

P A T H I N T E G R A L S

— in —

Quantum Mechanics

Statistics

and

Polymer Physics

P A T H INTEGRALS

———— in ————
**Quantum Mechanics
Statistics
and
Polymer Physics**

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Published by

World Scientific Publishing Co. Pte. Ltd.

P O Box 128, Farrer Road, Singapore 9128

USA office: 687 Hartwell Street, Teaneck, NJ 07666

UK office: 73 Lynton Mead, Totteridge, London N20 8DH

Library of Congress Cataloging-in-Publication Data

Kleinert, Hagen.

Path integrals in quantum mechanics, statistics, and polymer
physics / Hagen Kleinert.

p. cm.

Includes bibliographical references and index.

ISBN 9810201966. -- ISBN 9810201974 (pbk.)

1. Path integrals. 2. Quantum theory. 3. Statistical physics.
4. Polymers. I. Title.

QC174.17.P27K54 1990

530.1'2--dc20

90-45950

CIP

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*Ay, call it holy ground,
The soil where first they trod!*
F.D. HEMANS (1793-1835),
Landing of the Pilgrim Fathers

Chapter 1

Fundamentals

Before turning to the actual subject of this text, path integrals, it may be useful to recall some of the theoretical background underlying the theory to be developed.¹

1.1 Classical Mechanics

A classical mechanical system is described by a set of generalized coordinates q_1, \dots, q_N , the associated velocities, $\dot{q}_1, \dots, \dot{q}_N$, and a Lagrangian

$$L(q_i(t), \dot{q}_i(t), t). \quad (1.1)$$

The dot denotes the time derivative d/dt . The Lagrangian governs the dynamics and is, at most, a quadratic function of \dot{q}_i . The time integral

$$\mathcal{A}[q_i] = \int_{t_a}^{t_b} dt L(q_i(t), \dot{q}_i(t), t) \quad (1.2)$$

over the Lagrangian along an arbitrary path $q_i(t)$ is called the *action* of this path. The path $q_i(t)$ that is actually chosen by the system as a function of time is called the *classical path*, $q_i^{cl}(t)$. It has the property of extremizing the action in comparison with all neighboring paths

$$\underline{q_i(t)} \equiv q_i^{cl}(t) + \delta q_i(t) \quad (1.3)$$

with fixed end points $q(t_b)$, $q(t_a)$. To express this property formally one introduces the *variation* of the action as the linear term in $\delta q_i(t)$ of the change of $\mathcal{A}[q_i]$:

$$\delta \mathcal{A}[q_i] \equiv \{\mathcal{A}[q_i + \delta q_i] - \mathcal{A}[q_i]\}_{lin} \quad (1.4)$$

¹The reader familiar with classical and quantum mechanics may skip the first four sections and start with Section 1.5.

The extremal principle for the classical path is then

$$\delta \mathcal{A}[q_i] \Big|_{q_i(t)=q_i^{cl}(t)} = 0 \quad (1.5)$$

for all variations of the path around the classical path, $\delta q_i(t) \equiv q_i(t) - q_i^{cl}(t)$, which vanish at the end points:

$$\delta q_i(t_a) = \delta q_i(t_b) = 0. \quad (1.6)$$

Since the action is a time integral of a Lagrangian, this extremality property can be phrased in terms of differential equations. Let us calculate the variation of $\mathcal{A}[q_i]$ explicitly,

$$\begin{aligned} \delta \mathcal{A}[q_i] &= \{\mathcal{A}[q_i + \delta q_i] - \mathcal{A}[q_i]\}_{lin} \\ &= \int_{t_a}^{t_b} dt \{L(q_i(t) + \delta q_i(t), \dot{q}_i(t) + \delta \dot{q}_i(t), t) - L(q_i(t), \dot{q}_i(t), t)\}_{lin} \\ &= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i(t) \right\} \\ &= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right\} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta q_i(t) \Big|_{t_a}^{t_b}. \end{aligned} \quad (1.7)$$

The last expression arises by partially integrating the $\delta \dot{q}_i$ term. Here, as in the entire text, repeated indices are understood to be summed (*Einstein's summation convention*). The end point terms (*surface or boundary terms*) at t_a and t_b may be dropped, due to (1.6). Thus we find, for the classical orbit $q_i^{cl}(t)$, the so-called *Euler-Lagrange equations*:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}. \quad (1.8)$$

There is an alternative formulation of classical dynamics which is based on a Legendre transformed function of the Lagrangian called the *Hamiltonian*

$$H(p_i(t), q_i(t), t) \equiv \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i(t) - L(q_i(t), \dot{q}_i(t), t). \quad (1.9)$$

Its value at any time is identified with the energy of the system. According to the general theory of Legendre transformations,² the natural variables in H are no longer $q_i(t)$ and $\dot{q}_i(t)$, but $q_i(t)$ and the generalized momenta $p_i(t)$ defined by the equations

$$p_i(t) \equiv \frac{\partial}{\partial \dot{q}_i} L(q_i(t), \dot{q}_i(t), t). \quad (1.10)$$

²For an elementary introduction see the book H.B. Callan, *Classical Thermodynamics*, John Wiley and Sons, New York, 1960.

In order to specify the Hamiltonian $H(p_i(t), q_i(t), t)$ in terms of its proper variables $p_i(t), q_i(t)$, the equations (1.10) for $p_i(t)$ have to be solved for $\dot{q}_i(t)$,

$$\dot{q}_i(t) = v_i(p_i(t), q_i(t), t), \quad (1.11)$$

and inserted into (1.9), giving H as

$$H(p_i(t), q_i(t), t) = p_i(t)v_i(p_i(t), q_i(t), t) - L(q_i(t), v_i(p_i(t), q_i(t)), t). \quad (1.12)$$

Expressed in terms of H , the action becomes a functional of $p_i(t)$ and $q_i(t)$,

$$\mathcal{A}[p, q] = \int_{t_a}^{t_b} dt [p_i(t)\dot{q}_i(t) - H(p_i(t), q_i(t), t)]. \quad (1.13)$$

This is the so-called *canonical form* of the action. The classical orbits, now specified by $p_i^{cl}(t), q_i^{cl}(t)$, extremize the action in comparison with all neighboring orbits when $q_i(t)$ are varied at fixed end points [see (1.3), (1.6)], and $p_i(t)$ without restriction:

$$\begin{aligned} q_i(t) &= q_i^{cl}(t) + \delta q_i(t), & \delta q_i(t_a) = \delta q_i(t_b) &= 0, \\ p_i(t) &= p_i^{cl}(t) + \delta p_i(t). \end{aligned} \quad (1.14)$$

This gives a variation

$$\begin{aligned} \delta \mathcal{A}[p, q] &= \int_{t_a}^{t_b} dt \left[\delta p_i(t)\dot{q}_i(t) + p_i(t)\delta \dot{q}_i(t) - \frac{\partial H}{\partial p_i} \delta p_i - \frac{\partial H}{\partial q_i} \delta q_i \right] \\ &= \int_{t_a}^{t_b} dt \left\{ \left(\dot{q}_i(t) - \frac{\partial H}{\partial p_i} \right) \delta p_i - \left(\dot{p}_i(t) + \frac{\partial H}{\partial q_i} \right) \delta q_i \right\} \\ &\quad + p_i(t)\delta q_i(t) \Big|_{t_a}^{t_b} \end{aligned} \quad (1.15)$$

From this we find the *Hamilton equations* of motion for the classical orbits,

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i}, \\ \dot{q}_i &= \frac{\partial H}{\partial p_i}. \end{aligned} \quad (1.16)$$

These agree with the Euler-Lagrange equations (1.8) via (1.10), as can easily be verified.

The $2N$ -dimensional space of all p_i and q_i is called the *phase space*. An arbitrary function

$$F(p_i(t), q_i(t), t) \quad (1.17)$$