). A slight modification of the method used above will yield the desired result.

Instead of the kernel Min (s, t) we consider the kernel

$$\sqrt{p(s)}\,\mathrm{Min}\,(s,t)\sqrt{p(t)}$$

and denote again by λ_n and $\varphi_n(t)$ its eigenvalues and normalized eigenfunctions.

If we now expand $\sqrt{p(t)}x(t)$ in the system $\{\varphi_n\}$

$$\sqrt{p(t)}\,x(t) \sim \sum_{n=1}^{\infty} L_n \varphi_n(t)\,,$$

$$L_n = \int_0^1 \sqrt{p(t)}\,x(t)\,\varphi_n(t)\,dt$$

again the L_n are linear combinations of independent Gaussian variables each of mean zero and variance one and

$$E\{L_m L_n\} = \int_0^1\int_0^1 \sqrt{p(t)}\ \mathrm{Min}\,(s,t)\sqrt{p(s)}\,\varphi_m(t)\varphi_n(s)\,dt\,ds = \lambda_n \delta_{mn}\,.$$

Setting again

$$L_n = H_n\sqrt{\lambda_n}$$

we get

$$\int_0^1 p(t)x^2(t)\,dt = \sum_{n=1}^{\infty} \lambda_n H_n^2$$

where the H_n are independent Gaussian variables each with mean zero and variance one.

Finally, as before,

$$E\left\{\exp\left(i\xi\int_0^1 p(t)x^2(t)\,dt\right)\right\} = \prod_{k=1}^{\infty} \frac{1}{\sqrt{1-2i\xi\lambda_k}}\,.$$

The λ_k's now turn out to be the eigenvalues of the Sturm-Liouville problem

$$\varphi''(t) + \frac{1}{\lambda}p(t)\varphi(t) = 0\,,$$

with the boundary condition

$$\varphi(0) = \varphi'(1) = 0\,.$$

This result was also obtained by Cameron and Martin [6] (by a different method) and it was the first indication that there may be an intimate connection between Wiener integrals and problems of analysis.

It should also be mentioned that quite recently A. M. Garsia, E. Rodemich and H. Rumsey Jr. [5b] proved directly that

$$\sum_{n=1}^{\infty} H_n \sqrt{\lambda_n} \varphi_n(t)$$

(for arbitrary non-negative sufficiently regular $p(t)$) is uniformly convergent with probability one and hence it can be used to construct the Wiener measure in $C_0(0, 1)$ thus by passing the other representations.

(*d*) If $p(t)$, $0 < t < 1$, changes sign the kernel

$$\sqrt{p(s)}\, \mathrm{Min}\,(s, t) \sqrt{p(t)}$$

is not hermitian and the method above fails. The result nevertheless remains valid as the following alternative derivation shows (1). For simplicity assume that $p(t)$ is continuous and note that (since $x(t)$ is also continuous)

$$\int_0^1 p(t) x^2(t)\, dt = \lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} p\left(\frac{k}{n}\right) x^2\left(\frac{k}{n}\right).$$

Thus for every real ξ

$$\lim_{n \to \infty} \exp\left(\frac{i\xi}{n} \sum_{k=1}^{n} p\left(\frac{k}{n}\right) x^2\left(\frac{k}{n}\right)\right) = \exp\left(i\xi \int_0^1 p(t) x^2(t)\, dt\right)$$

and since

$$\left| \exp\left(\frac{i\xi}{n} \sum_{k=1}^{n} p\left(\frac{k}{n}\right) x^2\left(\frac{k}{n}\right)\right) \right| = 1$$

(1) For details see [7].

we have by the Lebesgue bounded convergence theorem

$$\lim_{n\to\infty} E\left\{\exp\left(\frac{i\xi}{n}\sum_{k=1}^{n} p\left(\frac{k}{n}\right)x^2\left(\frac{k}{n}\right)\right)\right\} =$$

$$= E\left\{\exp\left(i\xi\int_0^1 p(t)x^2(t)\,dt\right)\right\}.$$

By the definition of the Wiener integral

$$E\left\{\exp\left(\frac{i\xi}{n}\sum_{k=1}^{n} p\left(\frac{k}{n}\right)x^2\left(\frac{k}{n}\right)\right)\right\}=$$

$$= \frac{(\sqrt{n})^n}{(\sqrt{2\pi})^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(\frac{i\xi}{n}\sum_{k=1}^{n} p\left(\frac{k}{n}\right)x_k^2\right)\exp\left(-\frac{n}{2}\sum_{k=1}^{n}(x_k-x_{k-1})^2\right)dx_1\ldots dx_n$$

$$(x_0=0).$$

Setting

$$\sqrt{\frac{n}{2}}\,x_k = y_k, \qquad k=1,2,\ldots,n$$

we obtain

$$E\left\{\exp\left(\frac{i\xi}{n}\sum_{k=1}^{n} p\left(\frac{k}{n}\right)x^2\left(\frac{k}{n}\right)\right)\right\} = \left[\mathrm{Det}\left(A_0^{(n)}-\frac{2i\xi}{n^2}R^{(n)}\right)\right]^{-\frac{1}{2}},$$

where $A_0^{(n)}$ is the (slightly modified) Jacobi matrix

$$\begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0\\ -1 & 2 & -1 & 0 & \cdots & 0\\ 0 & -1 & 2 & -1 & \cdots & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & \cdots & 0 & -1 & 2 & -1\\ 0 & \cdots & 0 & 0 & -1 & 1 \end{pmatrix}$$

and $R^{(n)}$ the diagonal matrix

$$R^{(n)} = \begin{pmatrix} p\left(\frac{1}{n}\right) & & & 0 \\ & p\left(\frac{2}{n}\right) & & \\ & & \ddots & \\ 0 & & & p\left(\frac{n}{n}\right) \end{pmatrix}.$$

It is obvious that

$$\det A_0^{(n)} = 1$$

and almost equally obvious that

$$A_{ij}^{(n)-1} = \text{Min}\,(i, j)\,.$$

Thus

$$\det\left(A_0^{(n)} - \frac{2i\xi}{n^2} R^{(n)}\right) =$$

$$= \det\left(I - \frac{2i\xi}{n^2} A_0^{(n)-1} R^{(n)}\right).$$

The (i, j) element of $A_0^{(n)-1} R^{(n)}$ is

$$\text{Min}\,(i, j)\, p\left(\frac{j}{n}\right)$$

and by a classic theorem of Hilbert the limit, as $n \to \infty$, of our determinant is the Fredholm determinant $D(2i\xi)$ of the kernel

$$\text{Min}\,(s, t)\, p(t)$$

which can easily be shown to be equal to

$$\prod_{k=1}^{\infty} (1 - 2i\xi\lambda_k)$$

where λ's are again the eigenvalues of

$$\varphi'' + \frac{1}{\lambda} p(t)\varphi = 0$$

with boundary condition

$$\varphi(0) = \varphi'(1) = 0 .$$

(*e*) It should be emphasized that the very existence of the measure and the integral can have purely analytic implications. For example the existence of the limit as $n \to \infty$ of the multiple integral

$$\frac{(\sqrt{n})^n}{(\sqrt{2\pi})^n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left(\frac{i\xi}{n} \sum_{k=1}^{n} p\left(\frac{k}{n}\right) x_k^2\right) \exp\left(-\frac{n}{2} \sum_{k=1}^{n} (x_k - x_{k-1})^2\right) dx_1 \ldots dx_n \qquad (x_0 = 0) ,$$

is a consequence of Lebesgue's bounded convergence theorem (for the Wiener integral).

In the sequel many other instances of analytic implications of the underlying measure theory will be (explicitely or implicitely) encountered.

(*f*) Wiener's way of introducing his measure in $C_0(0, 1)$ by an explicit construction tends to hide a subtlety of the problem which was brought up by Doob in a series of works culminating in his book [8].

Doob starts with the space of *all* real valued functions $x(t)$ $(x(0) = 0, 0 < t < \infty)$ and keeps the assignment of measure to the sets of functions

$$\{\alpha_1 < x(t_1) < \beta_1,\ \alpha_2 < x(t_2) < \beta_2 \ldots \alpha_n < x(t_n) < \beta_n\}$$

as given by the Einstein-Smoluchowski theory of Brownian motion.

It turns however out that the Borel field generated by the above « elementary » sets is too small in the sense that many interesting non-elementary sets turn out to be non-measurable. In particular, the set $C_0(0, \infty)$ of continuous functions is non-measurable! Fortunately its *outer* measure is one and because of this it is possible to concentrate the measure on it while maintaining the original assignment of measures to

the elementary sets. One is then led to back to the original Wiener measure having been however a little frightened in the process.

Lest the reader gets the impression that the measure theoretic subtleties are by and large of an exotic nature let me reassure him that this is not necessarily the case.

Some measure theoretic features which smack of pathology have purely analytic classical counterparts and in the next sections I shall discuss some examples.

SECTION 3

Elements of Probabilistic Potential Theory

The reader is by now sufficiently familiar with the measure and integration theory in $C_0(0, \infty)$ to believe that the extension from one space dimension to several should present no real difficulties.

Let us then take for granted that we have at our disposal a measure and integration theory in the space of all continuous curves in R_3 (three-dimensional Euclidean spaces) starting at the origin

$$r(t)\,, \qquad r(0) = 0\,, \qquad 0 < t < \infty\,.$$

Just to remind ourselves that we are dealing with Brownian motion of a free particle in three dimensions I shall write down the analogue of (2.6) and (2.4)

$$(3.1) \qquad P\{r(t_1) \in \Omega_1,\ r(t_2) \in \Omega_2,\ \ldots,\ r(t_n) \in \Omega_n\} =$$

$$= \int_{\Omega_1} \ldots \int_{\Omega_n} P(0|r_1;\, t_1)\, P(r_1|r_2;\, t_2 - t_1) \ldots P(r_{n-1}|r_n;\, t_n - t_n)\, dr_1 \ldots dr_n\,,$$

$$(3.2) \qquad P(r|\rho;\, t) = \frac{1}{(2\pi t)^{\frac{3}{2}}} \exp\left\{-\frac{\|r-\rho\|^2}{2t}\right\},$$

$\Omega_1, \Omega_2, \ldots, \Omega_n$ are Borel sets (in R_3) and $\|\alpha\|$ denotes the length of the vector α.

Consider now a closed region Ω which is the closure of its interior Ω_0 and denote by $V_\Omega(r)$ the indicator function of Ω, i.e.

$$(3.3) \qquad V_\Omega(r) = \begin{cases} 1\,, & r \in \Omega\,, \\ 0\,, & r \notin \Omega\,. \end{cases}$$

Let

$$T_\Omega(y) = \int_0^\infty V_\Omega(y + r(\tau))\, d\tau \,. \tag{3.4}$$

$T_\Omega(y)$ is clearly the *total* time the curve $y + r(\tau)$, $0 < \tau < \infty$, spends in Ω and for some curves this time is infinite. However for *almost all* curves it is finite as can be seen by calculating

$$E\left\{\int_0^\infty V_\Omega(y + r(\tau))\, d\tau\right\}.$$

Since everything in sight is non-negative we can interchange the order of integration $\left(E \text{ and } \int_0^\infty\right)$ obtaining

$$E\left\{\int_0^\infty V_\Omega(y + r(\tau))\, d\tau\right\} =$$

$$= \int_0^\infty d\tau\, E\{V_\Omega(y + r(\tau))\} =$$

$$= \int_0^\infty P\{y + r(\tau) \in \Omega\}\, d\tau =$$

$$= \int_0^\infty d\tau \int_\Omega \frac{\exp\left\{-\dfrac{\|r - y\|^2}{2\tau}\right\}}{(2\pi\tau)^{\frac{3}{2}}}\, dr =$$

$$= \int_\Omega dr \int_0^\infty \frac{1}{(2\pi\tau)^{\frac{3}{2}}} \exp\left\{-\frac{\|r - y\|^2}{2\tau}\right\} d\tau =$$

$$= \frac{1}{2\pi} \int_\Omega \frac{1}{\|r - y\|}\, dr < \infty \,.$$

Since the expectation (Wiener integral) of $T_\Omega(y)$ is finite it follows that $T_\Omega(y)$ itself is finite with probability one (i.e. almost every three-

dimensional Brownian path spends a finite time in Ω). In two dimensions (as well as in one) with probability one the path spends an infinite time in every region.

Higher moments of $T_\Omega(y)$ can also be easily calculated. For example,

$$E\{T_\Omega^2(y)\} = E\left\{\left(\int_0^\infty V_\Omega(y + r(\tau))\, d\tau\right)^2\right\} =$$

$$= 2!\iint\limits_{0\leqslant\tau_1<\tau_2<\infty} E\{V_\Omega(y + r(\tau_1))\, V(y + r(\tau_2))\}\, d\tau_1\, d\tau_2 =$$

$$= 2!\iint\limits_{0\leqslant\tau_1<\tau_2<\infty} P\{y + r(\tau_1) \in \Omega,\ y + r(\tau_2) \in \Omega\}\, d\tau_1\, d\tau_2 =$$

$$= 2!\iint\limits_{0\leqslant\tau_1<\tau_2<\infty} \int_\Omega\int_\Omega P(y|r_1;\ \tau_1) P(r_1|r_2;\ \tau_2 - \tau_1)\, dr_1\, dr_2\, d\tau_1\, d\tau_2 =$$

$$= 2!\,\frac{1}{(2\pi)^2}\int_\Omega\int_\Omega \frac{1}{\|r_1 - y\|}\,\frac{1}{\|r_2 - r_1\|}\, dr_1\, dr_2$$

where it is understood that here as well as in the sequel

$$\int_\Omega d\rho \ldots$$

is a multiple integral (triple in our case) with $d\rho$ denoting the (multi-dimensional) element of integration.

Similarly for every positive integer k we have

$$E\{T_\Omega^k(y)\} = k!\,\frac{1}{(2\pi)_k}\int_\Omega\ldots\int_\Omega \frac{1}{\|r_1 - y\|}\,\frac{1}{\|r_2 - r_1\|}\,\frac{1}{\|r_k - r_{k-1}\|}\, dr_1 \ldots dr_k\,.$$

The kernel

$$\frac{1}{2\pi}\,\frac{1}{\|r - \rho\|} \qquad r, \rho \in \Omega\,,$$

is easily seen to be positive definite and of the Hilbert-Schmidt type. Denoting by $\lambda_1, \lambda_2, \ldots$ its eigenvalues by $\varphi_1(\rho), \varphi_2(\rho), \ldots$ the corresponding

normalized eigenfunctions, we obtain

$$E\{T_\Omega^k(y)\} = k! \sum_{j=1}^{\infty} \lambda_j^{k-1} \int_\Omega \varphi_j(\rho)\, d\rho \, \frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho\,.$$

For sufficiently small $|z|$ (z complex) it follows that

$$E\{\exp(zT_\Omega(y))\} = \tag{3.7}$$

$$= 1 + z \sum_{j=1}^{\infty} \frac{1}{1 - z\lambda_j} \int_\Omega \varphi_j(\rho)\, d\rho \, \frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho\,.$$

It is easily seen that both sides of (3.7) are analytic in the right half plane $\mathrm{Re}\, z > 0$ and that hence (3.7) is valid throughout this half plane. In particular, for $u > 0$ we have

$$1 - E\{\exp(-uT_\Omega(y))\} = \tag{3.8}$$

$$= u \sum_{j=1}^{\infty} \frac{1}{1 + \lambda_j u} \int_\Omega \varphi_j(\rho)\, d\rho \, \frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho\,.$$

Consider now the L^2 function $f_u(r)$ for $r \in \Omega$ defined by the formula

$$f_u(r) \sim \frac{1}{2\pi} \sum_{j=1}^{\infty} \frac{u}{1 + \lambda_j u} \int_\Omega \varphi_j(\rho)\, d\rho\, \varphi_j(r) \tag{3.9}$$

and note that

$$1 - E\{\exp(-uT_\Omega(y))\} = \int_\Omega \frac{f_u(\rho)}{\|\rho - y\|}\, d\rho\,.$$

For $y \in \Omega$

$$\frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho = \lambda_j \varphi_j(y)$$

and hence

$$1 - E\{\exp(-uT_\Omega(y))\} = \sum_{j=1}^{\infty} \frac{u\lambda_j}{1 + u\lambda_j} \int_\Omega \varphi_j(\rho)\, d\rho\, \varphi_j(y)\,. \tag{3.10}$$

Integrating both sides of (3.10) over a region A contained in Ω ($A \subset \Omega$) we have

$$\int_A [1 - E\{\exp(-uT_\Omega(y))\}]\, dy =$$

$$= \sum_{j=1}^{\infty} \frac{u\lambda_j}{1+u\lambda_j} \int_\Omega \varphi_j(\rho)\, d\rho \int_A \varphi_j(y)\, dy = |A| - \int_A f_u(y)\, dy\,,$$

use having been made of the Parseval relation

$$|A| = \sum_{j=1}^{\infty} \int_\Omega \varphi_j(\rho)\, d\rho \int_A \varphi_j(y)\, dy\,.$$

Since both u and $T_\Omega(y)$ are non-negative we have

$$0 < \int_A [1 - E\{\exp(-uT_\Omega(y))\}]\, dy < |A|\,,$$

where $|A|$ denotes the Lebesgue measure of A. It therefore follows that

$$0 < \int_A f_u(r)\, dr < |A|$$

and hence

$$\mu_u(A) = \int_A f_u(r)\, dr \tag{3.11}$$

is a bounded *positive* Radon measure.

We can now write

$$1 - E\{\exp(-uT_\Omega(y))\} = \int_\Omega \frac{\mu_u(d\rho)}{\|\rho - y\|} \tag{3.12}$$

and let $u \uparrow \infty$.

The left hand side of (3.12) aproaches

$$P\{T_\Omega(y) > 0\}$$

while (at least through an appropriate subsequence) the right hand side approaches

$$\int_{\Omega} \frac{\mu(d\rho)}{\|\rho - y\|}.$$

Thus

$$U(y) = P\{T_\Omega(y) > 0\} = \int_{\Omega} \frac{\mu(d\rho)}{\|\rho - y\|} \tag{3.13}$$

so that $P\{T_\Omega(y) > 0\}$ is a *potential of a non-negative mass distribution.*

It can be shown that

$$U(y) \to 0 \qquad \text{as} \qquad \|y\| \to \infty$$

and that

$$U(y) \to 1$$

as y approaches a (properly defined) regular point on the boundary of Ω. For a wide class of regions $U(y)$ is therefore its capacity potential.

Now, it is well known from the classical theory of the Newtonian potential that the charge $\mu(d\rho)$ is concentrated on the boundary of the region. What I want to emphasize is that this fact is intimately related (in fact, essentially equivalent) to the continuity of Brownian paths.

In fact, let $y \notin \Omega$ and cut out an arbitrarily large open subregion B contained in the open interior Ω_0 ($B \subset \Omega_0$). Now, because of continuity of the paths

$$P\{T_\Omega(y) > 0\} = P\{T_{\Omega - B}(y) > 0\}$$

and therefore μ is concentrated on $\Omega - B$ for every $B \subset \Omega_0$, i.e. on the boundary of Ω.

To dramatize a little more the interplay of measure theoretic and purely analytic aspects let me consider briefly the following problem.

The Wiener measure as we have seen was based on assigning the measures (2.3) to sets (2.2) with P given by the formula (2.4). The choice of P is *not* arbitrary since consistence of the assignment requires that P satisfy the Chapman-Kolmogorov (or more justly the Einstein-Smolu-

chowski) equation

$$P(x|y;\, t+\tau) = \int_{-\infty}^{\infty} P(x|\zeta;\, t)\, P(\zeta|y;\, r)\, d\zeta \tag{3.14}$$

for all positive t and τ. If we further assume that $P(x|y;\, t)$ be spatially homogeneous (i.e. dependend only on $y-x$) and symmetric, then the only solutions are of the form

$$P(y-x;\, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left(-t|\xi|^{\alpha}\right) \exp\left(i\xi(y-x)\right) d\xi$$

with $0<\alpha\leqslant 2$. Can one use these P's to construct a Wiener like measure? The answer is « yes », but the measure can no longer be concentrated on the space of continuous functions!

Let me prove it in the case $\alpha<1$ since it is simpler than the case $1\leqslant\alpha<2$.

We simply imitate word for word the potential theoretic considerations at the beginning of this section replacing Ω by the interval

$$(-1,\, 1) \quad \text{and} \quad r(\tau), \qquad 0\leqslant\tau<\infty$$

by the process

$$x(\tau), \qquad x(0)=0, \qquad 0\leqslant\tau<\infty,$$

based on P given by the formula (3.14).

We are then led to the result that

$$U(y) = P\{T_{\Omega}(y)>0\} = \int \frac{\mu(dx)}{|x-y|^{\alpha}}$$

and if the paths were continuous μ would be concentrated in points -1, $+1$ yielding

$$U(y) = \frac{\mu(1)}{|1-y|^{1-\alpha}} + \frac{\mu(-1)}{|1+y|^{1-\alpha}}.$$

On the other hand for $-1<y<1$, $U(y)$ must clearly be equal to 1 and it is equally clear that for no choice of $\mu(1)$ and $\mu(-1)$ is this possible.

SECTION 4

Asymptotics of the Number of Bound States of Certain Schrödinger Equations and Related Topics

The calculations of the preceeding section contain the seeds of a probabilistic approach to Potential Theory, a subject which has received much attention in the mathematical literature of the past thirty years. I shall not dwell farther upon Potential Theory having recently reviewed the subject in a monograph [9]. I shall, however, sketch a related development because it is closely tied to a subject which has recently been actively pursued by a number of investigators.

I shall do it in a partly historical (and even autobiographical) setting because I believe that something may be learned from such a presentation.

My own interest in probabilistic Potential Theory originated in an attempt to prove a conjecture of Erdös to the effect that for $\beta \to \infty$

$$P\{T_\Omega(y) > \beta\} \sim C \exp(-\mu\beta) . \tag{4.1}$$

The conjecture had nothing to say about the constants C and μ except, of course, that both depended on the region Ω and possibly on y.

This was in the late forties and we all knew much less about connections between differential and integral equations on the one hand and Probability Theory on the other, than we do now.

Mathematicians, or rather mathematical analysts, are divided roughly speaking into two classes: the « calculators », i.e. those who look for exact formulas, and the « estimators », i.e. those who live by inequalities. I belong to the first class while Erdös is one of the most brilliant

representative of the second. Naturally then I began to look for a formula for

$$P\{T_\Omega(y) > \beta\} .$$

This led to the calculation of the moments

$$E\{T_\Omega^k(y)\}$$

and the moment generating function

$$E\{\exp(-uT_\Omega(y))\}, \qquad u > 0 .$$

Setting

$$\sigma(\beta) = P\{T_\Omega(y) < \beta\}$$

we rewrite (3.8) in the equivalent form

$$\int_0^\infty \exp(-u\beta)\, d\sigma(\beta) = 1 - u \sum_{j=1}^\infty \frac{1}{1+u\lambda_j} \int_\Omega \varphi(\rho)\, d\rho \frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho$$

and in a few elementary steps we arrive at

$$P\{T_\Omega(y) > \beta\} = 1 - \sigma(\beta) = \sum_{j=1}^\infty \frac{a_j}{\lambda_j} \exp(-\beta/\lambda_j)$$

where

$$a_j = \int_\Omega \varphi_j(\rho)\, d\rho \frac{1}{2\pi} \int_\Omega \frac{\varphi_j(\rho)}{\|\rho - y\|}\, d\rho .$$

Thus

$$P\{T_\Omega(y) > \beta\} \sim a_1 \exp(-\beta/\lambda_1)$$

confirming Erdös' conjecture with $C = a_1/\lambda_1$ and $\mu = 1/\lambda_1$.

This as well as other results tended to focus attention on the integral equation

$$\frac{1}{2\pi} \int_\Omega \frac{\varphi(\rho)}{\|\rho - r\|}\, d\rho = \lambda\varphi(r) , \qquad r \in \Omega \tag{4.2}$$

and almost as an afterthought I tried to determine the asymptotic behavior of the eigenvalues λ_n as $n \to \infty$. The answer was easy to guess because the integral equation is equivalent to the differential equation

$$\frac{1}{2}\nabla^2\varphi + \frac{1}{\lambda}\varphi = 0\,, \qquad r \in \Omega_0\,,$$

with the « boundary conditions »

$$\int_S \left\{\varphi(\rho)\frac{\partial}{\partial n}\left[\frac{1}{\|r-\rho\|}\right] - \frac{\partial\varphi(\rho)}{\partial n}\,\frac{1}{\|r-\rho\|}\right\} d\sigma = 0 \tag{4.3}$$

for *every* $r \in \Omega_0$. S denotes the boundary surface of Ω and $d\sigma$ the surface element.

At the time these developments were taking place I have formulated H. Weyl's celebrated theorem about the asymptotic behavior of the eigenvalues of the Laplacian in terms of what I called « the principle of not feeling the boundary », and this principle implied (heuristically of course) that the asymptotic behavior of the eigenvalues of the Laplacian is the same ***regardless*** of the boundary condition.

This led to the conjecture that as $\lambda \to \infty$

$$\sum_{\lambda_j^{-1}<\lambda} 1 \sim \frac{\sqrt{2}}{3}\,\frac{|\Omega|}{\pi^2}\,\lambda^{\frac{3}{2}}$$

where $|\Omega|$ is the volume of Ω.

Since the « boundary condition » (4.3) was so unusual it seemed worthwhile to prove (4.3).

To do this it seemed useful to consider not just the *total* time

$$T_\Omega(y) = \int_0^\infty V_\Omega\big(y + r(\tau)\big)\,d\tau$$

the curve $y + r(\tau)$ spends in Ω but also the time « up to t »

$$T_\Omega(y;\,t) = \int_0^t V_\Omega\big(y + r(\tau)\big)\,d\tau\,;$$

and it seemed also useful to calculate

$$\int_0^\infty E\left\{\exp\left(-u\int_0^t V_\Omega(y+r(\tau))\,d\tau\right)V_A(y+r(t))\right\}dt$$

(V_A is, of course, the indicator function of the A).

It is just as easy as it was to derive (3.10) to obtain the formula

$$\int_0^\infty E\left\{\exp\left(-u\int_0^t V_\Omega(y+r(\tau))\,d\tau\right)V_A(y+r(t))\right\}dt = \sum_{j=1}^\infty \frac{\lambda_j}{1+u\lambda_j}\int_A \varphi_j(r)\,dr\,\varphi_j(y) \tag{4.6}$$

provided $A \subset \Omega$ and $y \in \Omega$. By a simple inversion we now obtain

$$\int_0^\infty P\left\{\int_0^t V_\Omega(y+r(\tau))\,d\tau > \beta;\ y+r(t)\in A\right\}dt = \sum_{j=1}^\infty \exp(-\beta/\lambda_j)\lambda_j\int_A \varphi_j(r)\,dr\,\varphi_j(y)\,.$$

Let now A be the sphere of radius δ center at y: dividing both sides by the volume of A and letting $\delta \to 0$ we obtain

$$\frac{1}{(\sqrt{2\pi})^3}\int_0^\infty \frac{1}{t^{\frac{3}{2}}}P\left\{\int_0^t V_\Omega(y+r(\tau))\,d\tau > \beta \mid r(t)=0\right\}dt = \sum_{j=1}^\infty \exp\left(-\beta(-\beta/\lambda_j)\right)\lambda_j\varphi(y)\,. \tag{4.7}$$

We have used here conditional probability defined by the usual formula

$$P\left\{\int_0^t V_\Omega(y+r(\tau))\,d\tau > \beta \mid r(t)=0\right\} = \lim_{\delta\to 0}\frac{P\left\{\int_0^t V_\Omega(y+r(\tau))\,d\tau > \beta,\ y+r(t)\in A\right\}}{P\{y+r(t)\in A\}}$$

and the trivial observation that

$$\lim_{\delta \to 0} \frac{P\{y + r(t) \in A\}}{|A|} = \frac{1}{(\sqrt{2\pi t})^3} .$$

Integrating (4.7) over Ω with respect to y we obtain

$$\frac{1}{(\sqrt{2\pi})^3} \int_\Omega dy \int_0^\infty \frac{1}{t^{\frac{3}{2}}} P\left\{ \int_0^t V_\Omega(y + r(\tau))\, d\tau > \beta | r(t) = 0 \right\} dt = \tag{4.8}$$

$$= \sum_{j=1}^\infty \exp(-\beta/\lambda_j)\, \lambda_j .$$

If we now set

$$t = \beta\xi , \qquad \tau = \beta\eta$$

we can rewrite (4.8) in the equivalent form

$$\sum_{j=1}^\infty \exp(-\beta/\lambda_j)\, \lambda_j =$$

$$= \frac{1}{\beta^{\frac{3}{2}}} \frac{1}{(\sqrt{2\pi})^3} \int_\Omega dy \int_0^\infty \frac{1}{\xi^{\frac{3}{2}}} P\left\{ \int_0^\xi V_\Omega(y + r(\beta\eta))\, d\eta > 1 | r(\beta\xi) = 0 \right\} d\xi .$$

The integration on ξ is actually from 1 to ∞ since for $\xi < 1$

$$\int_0^\xi V_\Omega(y + r(\beta\eta))\, d\eta < 1$$

and hence

$$P\left\{ \int_0^\xi V_\Omega(y + r + (\beta\eta))\, d\eta > 1 | r(\beta\xi) = 0 \right\} = 0 .$$

It is now convenient to observe that the statistical properties of

$r(\beta\eta)$ are the same as those of $\sqrt{\beta}\, r(\eta)$ so that

$$P\left\{\int_0^{\xi} V_\Omega(y + r(\beta\eta))\, d\eta > 1 | r(\beta\xi) = 0\right\} =$$

$$= P\left\{\int_0^{\xi} V_\Omega(y + \sqrt{\beta}\, r(\eta))\, d\eta > 1 | r(\xi) = 0\right\}.$$

Thus as $\beta \to 0$ this probability for $y \in \Omega$ and $\xi > 1$ clearly approaches 1.

We therefore have, asymptotically as $\beta \to 0$

$$\sum_{j=1}^{\infty} \exp(-\beta/\lambda_j)\, \lambda_j \sim \frac{2|\Omega|}{(\sqrt{2\pi})^3} \frac{1}{\beta^{\frac{3}{2}}}$$

and by a Tauberian theorem

$$\sum_{\lambda_j^{-1} < \lambda} \lambda_j \sim \frac{\sqrt{2}\,|\Omega|}{\pi^2} \sqrt{\lambda}\,, \qquad \lambda \to \infty$$

which implies almost at once that

$$\sum_{\lambda_j^{-1} < \lambda} 1 \sim \frac{\sqrt{2}\,|\Omega|}{3\pi^2} \lambda^{\frac{3}{2}}. \tag{4.9}$$

The above calculations can be immediately extended in two directions.

First, $V_\Omega(r)$ can be replaced by a general non-negative $V(r)$ which is integrable over the whole space

$$\int V(r)\, dr < \infty$$

and satisfies mild regularity conditions.

For example, formula (4.6) becomes now

$$\sqrt{V(y)} \int_0^{\infty} E\left\{\exp\left(-u \int_0^t V(y + r(\tau))\, d\tau\right) \sqrt{V(y + r(t))} \cdot \right.$$

$$\left. \cdot V_A(y + r(t))\right\} dt = \sum_{j=1}^{\infty} \frac{\lambda_j}{1 + u\lambda_j} \int_A \varphi_j(r)\, dr\, \varphi_j(y) \tag{4.10}$$

where the λ's and the φ's are now the eigenvalues and the (normalized) eigenfunctions of the kernel

$$\frac{1}{2\pi}\sqrt{V(r)}\,\frac{1}{\|r-\rho\|}\sqrt{V(\rho)} \tag{4.11}$$

and the asymptotic formula (4.9) becomes

$$\sum_{\lambda_j^{-1}<\lambda} 1 \sim \frac{\sqrt{2}}{3\pi^2}\int V^{\frac{3}{2}}(r)\,dr\,\lambda^{\frac{3}{2}}\,, \qquad \lambda\to\infty\,. \tag{4.12}$$

From the mathematical point of view this is not much of a generalization since no new idea is needed and the result doesn't seem to be, in itself, particularly interesting. But appearances are deceiving as we shall see in a moment.

Consider the Schrödinger equation

$$\tfrac{1}{2}\nabla^2\psi = AV(r)\psi = -E\psi \qquad (A>0)\,, \tag{4.13}$$

where $V(r)$ is non-negative, integrable (over the whole space) and satisfying (mild) regularity conditions needed to justify the formal steps leading to (4.10).

If we are interested in bound states, i.e. solutions of (4.13) which are square integrable we must have $E<0$ and we can therefore set

$$E = -\varkappa^2 \qquad (\varkappa \text{ real})\,.$$

The differential equation (4.13) with $E=-\varkappa^2$ is equivalent to the integral equation

$$\frac{1}{A}\psi(r) = \frac{1}{2\pi}\int \frac{\exp\{-\varkappa\sqrt{2}\,\|r-\rho\|\}}{\|r-\rho\|}\,V(\rho)\psi(\rho)\,d\rho \tag{4.14}$$

which by setting

$$\varphi(r) = \sqrt{V(r)}\,\psi(r)$$

becomes

$$\frac{1}{A}\varphi(r) = \frac{1}{2\pi}\int\sqrt{V(r)}\,\frac{\exp\{-\varkappa\sqrt{2}\,\|r-\rho\|\}}{\|r-\rho\|}\,\sqrt{V(\rho)}\varphi(\rho)\,d\rho\,. \tag{4.15}$$

If we denote by $\lambda_1(\varkappa)$, $\lambda_2(\varkappa)$, ... the eigenvalues of the kernel

$$\frac{1}{2\pi}\sqrt{V(r)}\,\frac{\exp\{-\varkappa\sqrt{2}\,\|r-\rho\|\}}{\|r-\rho\|}\,\sqrt{V(\rho)} \tag{4.16}$$

then we see that the energies $\varkappa_1^2$, $\varkappa_2^2$, ... of the bound states (if any) are obtained by solving the equations

$$\frac{1}{A}=\lambda_1(\varkappa_1)\,,\qquad \frac{1}{A}=\lambda_2(\varkappa_2)\,,\qquad \ldots\,.$$

Since for every $\varkappa$ $\lambda_n(\varkappa)\to 0$ (decreasingly) as $n\to\infty$ and since for

$$\varkappa\to 0\qquad \lambda_n(\varkappa)\to\lambda_n(0)=\lambda_n$$

the eigenvalues of the kernel (4.11) it follows that the number $n(A)$ of bound states is equal to the number of eigenvalues of the kernel (4.11) which exceed A^{-1}. In other words

$$n(A)=\sum_{\lambda_j^{-1}<A}1\,. \tag{4.17}$$

This elegant result connecting the number of bound states of the Schrödinger equation (4.13) and the number of eigenvalues of the kernel (4.11) whose inverses do not exceed A is due to J. Schwinger [10] and it immediately adds spice to formula (4.12) since it now reads

$$n(A)\sim\frac{\sqrt{2}}{3\pi^2}\int V^{\frac{3}{2}}(r)\,dr\,A^{\frac{3}{2}}\,,\qquad A\to\infty\,,$$

an asymptotic result first obtained by A. Martin [11].

The second direction in which the results of this section can be extended is to replace $r(\tau)$ by the process $x(\tau)$,

$$0<\tau<\infty\,,\qquad x(0)=0\,,$$

mentioned at the end of Section 3.

In this case as we have seen the paths are not continuous, but this does not prevent one from imitating the formal steps and we reach the

formula

$$\sqrt{V(y)}\int_0^\infty E\left\{\exp\left(-u\int_0^t V(y+x(\tau))\,d\tau\right)\sqrt{V(y+x(t))}\,V_\Delta(y+x(t))\right\}dt =$$

$$=\sum_{j=1}^\infty \frac{\lambda_j}{1+u\lambda_j}\int_\Delta \varphi_j(x)\,dx\,\varphi_j(y)$$

where the λ's and φ's are the eigenvalues and (normalized) eigenfunctions of the kernel

$$C(\alpha)\sqrt{V(x)}\,\frac{1}{|x-y|^{1-\alpha}}\sqrt{V(y)}$$

where

$$C(\alpha)\,\frac{1}{|x-y|^{1-\alpha}} = \int_0^\infty \frac{1}{2\pi}\int_{-\infty}^\infty \exp\left(-t|\xi|^\alpha\right)\exp\left(i\xi(x-y)\right)d\xi\,dt =$$

$$=\frac{1}{2\pi}\int_{-\infty}^\infty \frac{\cos\xi(x-y)}{|\xi|^\alpha}\,d\xi = \frac{1}{2\pi}\int_{-\infty}^\infty \frac{\cos\xi}{|\xi|^\alpha}\,d\xi\,\frac{1}{|x-y|^{1-\alpha}}$$

i.e.

$$C(\alpha) = \frac{1}{2\pi}\int_0^\infty \frac{\cos\xi}{|\xi|^\alpha}\,d\xi\,.$$

The analogue of (4.8) is now

$$\frac{1}{2\pi\alpha}\Gamma\left(\frac{1}{\alpha}\right)\int_{-\infty}^\infty V(y)\int_0^\infty \frac{1}{t^{1/\alpha}}P\left\{\int_0^t V(y+x(\tau))\,d\tau > \beta\,|\,x(t)=0\right\}dt\,dy =$$

$$=\sum_{j=1}^\infty \exp\left(-\beta/\lambda_j\right)\lambda_j$$

and again as before one obtains

$$\sum_{\lambda_j^{-1}<\lambda} 1 \sim \frac{1}{\pi}\int V^{1/\alpha}(x)\,dx\,\lambda^{1/\alpha}\,, \qquad \lambda\to\infty\,.$$

The result was first proved by me in [12] and subsequently by H. Widom [13] by a purely analytic method without any reference to probability or integration in function spaces.

Finally it should be mentioned that derivation of (4.6) can be trivially modified to give

$$(4.18)\qquad \sqrt{V(y)}\int_0^\infty \exp(-st)E\left\{\exp\left(-u\int_0^t V(y+r(\tau))\,d\tau\right)\sqrt{V(y+r(t))}\cdot\right.$$

$$\left.\cdot\sqrt{V_A(y+r(t))}\right\}dt=\sum_{j=1}^{\infty}\frac{\lambda_j(s)}{1+u\lambda_j(s)}\psi_j^{(s)}(y)\int_A\psi_j^{(s)}(r)\,dr\,,$$

where the $\gamma_j(s)$ and the $\psi_j^{(s)}$ are the eigenvalues and the (normalized) eigenfunctions of the kernel:

$$\sqrt{V(\varrho)}\,\frac{\exp\left(-\sqrt{2s}\,\|r-\varrho\|\right)}{2\pi\|r-\varrho\|}\,\sqrt{V(r)}\,.$$

If we multiply both sides of (4.18) by a suitable $h(u)$ and integrate (on u) from 0 to ∞ we obtain

$$\sqrt{V(y)}\int_0^\infty \exp[-st]E\left\{f\left(\int_0^t V(y+r(\tau)\,d\tau)\sqrt{V(y+r(t))}\sqrt{V_A(y+r(t))}\right\}dt=\right.$$

$$=\sum F(\lambda_j(s))\psi_j^{(s)}(y)\int_A\psi_j^{(s)}(r)\,dr\,,$$

where

$$f(x)=\int_0^\infty h(u)\exp(-ux)\,du$$

and

$$F(y)=y\int_0^\infty \exp(-x)f(xy)\,dx\,.$$

One can now pass to conditional expectations and integrate over y obtaining

$$\frac{1}{(\sqrt{2\pi})^3}\int dy\, V(y)\int_0^\infty \frac{\exp(-st)}{t^{\frac{3}{2}}}\, E\left\{f\left(\int_0^t V(y+r(\tau))\,d\tau\right)\middle| r(t)=0\right\}dt =$$

$$=\sum_{j=1}^{\infty} F(\lambda_j(s))\,.$$

This slight modification of (4.8) is called Lieb's formula in a recent book [14] by B. Simon.

SECTION 5

Scattering Length and Capacity

Closely related to the subject matter of the two preceding sections is the concept of scattering length. Apart from the intrinsic interest of this concept a discussion of this topic in these lectures is further justified by the fact that it was Enrico Fermi who introduced scattering length into nuclear physics (see e.g. [15]).

Let us begin with a brief review of the basic facts of quantum mechanical scattering theory.

Let, as before, $V(r)$ be a non-negative function such that

$$\int V(r)\,dr < \infty$$

and again satisfying mild regularity conditions.

The scattering problem is to find the solution of the Schrödinger equation

$$\frac{1}{2}\nabla^2\varphi - V(r)\varphi = -\varkappa^2\varphi \qquad (\varkappa \text{ real})$$

which at infinity (i.e. as $\|r\| \to \infty$) has the asymptotic behavior

$$\varphi_\varkappa(r) \sim \exp\left(i\varkappa\sqrt{2}\,z\right) + f_\varkappa(e)\frac{\exp\left(i\varkappa\sqrt{2}\,\|r\|\right)}{\|r\|} \tag{5.1}$$

where e is the unit vector in direction r i.e.

$$e = \frac{r}{\|r\|}\,.$$

The first term on the right hand side of (5.1) is the incident plane wave in the direction of z-axis and the second term represents the (asymptotically) principal part of the scattered wave. The complex scalar $f_\varkappa(e)$ is called the scattering amplitude and the integral

$$\sigma^2 = \int_{S(1)} |f_\varkappa(e)^2| \, d\sigma$$

over the surface $S(1)$ of the unit sphere of the absolute square of the scattering amplitude is called the scattering cross-section.

It is easy to see and not too difficult to show that $\varphi_\varkappa(r)$ is the (*unique*) solution of the integral equation

$$\varphi_\varkappa(r) = \exp(i\varkappa\sqrt{2}z) - \frac{1}{2\pi}\int \frac{\exp(i\varkappa\sqrt{2}\,\|r-\rho\|)}{\|\rho - r\|} V(\rho)\varphi_\varkappa(\rho)\, d\rho \tag{5.2}$$

from which it follows that

$$f_\varkappa(e) = -\frac{1}{2\pi}\int \exp(i\varkappa\sqrt{2}\,\|r\cdot e\|)\,\varphi_\varkappa(r)\, V(r)\, dr\,. \tag{5.3}$$

In the low energy limit $\varkappa \to 0$ the integral equation (5.2) assumes the form

$$\varphi_0(r) = 1 - \frac{1}{2\pi}\int \frac{\varphi_0(\rho)\, V(\rho)}{\|r-\rho\|}\, d\rho \tag{5.4}$$

and the scattering amplitude becomes independent of e

$$f_0(e) = -\Gamma = -\frac{1}{2\pi}\int V(r)\varphi_0(r)\, dr\,. \tag{5.5}$$

If due attention is paid to physical dimensions it turns out that Γ has the dimension of length and it is called the scattering length.

Consider now the expression

$$G_s(y) = s\int_0^\infty \exp(-st)\, E\left\{\exp\left(-\int_0^t V(y + r(\tau))\, d\tau\right)\right\} dt \tag{5.6}$$

where $s > 0$.

By calculations similar to those of Section 3 we find that G_s satisfies the integral equation

$$G_s(y) = 1 - \frac{1}{2\pi} \int \frac{\exp\left(-\sqrt{2s}\,\|y-r\|\right)}{\|y-r\|} V(r) G_s(r)\, dr \tag{5.7}$$

from which it follows almost at once that

$$\int (1 - G_s(y))\, dy = \frac{1}{s} \int V(r) G_s(r)\, dr\,. \tag{5.8}$$

Formula (5.8) can be rewritten in the equivalent form

$$\int_0^\infty \exp(-st) \int E\left\{1 - \exp\left(-\int_0^t V(y + r(\tau))\, d\tau\right) dy\right\} dt = \tag{5.9}$$

$$= \frac{1}{s^2} \int V(r) G_s(r)\, dr$$

and from (5.2) and (5.7) we see that

$$\lim_{s \to 0} G_s(r) = \varphi_0(r)\,.$$

Thus for $s \to 0$ we have the asymptotic formula

$$\int_0^\infty \exp(-st) \int E\left\{1 - \exp\left(-\int_0^t V(y + r(\tau))\, d\tau\right)\right\} dy\, dt \sim \frac{2\pi\Gamma}{s^2} \tag{5.10}$$

and hence, by a Tauberian theorem,

$$\int E\left\{1 - \exp\left(-\int_0^t V(y + r(\tau))\, d\tau\right)\right\} dy \sim 2\pi\Gamma t \tag{5.11}$$

as $t \to \infty$.

It is well known that for a « hard » potential, i.e.

$$V(r) = \begin{cases} +\infty\,, & r \in \Omega\,, \\ 0\,, & r \notin \Omega\,, \end{cases}$$

the scattering length is equal to the capacity of Ω (about the region Ω we make the same assumptions as in Section 3).

Let me sketch a derivation of this result to illustrate once again the interplay between probabilistic and purely analytic ideas.

If I set

$$V(r) = uV_\Omega(r)$$

then (5.7) becomes

$$G_s(y; u) = 1 - \frac{u}{2\pi} \int_\Omega \frac{\exp\left(-\sqrt{2s}\,\|y-r\|\right)}{\|y-r\|} G_s(r; u)\, dr$$

and denoting by $\lambda_j(s)$ the eigenvalues and by $\psi_j^{(s)}(r)$ the normalized eigenfunctions of the kernel

$$\frac{1}{2\pi} \frac{\exp\left(-\sqrt{2s}\,\|r-\rho\|\right)}{\|r-\rho\|}, \qquad r \in \Omega\,,\ \rho \in \Omega\,,$$

we obtain at once that for $r \in \Omega$

$$G_s(r; u) \sim \sum_{j=1}^{\infty} \frac{1}{1 + u\lambda_j(s)} \int_\Omega \psi_j^{(s)}(\rho)\, d\rho\, \psi_j^{(s)}(r)\,.$$

Formula (5.8) becomes now

$$\int \left(1 - G_s(y; u)\right) dy = \frac{1}{s} \int_\Omega u G_s(r; u)\, dr =$$

$$= \frac{1}{s} \sum_{j=1}^{\infty} \frac{1}{1/u + \lambda_j(s)} \left(\int_\Omega \psi_j^{(s)}(\rho)\, d\rho \right)^2$$

and letting $u \uparrow \infty$ we obtain

$$\int_0^\infty \exp(-st) \int P\left\{ \int_0^t V_\Omega(y + r(\tau))\, d\tau > 0 \right\} dy\, dt =$$

$$= \frac{1}{s^2} \sum_{j=1}^{\infty} \frac{1}{\lambda_j(s)} \left(\int_\Omega \psi_j^{(s)}(r)\, dr \right)^2. \tag{5.17}$$

By analogy with $\mu_u(A)$ of section 3 we can introduce the Radon measure $\mu_u^{(s)}(A)$ and obtain as before

$$1-G_s(y;u)=\int_\Omega \frac{\exp\left(-\sqrt{2s}\,\|y-\rho\|\right)}{\|y-\rho\|}\,\mu_u^{(s)}(d\rho) \tag{5.18}$$

and in the limit $u\uparrow\infty$

$$s\int_0^\infty \exp(-st)\,P\left\{\int_0^t V_\Omega(y+r(\tau))\,d\tau>0\right\}dt= \tag{5.19}$$

$$=\int \frac{\exp\left(-\sqrt{2s}\,\|y-\rho\|\right)}{\|y-\rho\|}\,\mu^{(s)}(d\rho)\,.$$

Also since

$$\int_\Omega \mu_u^{(s)}(d\rho)=\frac{1}{2\pi}\sum_{j=1}^\infty \frac{\left(\int_\Omega \psi_j^{(s)}(r)\,dr\right)^2}{1/u+\lambda_j^{(s)}}$$

we see that

$$\sum_{j=1}^\infty \frac{\left(\int_\Omega \psi_j^{(s)}(r)\,dr\right)^2}{\lambda_j^{(s)}}=2\pi\int \mu^{(s)}(d\rho)\,. \tag{5.20}$$

If in (5.18) we let $s\downarrow 0$ we obtain

$$P\{T_\Omega(y)>0\}=U(y)=\lim_{s\downarrow 0}\int \frac{\exp\left(-\sqrt{2s}\,\|y-\rho\|\right)}{\|y-\rho\|}\,\mu^{(s)}(d\rho)= \tag{5.21}$$

$$=\lim_{s\downarrow 0}\int \frac{\mu^{(s)}(d\rho)}{\|y-\rho\|}\,.$$

It is not difficult to prove that the measure $\mu^{(s)}$ approaches the measure μ as $s\downarrow 0$ and that also

$$\lim_{s\downarrow 0}\int \mu^{(s)}(d\rho)=\int \mu(d\rho)\,. \tag{5.22}$$

Now

$$\int \mu(d\rho)$$

is the capacity $C(\Omega)$ of Ω and finally (5.17) becomes

$$(5.23) \qquad \int_0^\infty \exp(-st) \int P\left\{\int_0^t V_\Omega(y + r(\tau))\, d\tau > 0\right\} dy\, dt \sim \frac{2\pi C(\Omega)}{s^2}, \qquad s \downarrow 0,$$

showing that indeed the scattering length of the « hard » potential on Ω is the capacity of Ω.

A final point of purely mathematical interest. The capacity $C(\Omega)$ is *not* the usual capacity.

The usual capacity $\gamma(\Omega)$ is defined as the inverse of

$$\inf \int_\Omega \int_\Omega \frac{\nu(dr)\,\nu(d\rho)}{\|r-\rho\|}$$

over all *measures* ν such that

$$\int_\Omega \nu(dr) = 1 .$$

The capacity $C(\Omega)$ is the inverse of

$$\inf \int_\Omega \int_\Omega \frac{f(r)\, f(\rho)}{\|r-\rho\|} dr\, d\rho$$

over *all* $f \in L^2(\Omega)$ such that

$$\int_\Omega f(r)\, dr = 1 .$$

There are regions which are closures of their interiors for which

$$\gamma(\Omega) > C(\Omega) .$$

These sets are in a sense pathological because for them the probability of hitting is not equal to the probability of spending a positive time in them. For such sets the probability that a Brownian motion curve will « hit and run » is not zero!

It is interesting that the natural extension of the concept of scattering length leads to $C(\Omega)$ rather than to $\gamma(\Omega)$. (For further details see [16].)

SECTION 6

Feynman's Approach to non-Relativistic Quantum Mechanics

In the preceding pages I made a number of references to problems of Quantum Mechanics which were closely related to Wiener integrals. The recognition however of the close ties between Wiener's theory and Quantum Mechanics came about through the work of R. P. Feynman, who in his doctoral dissertation (Princeton, 1942) picked up an idea of Dirac's and made it a starting point of a novel and, as it turned out, immensely fruitful way of looking at Quantum Mechanical problems.

Feynman began with ordinary non-relativistic Quantum Mechanic of systems with a finite number n of degrees of freedom, and I shall give here a brief presentation of his ideas restricting myself to the case $n = 1$, i.e. of a particle moving along the x-axis in a potential $V(x)$.

In classical Mechanics if we want to find the path $x(\tau)$, $0 < \tau < t$, which at $\tau = 0$ starts from x_0 $(x(0) = x_0)$ and which at $\tau = t$ terminates at x $(x(t) = x)$ we can use the Maupertuis-Hamilton principle, i.e. try to solve the variational problem

$$\delta\left\{\int_0^t \left[\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 - V(x(\tau))\right] d\tau\right\} = 0\,, \tag{6.1}$$

$$x(0) = x_0\,, \qquad x(t) = x\,. \tag{6.2}$$

The mass of the particle is assumed to be one ($m = 1$) and

$$S = \int_0^t \left[\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 - V(x(\tau))\right] d\tau$$

is of course the classical action, the integrand being the Lagrangean of the problem.

In Quantum Mechanics the fundamental quantity is the *propagator* $K(x_0|x, t)$, which allows one to calculate the probability of finding the system in state ψ at time t if it has started from state φ at time 0. « States » in Quantum Mechanics are vectors (of length one) in a Hilbert space, which in the coordinate representation, which I shall use, are simply square integrable functions over the set of reals. The rule for calculating the above probability is embodied in the formula

$$\left| \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_0\, dx\, \varphi(x_0) K(x_0|x, t) \psi^*(x) \right|^2 \tag{6.3}$$

where * denotes the complex conjugate.

In the standard theory the propagator is obtained by solving the (time-dependent) Schrödinger equation

$$i\hbar \frac{\partial K}{\partial t} = -\frac{\hbar^2}{2} \frac{\partial^2 K}{\partial x^2} + V(x) K \tag{6.4}$$

with the initial condition

$$K(x_0|x; 0) = \delta(x - x_0)\,. \tag{6.5}$$

Feynman showed (heuristically) that the propagator K can be written as the « path integral »

$$K(x_0|x, t) = \int \exp\left(\frac{iS[x]}{\hbar}\right) d(\text{path}) \tag{6.7}$$

where the « integration » is over all paths $x(\tau)$ such that $x(0) = x_0$ and $x(t) = x$ and $\hbar = h/2\pi$ with h being the usual Planck's constant.

The d(path) « integral » is defined (à la Riemann) as the limit of

$$\frac{1}{(2\pi i \Delta \hbar)^{N/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left\{\frac{i}{\hbar}\left[\frac{(x_1 - x_0)^2}{2\Delta} + \frac{(x_2 - x_1)^2}{2\Delta} + \right.\right. \tag{6.8}$$

$$\left.\left. + \cdots \frac{(x - x_{N-1})^2}{2\Delta} - \Delta \sum_{k=1}^{N-1} V(x_k)\right]\right\} dx_1 \cdots dx_{N-1}.$$

as $N \to \infty$, $\Delta \to 0$ and $N\Delta = t$. To make the definition unambiguous we set

$$\sqrt{i} = \exp\left(\frac{\pi i}{4}\right).$$

The occurrence of i (which is essential for Quantum Mechanics!) makes manipulations with integrals like (6.8) extremely tricky.

First the existence of the limit is, in general, difficult to establish, and secondly it is awkward to be dependent on a particular discretization of the action integral. Still the intuitive appeal of Feynman's definition is enormous, and it gave birth to a dream that perhaps all of Physics could be rewritten in terms of « sums over histories ».

Be this as it may, the formal analogy between (6.8) and integrals appearing in Wiener's theory is striking and since Wiener's theory is rigorously founded Feynman's heuristic connection between the Schrödinger equation and the path integral can be made into an unassailable theorem.

The theorem in question is the following:

Let $x(\tau)$, $x(0) = 0$, $0 \leqslant \tau < \infty$ be the Brownian path (Wiener process) then

$$(6.9) \qquad E\left\{\exp\left(\int_0^t V(x_0 + x(\tau))\, d\tau\right);\ y < x_0 + x(t) < y + \Delta y\right\} = \int^{y+\Delta y} Q(x_0|x;\, t)\, dx$$

where $Q(x_0|x, t)$ is the solution of

$$(6.10) \qquad \frac{\partial Q}{\partial t} = \frac{1}{2}\frac{\partial^2 Q}{\partial x^2} + V(x)\, Q$$

subject to the initial condition

$$(6.11) \qquad \lim_{t \to 0} Q(x_0|x;\, t) = \delta(x - x_0)\,.$$

Here

$$E\{(\ldots;\ y < x + x(t) < y + \Delta y)\}$$

denotes the Wiener integral of ... over that portion of the space of Brownian paths which satisfy the condition $y < x + x(t) < y + \Delta y$.

$V(x)$ must, of course, be subject to certain regularity conditions, but these are mild and of technical interest only. It is, however, important to stress that V can be also *a function of time* t, so that in (6.9) and (6.10) $V(x)$ can be replaced by $V(x, t)$.

Formula (6.9) is often called the Feynman-Kac formula and there are literally dozens of proofs of varying degrees of « slickness ». The least « slick » is my original proof [17] (which allowed only for V's not depending explicitely on t) and the most straightforward (though by no means the simplest) is the proof I sketched in [8]. A proof that is a candidate for the ultimate in streamlining can be found in the aforementioned book [14] by B. Simon.

Instead of repeating once again the proof of (6.9) I shall derive its analogue for a simple finite state Markov chain with continuously varying time. The idea behind the proof is the same and the technicalities are almost trivial. To simplify matters further I shall assume that V does not depend explicitely on t.

Let then $x(\tau)$ be a Markov process with states 1, 2, ..., n and transition probabilities matrix $P(t)$ which satisfies of course the equation

$$P(s+t) = P(s)\,P(t)\,, \qquad s>0\,,\ t>0\,.$$

Let now $V(i)$ be real (or complex) valued function on the states and consider the expectation

$$Q(i_0|i;\,t) = E_{i_0}\left\{\exp\left(\int_0^t V(x(\tau)\,d\tau);\, x(t)=i\right)\right\}. \tag{6.12}$$

The notation makes it clear that $x(0) = i_0$.

Expanding $\exp\left(\int_0^t V(x(\tau))\,d\tau\right)$ in powers of the argument we get

$$Q(i_0|i;\,t) = \tag{6.13}$$

$$= \sum_{k=0}^{\infty} \int\!\!\ldots\!\int \sum_{i_1,i_2,\ldots,i_k=1}^{n} V(i_1)\,\ldots\,V(i_k)\,P(i_0|i_1;\,\tau_1)\,P(i_1|i_2;\,\tau_2-\tau_1)\,\ldots$$

$$\ldots\,P(i_k|i;\,t-\tau_k)\,d\tau_1\,\ldots\,d\tau_k$$

where the integration is over the region

$$0<\tau_1<\tau_2<\ldots<\tau_k<t\,,$$

and upon taking Laplace transforms

$$(6.14)\qquad \int_0^\infty \exp(-st)Q(i_0|i;\,t)\,dt =$$

$$= \sum_{k=0}^{\infty} \sum_{i_1,i_2,\ldots,i_k=1}^{n} V(i_1)\ldots V(i_k)p_s(i_0|i_1)p_s(i_1|i_2)\ldots p_s(i_k|i)\,.$$

Here $P(i|j;\,t)$ is the $(i,\,j)$-th element of $P(t)$ and

$$p_s(i|j) = \int_0^\infty \exp(-st)P(i|j;\,t)\,dt\,.$$

Let

$$(6.15)\qquad V = \begin{pmatrix} V(1) & & & 0 \\ & V(2) & & \\ & & \ddots & \\ 0 & & & V(n) \end{pmatrix}$$

and p_s be the matrix with entries $p_s(i|j)$, i.e.

$$(6.16)\qquad p_s = \int_0^\infty \exp(-st)\,P(t)\,dt\,.$$

Thus denoting by $Q(t)$ the matrix with entries $Q(i_0|i;\,t)$ we have

$$(6.17)\qquad \int_0^\infty \exp(-st)Q(t)\,dt = \sum_{k=0}^{\infty} (p_sV)^k p_s = (I - p_sV)^{-1}p_s\,.$$

Now it is well known that

$$(6.18)\qquad P(t) = \exp(tR)$$

where the (infinitesimal generator) matrix R has negative elements on the main diagonal and the sum of elements in each row is zero. Con-

sequently

$$p_s = (sI - R)^{-1}$$

and therefore

$$\int_0^\infty \exp(-st)Q(t)\,dt = \big(I - (sI - R)^{-1}V\big)(sI - R)^{-1} = \big(sI - (R + V)\big)^{-1}$$

whence

$$Q(t) = \exp\big(t(R + V)\big) \tag{6.19}$$

or

$$\frac{dQ}{dt} = (R + V)Q\,, \tag{6.20}$$

$$Q(0) = I \tag{6.21}$$

a clear analogues of (6.10) and (6.11).

SECTION 7

Feynman's Approach Continued. Semi-Classical Quantum Mechanics and a Theorem of Morse

Returning to Feynman's ideas I shall now discuss the so-called semiclassical approximation to Quantum Mechanics.

A glance at Feynman's formula

$$K(x_0|x,t) = \int \exp\left(\frac{iS[x]}{\hbar}\right) d(\text{path}) \tag{7.1}$$

is sufficient to make it clear that for small $\hbar$ [2] the major contribution to the integral comes from around the *classical path* $x_{\text{cl}}(\tau)$ defined by

$$\delta S = 0\,, \qquad x(0) = x_0\,, \qquad x(t) = x\,. \tag{7.2}$$

In the semiclassical approximation one goes one step farther by setting

$$x(\tau) = x_{\text{cl}}(\tau) + y(\tau)\,, \tag{7.3}$$

expanding the action about x_{cl} and stopping at the quadratic term:

$$S[x(\tau)] \cong S[x_{\text{cl}}(\tau)] + \int_0^t \left[\frac{1}{2}\left(\frac{dy}{d\tau}\right)^2 - \frac{1}{2}\,V''(x_{\text{cl}}(\tau))\,y^2(\tau)\right] d\tau\,. \tag{7.4}$$

[2] Actually one must rewrite everything in terms of dimensionless quantities so that $\hbar$ would become a small *dimensionless* parameter.

One now replaces $K(x_0|x, t)$ by the (semi-classical) approximation

$$(7.5)\qquad \tilde{K}(x_0|x, t) = \exp\left(\frac{i}{\hbar} S[x_{\mathrm{cl}}(\tau)]\right)\cdot \cdot \int_0^t \exp\left\{\frac{i}{\hbar}\int\left[\frac{1}{2}\left(\frac{dy}{d\tau}\right)^2 - \frac{1}{2}V''(x_{\mathrm{cl}}(\tau))y^2(\tau)\right]d\tau\right\} d(\mathrm{path})$$

where the integration $d(\mathrm{path})$ is over the space of paths $y(\tau)$ such that

$$(7.6)\qquad y(0) = y(t) = 0\,.$$

Now, the path integral is again defined as the limit of the multiple integral

$$(7.7)\qquad \left(\frac{1}{\sqrt{2\pi i \Delta\hbar}}\right)^N \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left\{\frac{i}{\hbar}\left[\frac{y_1^2}{2\Delta} + \frac{(y_2-y_1)^2}{2\Delta} + \cdots + \frac{y_{N-1}^2}{2\Delta} - \frac{\Delta}{2}\sum_1^{N-1} r(k\Delta)y_k^2\right]dy_1 \ldots dy_{N-1}\right\}$$

where I have put

$$(7.8)\qquad r(\tau) = V''(x_{\mathrm{cl}}(\tau))\,.$$

The limit is, of course, as $N \to \infty$, $\Delta \to 0$ and $N\Delta = t$.

Il has been shown by Pauli [19] (see also R.F. Dashen, B. Hasslacher and A. Neven [20]) that the limit of (7.7) is

$$(7.9)\qquad \frac{1}{\sqrt{2\pi i\hbar}}\sqrt{\pm\frac{\partial^2 S}{\partial x_0\,\partial x}}$$

with some uncertainty concerning the $\pm$ sign. (I have tacitly assumed that the classical path is unique; if this is not the case the semiclassical approximation is a sum of contributions from *all* classical paths.)

It turns out that as far as eigenvalues (energy levels) are concerned the quadratic approximation is essentially equivalent to the Bohr-Sommerfeld « old » quantum theory. I shall not go into this especially since this aspect has been a subject of several recent reviews (for the latest

see [21]). It should however be remarked that most of the uses of Feynman's path integrals in recent physics literature are centered around the quasi-classical approximation.

I shall conclude this section by discussing briefly an aspect of a theory developped by Marston Morse.

If the classical path starts at $t = 0$ from x_0 with initial momentum p_0 its position x at time t is a function of x_0, p_0 (and, of course, t)

$$x = x(x_0, p_0; t) .$$

If we change p_0 by a small amount ε (leaving x_0 and t unchanged) then the final position $x(x_0, p_0 + \varepsilon; t)$ will, in general, differ from $x(x_0, p_0; t)$ by an amount of order ε. However it is possible that for some x and t the difference is of higher order in ε in which case (x, t) is called *conjugate* to $(x_0, 0)$.

The condition of conjugacy is clearly

$$\frac{\partial x(x_0, p_0; t)}{\partial p_0} = 0 \tag{7.10}$$

and it can be written in a much nicer way if one recalls that by the Hamilton-Jacobi theory (in its simplest form)

$$p_0 = -\frac{\partial S}{\partial x_0} . \tag{7.11}$$

Thus

$$\frac{\partial^2 S}{\partial x_0 \partial x} = -\frac{\partial p_0}{\partial x} \tag{7.12}$$

or

$$\frac{\partial x}{\partial p_0} = -\left(\frac{\partial^2 S}{\partial x_0 \partial x}\right)^{-1} . \tag{7.13}$$

The condition of conjugacy (7.10) is therefore equivalent to

$$\left(\frac{\partial^2 S}{\partial x_0 \partial x}\right)^{-1} = 0 . \tag{7.14}$$

On the other hand by changing p_0 to $p_0 + \varepsilon$ we change (to first order in ε) the classical path $x_{cl}(\tau)$

$$\big(x_{cl}(0) = x_0,\ x_{cl}(t) = x\big) \quad \text{into} \quad x_{cl}(\tau) + \varepsilon\varphi(\tau)$$

with $\varphi(0) = 0$ to preserve the initial condition. If (x, t) is to be conjugate to $(x_0, 0)$ we must also have $\varphi(t) = 0$.

Recalling now that the equation of motion of our particle is

$$\frac{d^2x}{d\tau^2} + V'\big(x(\tau)\big) = 0 \tag{7.15}$$

we obtain at once that in order that (x, t) be conjugate to $(x_0, 0)$ it is necessary and sufficient that a non-trivial solution

$$\varphi''(\tau) + V''\big(x_{cl}(\tau)\big)\varphi(\tau) = 0 \tag{7.16}$$

exists subject to the boundary condition

$$\varphi(0) = \varphi(t) = 0\,. \tag{7.17}$$

In other words (x, t) is conjugate to $(x_0, 0)$ if and only if $\lambda = 1$ is an eigenvalue of the problem

$$\lambda\varphi''(\tau) + V''\big(x_{cl}(\tau)\big)\varphi(\tau) = 0\,, \qquad \varphi(0) = \varphi(t) = 0\,. \tag{7.18}$$

Morse's theorem states that if 1 is the n-th eigenvalue (in decreasing order) i.e. $\lambda_n(t) = 1$, there are n conjugate points (x, τ) to $(x_0, 0)$ for $0 < \tau < t$.

There is an obvious generalization of this simple and elegant result to systems of any finite number of degrees of freedom.

I shall now show how one can obtain a vast extension of this result based on ideas of functional integration.

I shall in fact prove that

$$\left(\frac{\partial^2 S}{\partial x_0\,\partial x}\right)^{-1} = t\prod_{j=1}^{\infty}\big(1 - \lambda_j(t)\big)\,. \tag{7.19}$$

Actually (7.19) has little to do with Mechanics, and I shall carry out the derivation in, so to speak, a neutral setting.

Consider

$$I(x;t) = E\left\{\exp\left(\frac{1}{2}\int_0^t r(\tau)x^2(\tau)\,d\tau\right);\ x(t)=x\right\} = \tag{7.20}$$

$$= E\left\{\exp\left(\frac{1}{2}\int_0^t r(\tau)\,x^2(\tau)\,d\tau | x(t)=x\right)\right\}\frac{\exp(-x^2/2t)}{\sqrt{2\pi t}}\,.$$

Here $x(\tau)$, $x(0)=0$, in the Wiener process, and I have used conditional expectations.

To be specific I shall remind the reader that

$$I(x;t) = \lim_{\Delta x\to 0}\frac{1}{\Delta x}E\left\{\exp\left(\frac{1}{2}\int_0^t r(\tau)x^2(\tau)\,d\tau\right);\ x<x(t)<x+\Delta x\right\}. \tag{7.21}$$

To avoid non-essential complexities I shall assume that $r(\tau)$ is continuous.

I shall now direct the reader to part (*d*) of Section 2 and assure him that with only slight modifications he should obtain the result

$$I(x;t) = \frac{\exp(-x^2/2t)}{\sqrt{2\pi t}}\,\frac{\exp\left(x^2\int_0^t \tau\eta(\tau)\,d\tau/2t\right)}{\sqrt{\prod_j(1-\lambda_j(t))}} \tag{7.22}$$

where the λ's are the eigenvalues of the problem:

$$\lambda\varphi''(\tau)+r(\tau)\varphi=0\,,\qquad \varphi(0)=\varphi(t)=0\,, \tag{7.23}$$

and $\eta(\tau)$ the solution of the integral equation

$$\eta(\tau)-r(\tau)\int_0^t\left[\min(\sigma,\tau)-\frac{\sigma\tau}{t}\right]\eta(\sigma)\,d\sigma=\tau r(\tau)\,. \tag{7.24}$$

Setting

$$\eta(\tau)=s(\tau)\,r(\tau) \tag{7.25}$$

one gets easily that $s(\tau)$ satisfies the integral equation

$$s(\tau) - \int_0^t \left[\min(\sigma, \tau) - \frac{\sigma\tau}{t}\right] r(\sigma)\, s(\sigma)\, d\sigma = \tau \tag{7.26}$$

which is equivalent to the differential equation

$$\frac{d^2 s}{d\tau^2} + r(\tau)\, s(\tau) = 0 \tag{7.27}$$

with the boundary conditions

$$s(0) = 0\,, \qquad s(t) = t\,. \tag{7.28}$$

It now follows in a few steps that

$$\int_0^t \tau\eta(\tau)\, d\tau = -t\left(\frac{ds}{d\tau}\right)_{\tau=t} + t \tag{7.29}$$

and finally that

$$I(x;\, t) = \frac{\exp\left(-(x^2/2t)(ds/d\tau)_{\tau=t}\right)}{\sqrt{2\pi t}\prod_j \left(1 - \lambda_j(t)\right)}\,. \tag{7.30}$$

By (6.9) and (6.10) with

$$V(x,\, t) = \tfrac{1}{2} r(t) x^2$$

we see that $I(x;\, t)$ satisfies the differential equation

$$\frac{\partial I}{\partial t} = \frac{1}{2}\frac{\partial^2 I}{\partial x^2} + \frac{1}{2} r(t) x^2 I \tag{7.31}$$

and the initial condition

$$I(x;\, 0) = \delta(x)\,. \tag{7.32}$$

It is natural to seek the solution of (7.31) in the form

$$I(x, t) = A(t) \exp\left(-\tfrac{1}{2}B(t)x^2\right) \tag{7.33}$$

which upon substituting in (7.31) tields

$$\frac{dA}{dt} = -\frac{1}{2}AB \tag{7.34a}$$

and

$$-\frac{dB}{dt} = B^2 + r(t)\,. \tag{7.34b}$$

We recognize (7.34*b*) as the classical non-linear Riccati equation and by comparing (7.33) with (7.3) we see that

$$B(t) = \frac{1}{t}\left(\frac{ds}{d\tau}\right)_{\tau=t} \tag{7.35}$$

where s is the solution of the *linear* equation (7.27) with the boundary condition (7.28).

Let now $s_0(\tau)$ be the solution of (7.27) satisfying the *initial* conditions

$$s_0(0) = 0\,, \qquad s_0'(0) = 1\,. \tag{7.36}$$

Then clearly

$$s(\tau) = t\frac{s_0(\tau)}{s_0(t)} \tag{7.37}$$

(assuming that $s_0(t) \neq 0$) and hence

$$B(t) = \frac{s_0'(t)}{s_0(t)} \tag{7.38}$$

which also implies that

$$B(t) \sim \frac{1}{t}\,, \qquad t \to 0\,. \tag{7.39}$$

Formula (7.38) is, of course, the famous substitution which linearizes the Riccati equation and reduces it to

$$\frac{d^2 s_0}{dt^2} + r(t)\, s_0 = 0 \,.$$

From (7.38), (7.34*a*) and (7.30) we obtain that

$$s_0(t) = t \prod_{j=1}^{\infty} \left(1 - \lambda_j(t)\right) \tag{7.40}$$

and I leave it to the reader to derive (7.19) from (7.40).

Strictly speaking the above derivation is valid only for sufficiently small times, but by a simple argument based on considering $zr(\tau)$ and on analytic continuation one can extend the validity of (7.40) to all times t.

The extension to the multidimensional case is straightforward although the details are a little tedious.

The final result is the following: Let $s_0(t)$ be an $n \times n$ matrix solution of the differential equation

$$\frac{d^2 s_0}{dt^2} + R s_0 = 0 \tag{7.41}$$

with the initial condition

$$s_0(0) = 0 \,, \qquad s_0'(0) = I \,, \tag{7.42}$$

where

$$R = R(t) = \left(\!\left(r_{ij}(t)\right)\!\right)$$

is a matrix with continuous entries.

Let furthermore $\lambda_1, \lambda_2, \ldots$ be the eigenvalues of the problem

$$\lambda \frac{d^2 \varphi_i}{dt^2} + \sum_{j=1}^{n} r_{ij} \varphi_j = 0 \,, \qquad i = 1, 2, \ldots, n \,,$$

$$\varphi_i(0) = \varphi_i(t) = 0 \,, \qquad i = 1, 2, \ldots, n$$

then

$$\det s_0(t) = t^n \prod_{j=1}^{\infty} \left(1 - \lambda_j(t)\right) . \tag{7.43}$$

In deriving this result one encounters the matrix Riccati equation in the form

$$-\frac{dB}{dt} = B^2 + R$$

which is then linearized by the substitution

$$B = \frac{dP}{dt} P^{-1} .$$

The Riccati equation both in its scalar and in its matrix form is, of course, well known as are the linearizing substitutions. That they are encountered in an unexpected context is not only a source of amusement but also of hope that such miracles, minor as they are, may happen again.

Formula (7.40) was first discovered and proved by purely analytic methods by N. Levinson [22], and a purely analytic proof of (7.43) was given by L. Bers (unpublished) following a talk I gave at Columbia University at a seminar conducted by D. V. and G. V. Chudnovsky. L. Faddeev informed me that (7.43) was known to him and his collaborators, but while there is no reason to doubt this assertion I could not find an unambiguous statement of the formula in the published literature.

SECTION 8

Short Time Asymptotics and High Eigenvalues of the Schrödinger Equation

The Feynman-Kac formula ((6.9) with Q defined by (6.10)) allows one to obtain various results concerning the Schrödinger equation

$$\frac{1}{2}\frac{\alpha^2\psi}{dx^2} - V(x)\psi = -\lambda\psi \tag{8.1}$$

on the infinite line $-\infty < x < \infty$.

For example if $V(x)$ is such that

$$\lim_{x\to\pm\infty} V(x) = +\infty$$

and $V(x)$ is bounded from below (8.1) has only a discrete set of eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 \ldots$ and it is quite easy to obtain the asymptotic behavior of λ_n as $n \to \infty$. Although this has been repeatedly discussed in the literature it is so simple and intuitively appealing that I shall once again summarize (briefly) the underlying idea.

It is well known that $Q(x_0|x;\, t)$ can be written in terms of the normalized eigenfunctions and eigenvalues of (8.1) as follows:

$$Q(x_0|x;\, t) = \sum_{n=1}^{\infty} \exp(-\lambda_n t)\,\psi_n(x_0)\,\psi_n(x) \tag{8.2}$$

and hence by (6.9) and using conditional probability

$$(8.3)\qquad \frac{\exp\left(-(x-x_0)^2/2t\right)}{\sqrt{2\pi t}}\,E\left\{\exp\left(-\int_0^t V(x_0+x(\tau))\,d\tau \,|\, x_0+x(t)=x\right)\right\} = \sum_{n=1}^{\infty}\exp\left(-\lambda_n t\right)\psi_n(x_0)\psi_n(x)\,.$$

Setting $x = x_0$ and integrating both sides over x we get

$$(8.4)\qquad \sum_{n=1}^{\infty}\exp\left(-\lambda_n t\right) = \frac{1}{\sqrt{2\pi t}}\int_{-\infty}^{\infty} dx\, E\left\{\exp\left(-\int_0^t V(x+x(\tau))\,d\tau\right)\Big| x(t)=0\right\}.$$

For $t \to 0$ it is intuitively obvious that

$$E\left\{\exp\left(-\int_0^t V(x+x(\tau))\,d\tau\right)\Big| x(t)=0\right\} \sim \exp\left(-tV(x)\right),$$

and one hould therefore expect that as $t \to 0$ we have asymptotically

$$(8\,5)\qquad \sum_{n=1}^{\infty}\exp\left(-\lambda_n t\right) \sim \frac{1}{\sqrt{2\pi t}}\int_{-\infty}^{\infty}\exp\left(-tV(x)\right)dx$$

provided, of course, V satisfies certain conditions.

The right hand side of (8.5) can be written as

$$(8.6)\qquad \frac{1}{2\pi}\iint\exp\left(-t\left(\frac{p^2}{2}+V(x)\right)\right)dx\,dp = \frac{1}{2\pi}\int\exp\left(-t\lambda\right)dA(\lambda)$$

where $A(\lambda)$ is the area of the set in the (x, p) (phase) plane defined by the inequality

$$\frac{p^2}{2}+V(x)<\lambda\,.$$

The left hand side (of (8.5)) can be written as

$$\int\exp\left(-t\lambda\right)dN(\lambda)$$

where $N(\lambda)$ is the number of eigenvalues λ_k do not exceed λ i.e.

$$N(\lambda) = \sum_{\lambda_k < \lambda} 1 .$$

Thus (8.5) can be written in the form

$$\int \exp(-t\lambda)\, dN(\lambda) \sim \frac{1}{2\pi} \int \exp(-t\lambda)\, dA(\lambda) , \qquad t \to 0 ,$$

which (under appropriate Tauberian conditions) should imply that

$$N(\lambda) \sim \frac{1}{2\pi} A(\lambda) , \qquad \lambda \to \infty . \tag{8.7}$$

If $\lambda = \lambda_n$ we have

$$A(\lambda_n) \sim 2\pi n , \qquad n \to \infty$$

and we hould recognize that

$$A(\lambda_n) = 2\pi n$$

is precisely the quantization rule which Planck first introduced into Physics.

Rigorous justifications of (8.5) and (8.7) are subtle and were first given by D. B. Ray [23] in 1954 (3); the intuitive background is however completely transparent and closely related to considerations of Section 4. Because only the limit $t \to 0$ is involved very little information about the paths is used. In fact, all we use is that for small t the path originating at zero and terminating at zero can be replaced by the chord connecting $(0, 0)$ and $(0, t)$, (i.e. a piece of the x-axis).

The standard way of deriving (8.7) based on the familiar WKB method is limited to the one-dimensional case while our argument is quite general.

(3) Considerable simplification of some of Ray's arguments was given recently by Mr. van den Berg of the University of Groningen as I learned while attending a conference on Statistical Mechanics on April 18, 1980 in Groningen, Holland.

SECTION 9

Introduction to the Donsker-Varadhan Long Time Asymptotics

This and the following section is devoted to a brief introduction to the recent work of Donsker and Varadhan (4), which, in my opinion, is the most interesting and novel development in the field of functional integration since the ascendency of the subject in the early fifties.

The origin of the work goes back to a formula for the lowest eigenvalue of the Schrödinger equation.

From (6.9), (6.10) and (8.2) we get

$$(9.1)\qquad E\left\{\exp\left(-\int_0^t V(x(\tau))\,d\tau\right)\right\} = \int_{-\infty}^{\infty} Q(0|x;\,t)\,dx = \sum_{n=1}^{\infty} \exp(-\lambda_n t)\,\psi_n(0)\int_{-\infty}^{\infty}\psi_n(x)\,dx$$

and therefore

$$(9.2)\qquad \lambda_1 = -\lim_{t\to\infty}\frac{1}{t}\log E\left\{\exp\left(-\int_0^t V(x(\tau))\,d\tau\right)\right\}$$

(since we are dealing with the infinite interval term by term integration of (8.2) requires justification).

(4) Donsker and Varadhan developed their theory in a series of papers of which [24] is the most useful as a start.

On the other hand we have by the well known Raleigh-Ritz principle

$$\lambda_1 = \inf_{\psi} \int_{-\infty}^{\infty} \left[\left(\frac{d\psi}{dx} \right)^2 + V(x)\psi^2 \right] dx \tag{9.3}$$

the infimum being over functions ψ satisfying the condition

$$\int_{-\infty}^{\infty} \psi^2(x)\, dx = 1 . \tag{9.4}$$

The question now arises how are (9.3) and (9.2) related and Donsker suspected for a long time that lurking in the background was a kind of steepest descent method in function space. This turns out to be entirely right, but in a somewhat unexpected way.

Let me first try to explain the underlying ideas on the simple case of a finite state Markov chain with continuously varying time.

I shall assume that the Markov chain is ergodic (5), and I shall denote by $W(i)$ the stationary probabilities, i.e.

$$\sum_{i=1}^{n} W(i) P(i|j;\, t) = W(j) . \tag{9.5}$$

Ergodicity means that

$$\lim_{t\to\infty} P(i|j;\, t) = W(j) \tag{9.6}$$

(though less would suffice) and it implies the occupation time $\Theta_i(t)$ of the state i (i.e. the time up to t which $x(\tau)$ spends in the state i) obeys the (weak) ergodic theorem, i.e.

$$\lim_{t\to\infty} \frac{\Theta_i(t)}{t} = W(i) \tag{9.7}$$

in probability (actually the process also obeys the strong ergodic theorem).

(5) This is actually not really necessary in our simple case, but in the continuous version discussed in the next section ergodicity becomes important.

Let us also note that

$$E\left\{\exp\left(\int_0^t V(x(\tau))\,d\tau\right)\right\} = \sum_{i=1}^{n}\sum_{i_0=1}^{n} W(i_0)Q(i_0|i;\,t)\,. \tag{9.8}$$

From (6.12) and (6.19) it follows at once that

$$\lim_{t\to\infty}\frac{1}{t}\log E\left\{\exp\left(\int_0^t V(x(\tau))\,d\tau\right)\right\} = \lambda_{\max}(R+V)\,, \tag{9.9}$$

where $x(\tau)$ is now our finite state Markov chain and $\lambda_{\max}(R+V)$ the maximum eigenvalue of the matrix $R+V$ (which as a consequence of a classical theorem of Frobenius-Perron must be real). It is clear that (9.9) is the analogue of (9.2), but it will be more convenient to write it in the form

$$E\left\{\exp\left(\int_0^t V(x(\tau))\,d\tau\right)\right\} \sim \exp\left(t\lambda_{\max}(R+V)\right)\,. \tag{9.10}$$

Now,

$$\int_0^t V(x(\tau))\,d\tau = t\sum_{i=1}^{n} V(i)\frac{\Theta_i(t)}{t}$$

and hence

$$E\left\{\exp\left(\int_0^t V(x(\tau))\,d\tau\right)\right\} = \int_{\alpha_1+\ldots+\alpha_n=1}\cdots\int\exp\left(t\sum_{i=1}^{n} V(i)\alpha_i\right)d\sigma_t(\alpha_1,\,\ldots,\,\alpha_n)\,,$$

where

$$\sigma_t(\alpha_1,\,\ldots,\,\alpha_n)$$

is the joint distribution of the relative occupation times

$$\frac{\Theta_1(t)}{t},\,\ldots,\,\frac{\Theta_n(t)}{t}\,.$$

If one thinks of $d\sigma_t(\alpha_1, \ldots, \alpha_n)$ as $P_t(\alpha_1, \ldots, \alpha_n)/dO_n$ (dO_n being the surface element of $\alpha_1 + \ldots + \alpha_n = 1$) then the asymptotic relation (9.10) suggests that

$$P_t(\alpha_1, \ldots, \alpha_n) \sim \exp\left(tI(\alpha_1, \ldots, \alpha_n)\right), \qquad t \to \infty, \tag{9.11}$$

and

$$\lambda_{\max}(R+V) = \max\left\{\sum_{i=1}^{n} \alpha_i V(i) + I(\alpha_1, \ldots, \alpha_n)\right\} \tag{9.12}$$

the maximum being over non-negative α's, $\alpha_i \geqslant 0$, $i = 1, 2, \ldots, n$, whose sum is one

$$\sum_{i=1}^{n} \alpha_i = 1 .$$

The I-function is the principal discovery of Donsker and Varadhan and it depends *only on the process* $x(\tau)$.

Actually (9.11) may be slightly misleading and the definition of the I-function can be given differently. Roughly speaking one can proceed as follows:

First partition the set

$$\alpha_i \geqslant 0, \qquad i = 1, 2, \ldots, n, \qquad \sum_{i=1}^{n} \alpha_i = 1$$

into two disjoint sets E_0 and E_1, then in turn partition each of these into two disjoint sets, etc. We thus obtain a sequence of partitions, the sets of the n-th partition being labelled

$$E_{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n}, \qquad \varepsilon_i = 0, 1 .$$

We have, of course,

$$E_{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_{n+1}} \subset E_{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n} \quad \text{etc.} .$$

We also make sure that the *maximal* diameter of the sets of the n-th partition approaches zero as $n \to \infty$.

Given now a point $(\bar{\alpha}_1, \ldots, \bar{\alpha}_n)$ there is a sequence of sets E_p (p standing for a sequence of binary ε's) such that

$$E_1 \supset E_2 \ldots$$

and whose intersection consists of the single point $(\bar{\alpha}_1, \ldots, \bar{\alpha}_n)$. We define $I(\bar{\alpha}_1, \ldots, \bar{\alpha}_n)$ by the formula

$$I(\bar{\alpha}_1, \ldots, \bar{\alpha}_n) = \lim_{p \to \infty} \limsup_{t \to \infty} \left(\int_{E_p} d\sigma_t(\alpha_1, \ldots, \alpha_n) \right)^{1/t}. \tag{9.13}$$

To see why this is so, note that

$$\int_{\alpha_1 + \ldots + \alpha_n = 1} \exp\left(t \sum_{i=1}^{n} \alpha_i V(i) \right) d\sigma_t(\alpha_1, \ldots, \alpha_n) =$$

$$= \sum_{p} \int_{E_p} \exp\left(t \sum_{i=1} \alpha_i V(i) \right) d\sigma_t(\alpha_1, \ldots, \alpha_n) \sim \exp\left(t \lambda_{\max}(R + V) \right)$$

where the E's are the sets comprising the n-th partition.

Hence

$$\lambda_{\max}(R + V) = \lim_{t \to \infty} \left(\int_{E_{p_0}} \exp\left(t \sum_{i=1}^{n} V(i) \alpha_i \right) d\sigma_t(\alpha_1, \ldots, \alpha_n) \right)^{1/t}$$

where

$$\int_{E_{p_0}} \exp\left(t \sum_{i=1}^{n} V(i) \alpha_i \right) d\sigma_t(\alpha_1, \ldots, \alpha_n)$$

is the *largest* of the integrals $\int_{E_p}$. Since diameters of sets comprising partitions of high order are small,

$$\sum_{i=1}^{n} V(i) \alpha_i$$

varies little over each such set and consequently the limit superior and

limit inferior of

$$\left(\int_{E_p} \exp\left(t \sum_{i=1}^{n} V(i)\alpha_i\right) d\sigma_t(\alpha_1, \ldots, \alpha_n)\right)^{1/t}$$

as $t \to \infty$ differs little and in fact their difference goes to zero as the order of the partition goes to infinity.

Let us then take it for granted that there exists a function $I(\alpha_1, \ldots, \alpha_n)$ associated with the process $x(\tau)$ such that

$$\lambda_{\max}(R+V) = \max\left\{\sum_{i=1}^{n} \alpha_i V(i) + I(\alpha_1, \ldots, \alpha_n)\right\}$$

with $\alpha_i \geqslant 0$ and

$$\sum_{i=1}^{n} \alpha_i = 1 .$$

How does one find I?

First note that the eigenvector corresponding to the maximum eigenvalue of $R+V$ must have non-negative components. This follows at once from the fact that for sufficiently large a the entries of $R+V+aI$ are non-negative and hence the principal eigenvector of $R+V+aI$ (which is the *same* as the principal eigenvector of $R+V$) has non-negative components. Next if $u_1, u_2, \ldots, u_n$ are all positive and if we set

$$\hat{V}(i) = -\frac{1}{u_i} \sum_{j=1}^{n} r_{ij} u_j \tag{9.14}$$

then the maximum eigenvalue is 0 (the components of the corresponding eigenvector being $u_1, u_2, \ldots, u_n$).

Thus

$$0 = \lambda_{\max}(R + \hat{V}) = \max_{(\alpha)}\left\{-\sum_{i=1}^{n} \frac{\alpha_i}{u_i} \sum_{j=1}^{n} r_{ij} u_j + I(\alpha_1, \ldots, \alpha_n)\right\} \tag{9.15}$$

for *all* $u_1, \ldots, u_n$ which are positive. It is now a small step to conclude that

$$I(\alpha_1, \ldots, \alpha_n) = \inf_{u_j > 0} \sum_{i=1}^{n} \frac{\alpha_i}{u_i} \sum_{j=1}^{n} r_{ij} u_j . \tag{9.16}$$

Finally one gets

$$\lambda_{\max}(R+V) = \max_{(\alpha)} \left\{ \sum_{i=1}^{n} \alpha_i V(i) + \inf_{u_j>0} \sum_{i=1}^{n} \frac{\alpha_i}{u_i} \sum_{j=1}^{n} r_{ij} u_j \right\}. \tag{9.17}$$

If the chain is time reversible i.e.

$$W(i)P(i|j;\, t) = W(j)P(j|i;\, t)$$

it follows that

$$W(i) r_{ij} = W(j) r_{ji}\,,$$

$$s_{ij} = \frac{\sqrt{W(i)}\, r_{ij}}{\sqrt{W(j)}} = \frac{\sqrt{W(j)}}{\sqrt{W(i)}} r_{ji} = s_{ji}\,.$$

Setting

$$\frac{u_j}{\sqrt{\alpha_j}} \sqrt{W(j)} = v_j$$

we see that

$$\sum_{i=1}^{n} \frac{\alpha_i}{u_i} \sum_{j=1}^{n} r_{ij} u_j = \frac{1}{2} \sum_{ij=1}^{n} s_{ij} \sqrt{\alpha_i} \sqrt{\alpha_j} \left(\frac{v_i}{v_j} + \frac{v_j}{v_i} \right).$$

But

$$\frac{v_i}{v_j} + \frac{v_j}{v_i} > 2$$

(the equality occurring when $v_i = v_j$) and hence

$$\inf_{u_i>0} \sum_{i=1}^{n} \frac{\alpha_i}{u_i} \sum_{j=1}^{n} r_{ij} u_j = \sum_{i,j=1}^{n} s_{ij} \sqrt{\alpha_i} \sqrt{\alpha_j}\,.$$

Finally in this case

$$\lambda_{\max}(R+V) = \max_{(\alpha)} \left\{ \sum_{i=1}^{n} \alpha_i V(i) + \sum_{i,j=1}^{n} s_{ij} \sqrt{\alpha_i} \sqrt{\alpha_j} \right\}$$

which upon setting

$$\sqrt{\alpha_i} = x_i$$

becomes

$$\lambda_{\max}(R+V) = \max\left\{\sum_{i=1}^{n} V(i)x_i^2 + \sum_{i,j=1}^{n} s_{ij}x_i x_j\right\} \tag{9.18}$$

the maximum being over x's satisfying

$$\sum_{i=1}^{n} x_i^2 = 1\,. \tag{9.19}$$

Thus in a roundabout way we have arrived at the Raleigh-Ritz principle for a special case of Markov chains (namely those whose infinitesimal generators are symmetrizeable).

What is however more interesting is that the Donsker-Varadhan method led to (9.17) which in a slightly disguised way gives a variational characterization of the maximum eigenvalue of an *arbitrary* matrix with non-negative elements since every such matrix can be written in the form $R+V$ (with R an infinitesimal generator of a Markov process). As far as I know such a characterization is new and thus a new theorem about non-negative finite matrices was discovered. Direct proofs (i.e. not using Markov processes and Donsker-Varadhan ideas) of (9.17) were given (post factum!) by Paul Chernoff and by I. M. Singer and Don Friedan (in response to my challenge in a lecture last January at I. M. Singer's Seminar in Berkeley).

SECTION 10

Introduction to the Donsker-Varadhan Theory Continued

Formally, the extension of the ideas presented in Section 9 to the Wiener process is almost immediate.

We consider

$$E\left\{\exp\left(-\int_0^t V(x(\tau))\,d\tau\right)\right\} \tag{10.1}$$

and introduction the distribution function

$$L_t(dx;\, x(\tau),\, 0<\tau<t) =$$

$$= \frac{1}{t}\times \text{time up to } t \text{ spent by } x(\tau) \text{ in } dx$$

so that

$$\int_0^t V(x(\tau))\,d\tau = t\int_{-\infty}^{\infty} V(x)\,L_t(dx)\,.$$

One can now think of the integral (10.1) over the space of paths as the integral of

$$\exp\left(-t\int_{-\infty}^{\infty} V(x)\,F(dx)\right)$$

over the space of distribution functions F which is the analogue of the set

$$\sum_{i=1}^{n} \alpha_i = 1\,, \qquad \alpha_i \geqslant 0\,, \qquad i = 1, 2, \ldots, n$$

of the preceding section.

It is harder to think of the analogue of $\sigma_t(\alpha_1, \ldots, \alpha_n)$ but the analogue of

$$\int_E d\sigma_t(\alpha_1, \ldots, \alpha_n)$$

is clearly the probability that $L_t(dx)$ belongs to a set E of distribution functions.

If one closes one's eyes and waves one's hands one can convince oneself that there is a functional $I(F)$ such that

$$\lambda_1 = \sup_F \left\{ -\int_{-\infty}^{\infty} V(x) F(dx) + I(F) \right\} \tag{10.2}$$

and that even if E_ν is a sequence of sets (in space of distribution functions) such that

$$E_1 \supset E_2 \supset \ldots$$

and whose intersection contains the single distribution function $\overline{F}$ then

$$I(\overline{F}) = \lim_{\nu \to \infty} \limsup_{t \to \infty} \left(P\{L_t(dx) \in E_\nu\} \right)^{1/t}. \tag{10.3}$$

Once we grant the existence of the I-functional such that (10.2) holds we can proceed as in Section 9 and consider the class of $\tilde{V}$'s given by the formula

$$\tilde{V}(x) = -\frac{1}{2} \frac{u''(x)}{u(x)}$$

with $u(x) > 0$.

We then have for every $u(x) > 0$

$$0 = \lambda_1 = \sup_F \left\{ -\frac{1}{2} \int_{-\infty}^{\infty} \frac{u''(x)}{u(x)} F(dx) + I(F) \right\}$$

and as before

$$I(F) = \frac{1}{2} \inf_{u>0} \int_{-\infty}^{+\infty} \frac{u''(x)}{u(x)} F(dx) . \tag{10.4}$$

Assuming (optimistically) that we may restrict ourselves to F's which have a differentiable derivative f which also behaves well at $\pm \infty$ we have

$$I(F) = \frac{1}{2} \inf_{u>0} \int_{-\infty}^{\infty} \left(\frac{u''(x)}{u(x)}\right) f(x)\, dx =$$

$$= \frac{1}{2} \inf_{u>0} \int_{-\infty}^{\infty} \left[f(x) \left(\frac{u'(x)}{u(x)}\right)^2 - f'(x) \frac{u'(x)}{u(x)} \right] dx .$$

Since $f > 0$ (being the derivative of a non-decreasing function F) we have (wherever $f > 0$)

$$f(x) \left(\frac{u'(x)}{u(x)}\right)^2 - f'(x) \frac{u'(x)}{u(x)} > -\frac{1}{4} \frac{f'^2}{f}$$

the equality occurring only when

$$\frac{u'(x)}{u(x)} = \frac{1}{2} \frac{f'(x)}{f(x)} .$$

Finally,

$$I(F) = -\frac{1}{8} \int_{-\infty}^{\infty} \frac{f'^2}{f}\, dx$$

and (by 10.2)

$$\lambda_1 = -\sup \left\{ -\int_{-\infty}^{\infty} V(x) f(x)\, dx - \frac{1}{8} \int_{-\infty}^{\infty} \frac{f'^2}{f}\, dx \right\} = \tag{10.5}$$

$$= \inf \left\{ \int_{-\infty}^{\infty} V(x) f(x)\, dx + \frac{1}{8} \int_{-\infty}^{\infty} \frac{f'^2}{f}\, dx \right\} .$$

The sup and the inf are taken over all f's such that

$$f > 0 \qquad \text{and} \qquad \int_{-\infty}^{+\infty} f\,dx = 1\,.$$

Setting

$$f = \psi^2$$

we obtain the Raleigh-Ritz principle in the form (9.3).

To tighten up this argument and to apply the theory to more complicated functionals of $L_t(dx)$ than the simple linear functional

$$\int_{-\infty}^{\infty} V(x)\,L_t(dx)$$

is not at all easy and, in fact, the complete theory is directly applicable only to ergodic processes (the Wiener process is clearly not ergodic). Still the underlying ideas are simple and elegant, and they are attracting more and more attention. There is therefore little doubt that much simplification of the apparatus which at present depends on rather subtle estimates will be forthcoming.

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