Topics in Path Integration

by

Anwar Yunas Shiekh

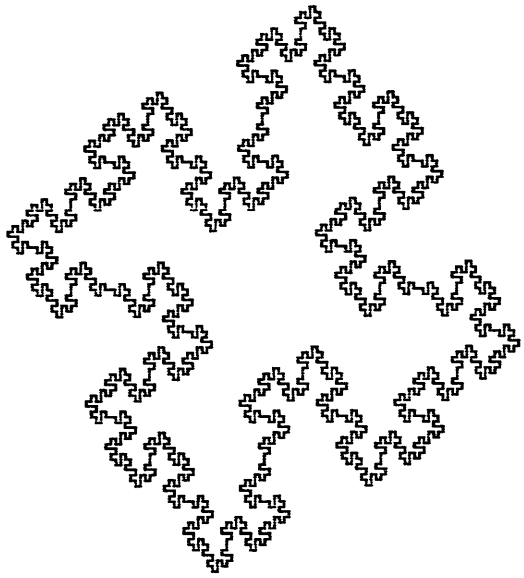
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Theoretical Particle Physics Group
Blackett Laboratory
Imperial College
London SW7 2BZ
England

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To the manner of people
that make such work
possible

Topics in Path Integration



"I think that it is a general rule that the originator of a new idea is not the most suitable person to develop it because his fears of something going wrong are really too strong and prevent his looking at the method from a purely detached point of view in the way that he ought to"

P. A. M. Dirac

J. Robert Oppenheimer Memorial Prize
acceptance speech, 1968.

Abstract

Several aspects of the application of path integrals to quantum mechanics are considered.

In chapter one, the path integral is used to form gauge invariant variables *[Mandelstam, 1962]* and these are used in the specific calculation of the non-relativistic scattering of charged scalar particles from a classical Aharonov-Bohm solenoid. This allows the calculation to be done without an explicit gauge choice.

Chapter two continues with the application of the path integral on a multiply connected space, and forms a constructive derivation for exact scalar diffraction from an impenetrable two dimensional wedge, first investigated by Sommerfeld *[1896]*.

Chapter three is more speculative; and represents a preliminary attempt to obtain a path integral, invariant under general (time dependent) canonical transformations. This would lead the way to a consistent quantization scheme, and a quantum mechanical application of the Hamilton-Jacobi philosophy *[Goldstein, 1980; Schulman, 1980]*.

Chapter four is a review of the ambiguities in the Dirac quantization scheme from a minimum set of postulates.

Preface

The work presented in this thesis was carried out in the Theoretical Particle Physics Group of Imperial College (1983-1986), London and (during the summer of 1985) at the Center for Relativity, Austin Texas, under the kind invitation of Cecile DeWitt-Morette. This labour was performed under the supervision of C.J.Isham.

The material presented is original except where otherwise stated and has not been submitted for a degree of this or any other university. The contents of chapters one and two have been separately published, while that of chapter three is still preliminary. Much of chapter four is a review, as is the introduction, although the approach may be novel, and in places original.

I acknowledge with gratitude the financial support of the Science and Engineering Research Council of England, without which I could not have been so employed.

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Introduction

The Path Integral Approach to Quantum Mechanics

Based on:

[Schulman, 1981; Feynman, 1948; Feynman and Hibbs, 1965; Langouche, Roekaerts and Tirapegui, 1965; Klauder, 1980; Feynman, 1985]

§1 Quantization

Classical mechanics is a description of nature using commuting variables that is well formulated by the Hamilton least action principle. But classical mechanics is not a complete model of nature; leaving several features unexplained. In fact classical electrodynamics predicts non-causal behavior for an accelerating charge *[Jackson, 1975]*, and might be considered incomplete on these grounds alone. It might even be speculated that there is only one self consistent theory of everything; that might then be deduced on consistency grounds without resort to observing the real thing. Some of the discrepancies in the classical theory have been overcome in the quantum generalization.

Dirac *[1925, 1958]* proposed how a quantum theory might be induced from the classical theory. He postulated that the classical commuting variables become non-commuting operators and suggested how the quantum dynamics be obtained from the classical Hamilton equations of motion. Since the quantum theory is the more fundamental theory (the classical predictions following in the $\hbar \to 0$ limit), it might be argued that this should be the starting point. Dirac's scheme, however has the advantage of starting from a well understood theory. In this scheme, to each classical system corresponds many quantum generalizations, (each yielding the same classical predictions for $\hbar \to 0$). Dirac's method however is ambiguous in not generating one unique member of the quantum generalizations. Some further specification (such as normal ordering) is required to completely specify the quantum theory (these features are reviewed in more detail in chapter four). This might not seem a disadvantage; but due to this ambiguity, classical techniques such as the

use of canonical transformations cannot be used to directly induce a quantum counterpart. This results in the loss of powerful techniques such as the Hamilton-Jacobi approach so often employed in classical mechanics *[Goldstein, 1980]*.

The work of chapter three is a preliminary investigation of the alternative path integral quantization technique of Feynman, in an attempt to overcome some of these problems. The path integral technique, although equivalent, differs significantly from the usual operator formulation of quantum mechanics, in that it employs commuting (or badly called 'classical') variables. Although these variables commute; the theory being equivalent to the operator formalism must contain 'operator ordering' within its structure. Understanding just how this occurs is crucial in the use of the path integral and is reviewed below.

§II Translating between formalisms

Although no formalism of quantum mechanics is more fundamental than any other, each is supposed to be equivalent and so one should be derivable from another. Assuming a knowledge of traditional quantum mechanics one may deduce the path integral formalism. Starting from the position to position amplitude for Heisenberg eigenstates:

$$\langle q_b,t_b|q_a,t_a\rangle$$

(This may be generalized to the transition between any two states.)

Inserting a set of position resolutions of unity;

$$1 = \int_{-\infty,\infty} dq\, |q\rangle\langle q|$$

leads to:

$$\langle q_b,t_b|q_a,t_a\rangle =$$

$$\int_{-\infty,\infty} dq(1) \int_{-\infty,\infty} dq(2) \ldots \int_{-\infty,\infty} dq(N-1)$$

$$\langle q(N),t(N)|q(N-1),t(N-1)\rangle\langle q(N-1),t(N-1)| \ldots |q(1),t(1)\rangle\langle q(1),t(1)|q(0),t(0)\rangle$$

where:

$$q_b = q(N)$$
$$q_a = q(0)$$

and are not integrated over.

$$= \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{k=1,N} \langle q(k),t(k)|q(k-1),t(k-1)\rangle$$

Recall that for a Heisenberg eigenstate:

$$|q(k),t(k)\rangle = \exp[i\overline{H}(\bar{q},\bar{p})t/\hbar]\,|q(k)\rangle$$

where $|q(k)\rangle$ is the state at time zero and $\overline{H}(\bar{q},\bar{p})$ is the Hamiltonian operator.

So:

$$\langle q_b,t_b|q_a,t_a\rangle = \int_{-\infty,\infty}\cdots\prod_{j=1,N-1}dq(j)\prod_{k=1,N}\langle q(k)|\exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|q(k-1)\rangle$$

continue by inserting momentum resolutions of unity:

$$\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\cdots\prod_{j=1,N-1}dq(j)\prod_{i=1,N}dp(i)$$
$$\prod_{k=1,N}\langle q(k)|p(k)\rangle\langle p(k)|\exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|q(k-1)\rangle$$

or

$$\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\cdots\prod_{j=1,N-1}dq(j)\prod_{i=1,N}dp(i)$$
$$\prod_{k=1,N}\langle q(k)|\exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|p(k)\rangle\langle p(k)|q(k-1)\rangle$$

Considering the first alternative (the consequences of the second are discussed later) and looking at the factor:

$$\langle p(k)|\exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|q(k-1)\rangle$$

define a function **H** through:

$$\exp[-i\mathbf{H}(q,p)\Delta t/\hbar] = \langle p|\exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|q\rangle/\langle p|q\rangle$$

Even though it is intended to take the $\Delta t\to 0$ limit; one must work to order Δt, since there are N such terms, where $N\Delta t = T$ (the 'time of flight'). In general a physical Hamiltonian hides $(\Delta t)^{-1}$ contributions (discussed later) and so agreement between all terms of the expanded exponentials is required. Agreement to lowest order yields:

$$\mathbf{H}(q,p) = \langle p|\bar{\mathbf{H}}(\bar{q},\bar{p})|q\rangle/\langle p|q\rangle$$

So for a Hermitean Hamiltonian:

$$\langle p|q\rangle\langle q|p\rangle\mathbf{H}^2(q,p) = \langle p|\bar{\mathbf{H}}(\bar{q},\bar{p})|q\rangle\langle q|\bar{\mathbf{H}}(\bar{q},\bar{p})|p\rangle$$

Integrating over q and using the resolution of unity for q:

$$\int_{-\infty,\infty}dq\,\langle p|q\rangle\langle q|p\rangle\mathbf{H}^2(q,p) = \int_{-\infty,\infty}dq\,\langle p|\bar{\mathbf{H}}(\bar{q},\bar{p})\bar{\mathbf{H}}(\bar{q},\bar{p})|q\rangle\langle q|p\rangle$$

Since the Hamiltonians are to agree for all q, equating the integrands yields:

$$\mathbf{H}^2(q,p) = \langle p|\bar{\mathbf{H}}^2(\bar{q},\bar{p})|q\rangle / \langle p|q\rangle$$

similarly for higher powers of the Hamiltonian.

In this way one may replace:

$$\langle p| \exp[-i\bar{\mathbf{H}}(\bar{q},\bar{p})\Delta t/\hbar]|q\rangle$$

by:

$$\langle p|q\rangle \exp[-i\mathbf{H}(q,p)\Delta t/\hbar]$$

where:

$$\mathbf{H}(q,p) = \langle p|\bar{\mathbf{H}}(\bar{q},\bar{p})|q\rangle / \langle p|q\rangle$$

To evaluate this one should commute factors in the Hamiltonian operator (using $[\bar{q},\bar{p}] = i\hbar\bar{\mathbf{1}}$), such that $\bar{q}$ operators are shifted to the right and can be applied to the position eigenstate, while $\bar{p}$ operators (now on the left) apply to their eigenstates. This sifting induces additional terms that carry the operator ordering information for the path integral.

Now recall:

$$\langle q|p\rangle = 1/\sqrt{(2\pi\hbar)} \exp[iqp/\hbar]$$

Substituting these results leads to:

$$\mathrm{Lim}_{N\to\infty} \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$
$$\exp\Big[\, i/\hbar \sum_{k=1,N} \{p(k)(q(k) - q(k-1)) - \mathbf{H}(q(k-1),p(k))\Delta t\}\Big]$$

$$\Delta t = T/N$$

The phase space (Hamilton) Path Integral

where:

$$\mathbf{H}(q,p) = \langle p|\bar{\mathbf{H}}(\bar{q},\bar{p})|q\rangle / \langle p|q\rangle$$

which may be **formally** written as:

$$\langle q_b,t_b|q_a,t_a\rangle = \int\int Dq\,(Dp/2\pi\hbar) \exp[i/\hbar\, \mathbf{S}(q,p)]$$

$$q(t_a) = q_a \qquad q(t_b) = q_b$$

$$S(q,p) = \int_{ta,tb} dt\ (p\dot{q} - H)$$

This is formal due to the fact that this expression depends upon which finite difference scheme is adopted in the discretization. The reasoning behind this will become clear later.

Why this object is referred to as a "path integral" or "sum over histories" follows from considering the points q(j), p(j) connected by lines. Then we have a broken line path from q_a to q_b; the sum in the exponent being the action of classical mechanics. But unlike classical mechanics the least action path is not, a priori, preferred over any other. Each path is equally considered and carries a phase weighting. The amplitude contribution from each and every path is then summed to yield the total end amplitude.

In many cases the p integrations may be explicitly performed to yield a configuration space (Lagrange) path integral. For example if:

$$\bar{H}(\bar{q},\bar{p}) = \bar{p}^2/2m + \bar{V}(\bar{q})$$

(i.e. the non-relativistic case with a conservative potential). In this case the path integral becomes:

$$Lim_{N\to\infty} \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$

$$\exp\left[i/\hbar \sum_{k=1,N} \{ p(k)(q(k) - q(k-1)) - (p^2(k)/2m + V(q(k-1)))\Delta t \} \right]$$

which may be evaluated using the Gaussian integral:

$$\int_{-\infty,\infty} \exp[-\alpha p^2 + \beta p]\, dp = \sqrt{(\pi/\alpha)}\, \exp[\beta^2/4\alpha]$$

(Re $\alpha > 0$)

There are many approaches to evaluating this, but perhaps the one with

the most generality is to adopt a matrix notation.

Denote $\mathbf{p}^t = (p(1),p(2), \ldots p(N))$

then

$$\int_{-\infty,\infty} \cdots \prod_{j=1,N} dp(j)\, \exp[-F(p)] = 1/\sqrt{(\det(\boldsymbol{\alpha}/2\pi))}\, \exp[-F_0]$$

where

$$F(p) = [\mathbf{p}^t\boldsymbol{\alpha}\mathbf{p}/2 + \boldsymbol{\beta}^t\mathbf{p} + \boldsymbol{\gamma}]$$

and F_0 is the minimum of $F(p)$ w.r.t. p i.e.

$$F_0 = \boldsymbol{\gamma} - \boldsymbol{\beta}^t\boldsymbol{\alpha}^{-1}\boldsymbol{\beta}/2$$

which may be seen from the fact that, since $\boldsymbol{\alpha}$ can be chosen Hermitean, it may be diagonalized by a unitary transformation (which has unit Jacobian) and the resulting Gaussian integrals trivially performed.

Identifying:

$$\boldsymbol{\alpha} = i\mathbf{1}\Delta t/\hbar m$$

where $\mathbf{1}$ is the N x N unit matrix, and noting that minimizing the action (w.r.t. p) fixes:

$$p = m\dot{q}$$

This leads to:

$$\mathrm{Lim}_{N\to\infty}\, 1/(2\pi\hbar i\Delta t)^{N/2} \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j)$$

$$\exp\Big[\, i\Delta t/\hbar \sum_{k=1,N} \big\{ m/2\, ((q(k) - q(k-1))/\Delta t)^2 - V(q(k-1)) \big\} \Big]$$

A configuration space (Lagrange) Path Integral

In fact looking back at the derivation it is seen that in this case the potential V(q) could be taken at $q(k-1)$ **or** $q(k)$ (taking the second of the two previous alternatives). This reflects the fact that there is no operator ordering problem in this Hamiltonian. To illustrate this feature, consider

the example given by the introduction of the electromagnetic vector potential.

Here (setting c=1):

$$\bar{\mathbf{H}}(\bar{q},\bar{p}) = (\bar{p} + e\bar{A})^2/2m - e\bar{\phi}(\bar{q}) + \bar{V}(\bar{q})$$

$$= (\bar{p}^2 + e\bar{p}\bar{A} + e\bar{A}\bar{p} + e^2\bar{A}^2)/2m - e\bar{\phi}(\bar{q}) + \bar{V}(\bar{q})$$

The freedom on where to insert resolutions of p can then be exploited to match operators against their eigenstates.

Consider the factor:

$$\langle q_{(k)}| \bar{\mathbf{H}}(\bar{q},\bar{p}) |q_{(k-1)}\rangle =$$

$$\langle q_{(k)}| (\bar{p}^2 + e\bar{p}\bar{A} + e\bar{A}\bar{p} + e^2\bar{A}^2)/2m - e\bar{\phi}(\bar{q}) + \bar{V}(\bar{q}) |q_{(k-1)}\rangle$$

Because of the non-commuting of factors, the A from $\bar{p}\bar{A}$ should be evaluated at $q_{(k-1)}$ while that from $\bar{A}\bar{p}$ acts at $q_{(k)}$. This illustrates how operator ordering is encoded into the path integral. Freedom remains within the term $(\bar{A}^2)$ not possessing ordering. This was the reason behind the use of the mid-point rule in the path integral *[Feynman, 1948]*. Having obtained the path integral, we can then take it as our primary object and investigate how it reduces to classical mechanics. This is done in the next section.

For numerical simulations the cancelling of phases is very vulnerable to rounding errors and if there are no poles in the complex plane it becomes possible to Wick rotate to imaginary time and work with the Euclidean (as opposed to Minkowski) Lagrange path integral:

$$\int Dq \exp[-\mathbf{S}(q,\dot{q})/\hbar]$$

(an analogous thing cannot be done for the Hamilton path integral).

This Euclidean object appears naturally in statistical mechanics. Here

the contributions from all paths are no longer taken equally, but rather those from around the minimum action path are strongly favoured. cancellation is replaced by suppression. in practice even the task of numerically performing the complete Euclidean path integral for reasonably large N is beyond present computational power and in practice a random selection (Monte Carlo) of paths is sampled and taken as representative. Clever numerical schemes exist, such as Metropolis, which randomly selects paths with the required exponential weighting, so avoiding over sampling the many unimportant paths. The field theoretic case follows from taking an infinite number of dimensions, when one is then summing over field configurations.

§III The Classical Limit

A heuristic but very appealing argument for the classical limit *[Feynman, 1965]* runs as follows. Paths around the classical path contribute amplitudes that are in phase (since the classical path is that with an extremum action); while those far from it contribute largely differing phases and so tend to cancel each other out. In this way contributions around the classical path are favoured and classical mechanics recovered in the $\hbar \to 0$ limit. These arguments are made more precise below.

Starting from the Hamilton path integral, derived earlier as:

$$\mathrm{Lim}_{N\to\infty} \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$
$$\exp\left[i/\hbar \sum_{k=1,N} \{ p(k)(q(k) - q(k-1)) - H(q(k-1),p(k))\Delta t \} \right]$$

$$\Delta t = T/N$$

This consists of many integrals of the form:

$$I(\lambda) \equiv \int_{-\infty,\infty} \int_{-\infty,\infty} dq\, dp\, \exp[i\lambda f(q,p)]$$

where $\lambda \to \infty$ is the classical limit ($\hbar \to 0$).

Assuming f to be analytic, we may Taylor expand about an extremum point (q_0,p_0), where q_0 and p_0 are determined from:

$$(\partial f(q_0,p_0)/\partial q)_p = 0, \quad (\partial f(q_0,p_0)/\partial p)_q = 0$$

So:

$$I(\lambda) = \int_{-\infty,\infty} \int_{-\infty,\infty} dq\, dp\, \exp[i\lambda f(q_0,p_0) + i\lambda/2\, (q-q_0)^2\, \partial^2 f(q_0,p_0)/\partial q^2$$
$$+ i\lambda/2\, (p-p_0)^2\, \partial^2 f(q_0,p_0)/\partial p^2$$
$$+ \ldots]$$

Choosing to expand the terms in the exponent of higher than second power

and setting $u \equiv q - q_0$, $v \equiv p - p_0$; yields a double integral of the form:

$$I(\lambda) = \exp[i\lambda C_{00}] \int_{-\infty,\infty} \int_{-\infty,\infty} du\, dv\, \exp[i\lambda C_{20} u^2] \exp[i\lambda C_{02} v^2]$$

$$[1 + i\lambda C_{40} u^4 + i\lambda C_{04} v^4 + \ldots]$$

where C is a constant matrix.

These integrals may be extracted from the Gaussian integral with source:

$$\int_{-\infty,\infty} \exp[i\alpha s^2 - \beta s]\, ds = \sqrt{(i\pi/\alpha)}\, \exp[i\beta^2/4\alpha]$$

by differentiating w.r.t. β (or α).

For example:

$$\int_{-\infty,\infty} \exp[i\alpha s^2]\, ds = \sqrt{(i\pi/\alpha)}$$

$$\int_{-\infty,\infty} s^2 \exp[i\alpha s^2]\, ds = \sqrt{(i\pi/\alpha)}\, (i/2\alpha)$$

$$\int_{-\infty,\infty} s^4 \exp[i\alpha s^2]\, ds = -\sqrt{(i\pi/\alpha)}\, (3/4\alpha^2)$$

etc.

(odd integrals disappearing)

From this one can see that in the classical limit of $\lambda \to \infty$; the first term, which stems from paths around the classical path, dominates.

§IV Stochastic Terms

A similar line of argument as before may be used to investigate the nature of the contributing paths. Beginning again from the Hamiltonian path integral:

$$\mathrm{Lim}_{N\to\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\cdots\prod_{j=1,N-1}dq(j)\prod_{i=1,N}(dp(i)/2\pi\hbar)$$

$$\exp\left[\,i/\hbar\sum_{k=1,N}\{p(k)(q(k)-q(k-1))-\mathbf{H}(q(k-1),p(k))\Delta t\}\right]$$

$$\Delta t = T/N$$

This consists of many integrals of the form:

$$I=\int_{-\infty,\infty}\int_{-\infty,\infty}dq\,dp\,\exp[i/\hbar\,\{p\Delta q-\mathbf{H}(q,p)\Delta t\}]$$

Taylor expand **H** about q,p = 0 to yield:

$$I=\int_{-\infty,\infty}\int_{-\infty,\infty}dq\,dp\,\exp[i/\hbar\,\{p\Delta q-p^2\Delta t/2m(q)\}]\,(C_{00}+C_{10}q+C_{01}p+\ldots)$$

further, temporarily expand $\exp[i/\hbar\,p\Delta q]$ to yield:

$$I=\int_{-\infty,\infty}\int_{-\infty,\infty}dq\,dp\,\exp[-i/\hbar\,p^2\Delta t/2m(q)]\,(D_{00}+D_{20}q^2+D_{02}p^2+\ldots)$$

Having held only p^2 in the exponential. The p integrals may then be performed using:

$$\int_{-\infty,\infty}\exp[i\alpha s^2]\,ds=\sqrt{(i\pi/\alpha)}$$

$$\int_{-\infty,\infty}s^2\exp[i\alpha s^2]\,ds=\sqrt{(i\pi/\alpha)}\,(i/2\alpha)$$

$$\int_{-\infty,\infty}s^4\exp[i\alpha s^2]\,ds=-\sqrt{(i\pi/\alpha)}\,(3/4\alpha^2)$$

etc.

(odd integrals disappearing)

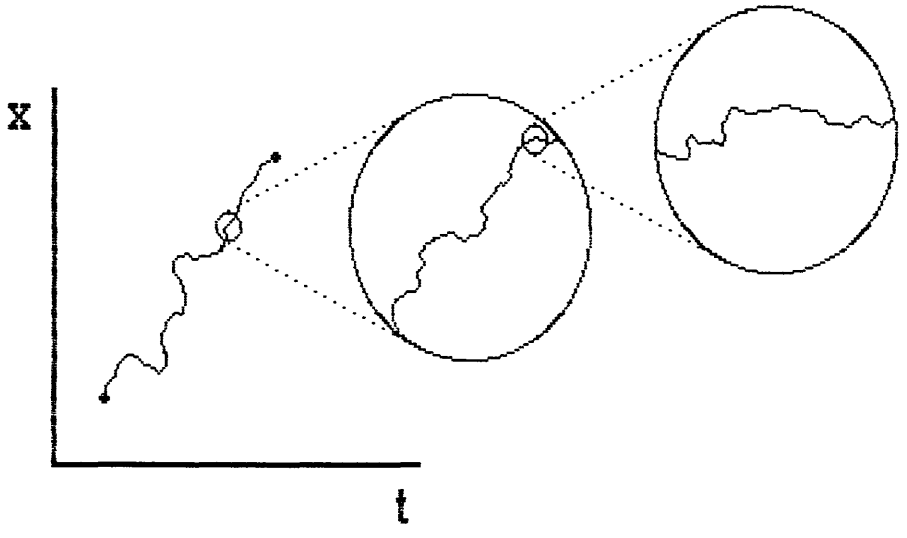
which shows that each p contributes like $(\Delta t)^{-1/2}$, since each p^2 generates a i/α, where $\alpha = -\Delta t/2m\hbar$.

In performing the p integrals in:

$$I = \int_{-\infty,\infty}\int_{-\infty,\infty} dq\, dp\, \exp[i/\hbar\,\{p\Delta q - p^2\Delta t/2m(q)\}]\,(C_{00} + C_{10}q + C_{01}p + \dots)$$

and obtaining the Lagrange formalism; p becomes $m\Delta q/\Delta t$, so that in the Lagrange formalism $\Delta q \sim (\Delta t)^{1/2}$ (c.f. $p \sim (\Delta t)^{-1/2}$ in the Hamiltonian formalism).

It is in this way that the contributing class of paths are seen to be stochastic (or Brownian) in nature (see figure below).



Stochastic path

(continuous but not differentiable)

This behavior must be carefully taken into account when working to order Δt (as before); and is the manifestation of the path integrals sensitivity to the finite difference scheme adopted in discretization. Terms, such as

$(\Delta q)^4/\Delta t$ in the Lagrangian, give (in the $\Delta t \to 0$ limit), for paths smooth in p and q, no contribution. This is because finite p implies $\Delta q \sim \Delta t$ and so $(\Delta q)^4/\Delta t \sim (\Delta t)^3$. But such terms are finitely contributing for the dominating unsmooth paths ($\Delta q \sim (\Delta t)^{1/2}$) and will be referred to as stochastic. This dependence on stochastic paths is where operator ordering is concealed.

The mid-point rule (being accurate to second order) generates no stochastic terms and is the reason why it correctly reproduces the quantum mechanics. This is seen when looking at the **usual** definition of the differential:

$$df(t)/dt \equiv \mathrm{Lim}_{\Delta t \to 0}\big(f(t+\Delta t) - f(t)\big)/\Delta t$$

Higher order differentials following from repeated application.

$$= \mathrm{Lim}_{\Delta t \to 0}\big(df(t)/dt + d^2f(t)/dt^2\, \Delta t/2! + \dots\big)$$

from Taylor expansion (f being assumed analytic)

The 'strongest' terms in the action (such as that stemming from $p\dot{q}$) are of order $(\Delta t)^0$, stronger terms not occurring physically as they lead to infinities in the $\Delta t \to 0$ limit. Time derivatives appearing in such terms should be represented accurately to order Δt, since we must work to this order. In this way the formula given above for the derivative is seen to be an inconsistent definition if used in a formalism, such as path integration, that is sensitive to first order in Δt. Alternatively using a symmetric (mid-point) definition:

$$\mathrm{Lim}_{\Delta t \to 0}\big(f(t+\Delta t) - f(t-\Delta t)\big)/2\Delta t$$

$$= \mathrm{Lim}_{\Delta t \to 0}\big(df(t)/dt + d^3f(t)/dt^3\, (\Delta t)^2/3! + \dots\big)$$

This has all the error terms disappearing for the path integral in the

$\Delta t \rightarrow 0$ limit, and so is a correct definition for use within the path integral. Other schemes might, in context, give no contribution, but the mid-point scheme is guaranteed not to. It might now be argued that the formal expression:

$$\langle q_b, t_b | q_a, t_a \rangle = \int\int Dq \, (Dp/2\pi\hbar) \exp[i/\hbar \, S(q,p)]$$

$$q(t_a) = q_a \qquad q(t_b) = q_b$$

$$S(q,p) = \int_{ta,tb} dt \, (p\dot{q} - H)$$

can be made unambiguous if it is noted that all consistent discretization schemes lead to no stochastic terms and so the same answer in the $\Delta t \rightarrow 0$ limit. As was seen earlier, this use of mid-point expansion was not always necessary in Cartesian coordinates; but becomes essential when in a general coordinate system and is a matter approached in more detail in chapter three.

An example on how to actually go about performing a path integral constitutes much of chapter one.

§V The Wave Equation

If we are to take the path integral as our primary object, as did Feynman *[1948]*, then we should understand how to obtain the wave equation from it. This may be illustrated by deducing Schrödinger's equation corresponding to the previous example of a non-relativistic particle in an electromagnetic field. Before proceeding with this one might investigate the gauge invariance of this object. So long as we use the mid-point rule we may proceed naively with the 'formal' object, since no stochastic terms appear.

$$I \equiv \int\int Dq\,(Dp/2\pi\hbar)\,\exp\Big[\,i/\hbar \int_{ta,tb} (p\dot{q} - (p + eA)^2/2m - e\phi - V)\,dt\,\Big]$$

translating, $p \rightarrow p - eA$:

$$= \int\int Dq\,(Dp/2\pi\hbar)\,\exp\Big[\,i/\hbar \int_{ta,tb} ((p - eA)\dot{q} - p^2/2m - e\phi - V)\,dt\,\Big]$$

performing the gauge transformation:

$$A \rightarrow A - \partial\chi/\partial q$$
$$\phi \rightarrow \phi - \partial\chi/\partial t$$

yields:

$$I \rightarrow I\,\exp\Big[\,ie/\hbar \int_{ta,tb} (\partial\chi/\partial q\,\dot{q} + \partial\chi/\partial t)\,dt\,\Big]$$

$$= I\,\exp[ie\chi/\hbar]_{a,b}$$

which confirms gauge invariance for the mid-point path integral. Stochastic terms would in general spoil gauge invariance.

To develop the wave equation, start from the mid-point Hamiltonian path integral:

$$K(y,t) \equiv \mathrm{Lim}_{N\to\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\cdots\prod_{j=1,N-1}dq(j)\prod_{i=1,N}(dp(i)/2\pi\hbar)$$

$$\exp\left[\, i/\hbar \sum_{k=1,N}\left\{p(k)(q(k)-q(k-1)) - \mathbf{H}(q(k-1),p(k))\Delta t\right\}\right]$$

where:

$$\mathbf{H}(q(k-1),p(k)) =$$

$$i/2m\left\{p^2(k) + ep(k)\left(A(q(k)) + A(q(k-1))\right) + e^2/4\left(A(q(k)) + A(q(k-1)\right)^2\right\}$$

$$- e\phi(q(k-1)) + V(q(k-1))$$

Here the freedom to assign A^2 at $q(k)$ or $q(k-1)$ has been exploited to simplify the working.

Performing the p integrals leads to:

$$K(y,t) = \mathrm{Lim}_{N\to\infty}\int_{-\infty,\infty}\cdots 1/Z^N\prod_{j=1,N-1}dq(j)\exp\left[\, i/\hbar\sum_{k=1,N}\mathbf{S}(q(k),q(k-1))\right]$$

where:

$$\mathbf{S}(q(k),q(k-1)) =$$

$$\left\{m/2\,(q(k)-q(k-1))^2/\Delta t - 1/2\,(q(k)-q(k-1))\left(eA(q(k)) + eA(q(k-1))\right)\right.$$

$$\left. + e\phi(q(k-1))\Delta t - V(q(k-1))\Delta t\right\}$$

We shall in fact leave the normalization constant (Z) undetermined, as it also follows later from consistency requirements. It should be noted that in this case the canonical momentum $p = m\dot{q} - eA$.

The way to proceed is to propagate forward one time step, since it is a differential equation in time we wish to develop for K. It follows from the previous equation (for any $\mathbf{S}$) that in the $\Delta t\to 0$ limit:

$$K(x,t+\Delta t) = \int_{-\infty,\infty}dy/Z\,\exp[i/\hbar\,\mathbf{S}(x,y)]\,K(y,t)$$

a statement of locality.

Explicitly, for the case in question:

$$K(x,t+\Delta t) = \int_{-\infty,\infty} dy/Z$$

$$\exp[i/\hbar\,(m/2\,(x-y)^2/\Delta t - i/2\,(x-y)(eA(x,t) + eA(y,t))$$

$$+ e\phi(y,t)\Delta t - V(y,t)\Delta t)]\,K(y,t)$$

working to order Δt and setting $\xi \equiv x-y$ (recall $\xi \sim (\Delta t)^{1/2}$):

$$K(x,t+\Delta t) = \int_{-\infty,\infty} d\xi/Z\,\exp[i/\hbar\,(m\xi^2/2\Delta t)]$$

$$(1 - i\xi/\hbar\,eA(x,t) - i\xi^2/2\hbar\,e\partial A(x,t)/\partial x + \ldots$$

$$+ i/\hbar\,e\phi(x,t)\Delta t + \ldots$$

$$- i/\hbar\,V(x,t)\Delta t - \ldots$$

$$- \xi^2/2\hbar^2\,e^2A^2(x,t) - \ldots\,)\,(K(x,t) + \partial K(x,t)/\partial x\,\xi + 1/2\,\partial^2 K(x,t)/\partial x^2\,\xi^2 + \ldots\,)$$

$$= \int_{-\infty,\infty} d\xi/Z\,\exp[i/\hbar\,(m\xi^2/2\Delta t)]$$

$$\{(1 - i/\hbar\,(\xi eA(x,t) - \xi^2/2\,e\partial A(x,t)/\partial x + e\phi(x,t)\Delta t - V(x,t)\Delta t)$$

$$- \xi^2/2\hbar^2\,e^2A^2(x,t)\big)\,K(x,t)$$

$$+ (\xi - i/\hbar\,\xi^2 eA(x,t))\,\partial K(x,t)/\partial x$$

$$+ \xi^2/2\,\partial^2 K(x,t)/\partial x^2 + \ldots\,\}$$

Z is determined from the consistency requirement that each side must agree in zero order, i.e.:

$$1 = \int_{-\infty,\infty} d\xi/Z\;\exp[i/\hbar\,(m\xi^2/2\Delta t)]$$

from which we deduce:

$$Z = (2\pi i\hbar\Delta t/m)^{1/2}$$

as before, by:

$$\int_{-\infty,\infty} \exp[i\alpha s^2]\, ds = \sqrt{(i\pi/\alpha)}$$

Performing the main integral using also:

$$\int_{-\infty,\infty} s^2 \exp[i\alpha s^2]\, ds = \sqrt{(i\pi/\alpha)}\,(i/2\alpha)$$

(odd integrals disappearing) leads to:

$$(K(x,t+\Delta t) - K(x,t))/\Delta t =$$

$$\left(1/2m\; e\partial A(x,t)/\partial x - ie\phi(x,t)/\hbar - iV(x,t)/\hbar - i/2m\hbar\; e^2A^2(x,t)\right) K(x,t)$$

$$+ 1/m\; eA(x,t)\,\partial K(x,t)/\partial x$$

$$+ i\hbar/2m\;\partial^2 K(x,t)/\partial x^2$$

In the limit $\Delta t \to 0$ we then obtain:

$$\mathbf{i\hbar\,\partial K/\partial t = 1/2m\,(i\hbar\,\partial/\partial x + eA)^2\,K - e\phi\,K + V\,K}$$

Schrödinger's equation for a non-relativistic particle in the presence of an electromagnetic field

The differential is correctly represented here since we are no longer within the path integral. Had we not taken care of where A was evaluated, additional 'anomalous' terms would in general appear, the path integral Hamiltonian would then no longer correspond directly to that appearing in the corresponding Schrödinger's equation. These anomalous terms would be responsible for spoiling gauge invariance. In summary, the mid-point rule hides no secrets, and for this reason is favoured.

This analysis was true for positive times of propagation. Choosing K = 0 for negative times and investigating the short time propagator:

$$K^+ = \mathrm{Lim}_{\Delta t \to 0^+} \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$

$$\exp\Big[\, i/\hbar \sum_{k=1,N} \{ p(k)(q(k) - q(k-1)) - H(q(k-1),p(k))\Delta t \} \Big]$$

For a short time of propagation, since the 'time of flight' tends to zero; we need only work to order $(\Delta t)^0$.

$$K^+ = \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} dq(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$

$$\exp\Big[\, i/\hbar \sum_{k=1,N} \{ p(k)(q(k) - q(k-1)) - p^2(k)\,\Delta t/2m \} \Big]$$

the only leading order term in the Hamiltonian being of the form $p^2/2m(q)$.

Setting $u(k) \equiv q(k) - q(k-1)$ this may be evaluated from:

$$K^+ = \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \cdots \prod_{j=1,N-1} du(j) \prod_{i=1,N} (dp(i)/2\pi\hbar)$$

$$\exp\Big[\, i/\hbar \sum_{k=1,N} \{ -p^2(k)\,\Delta t/2m + p(k)u(k) \} \Big]$$

$$= \delta(q - q_0) \quad \text{for } t^+$$

$$= 0 \qquad \text{for } t^- \quad \text{by choice}$$

from which it follows that:

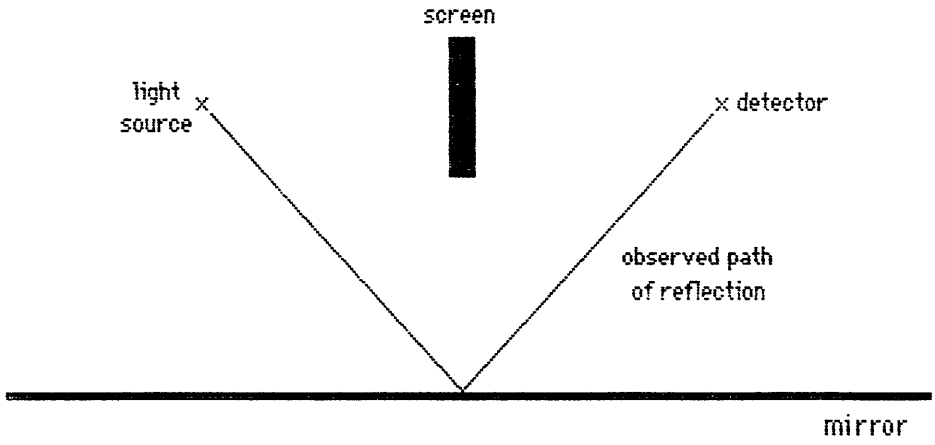
$$i\hbar\, \partial K/\partial t - H\,K = i\hbar\, \delta(q - q_0)\, \delta(t - t_0)$$

so that K is in fact seen to be the Green's function of the Schrödinger equation. This is consistent with the picture of a particle appearing at the space time point q_0, t_0.

§VI Are all paths explored by nature?

Fascinating is the question as to whether the probability amplitude wave really explores every path (reference to a particle or localized object should not be made outside of the act of localized interaction). This is aptly answered by Feynman *[1985]* in a discussion of mirrors and diffraction gratings. So intriguing is the argument that it is presented here as an illustration of the insight offered by the path integral picture.

Consider reflection from a large mirror (a screen preventing direct observation).



Reflection from a Mirror

We expect (from observation) in the symmetric case illustrated, for reflection to occur from the middle, and not the ends of the mirror. But the path integral postulates that all paths contribute equally. The resolution to this dilemma is contained in recalling that the classical contribution is from around the least action path, so recovering the law of reflection that

states the angle of incidence equals that of reflection. Although all other paths contribute, they are mutually cancelling. But if contributions from the mirror ends effectively cancel, one might wonder if they really are explored at all. This can be answered by modifying the mirror ends through selectively darkening regions such that the remaining reflecting parts contribute in phase. Now we see that we have created nothing but a diffraction grating, and behold the mirror ends now strongly contributing. In this way we see that the probability amplitude wave does indeed explore all regions, although often in vain.

Chapter One

Calculation of Non-Relativistic Scattering of Charged Scalar Particles from a Classical Aharonov-Bohm Solenoid without an explicit Gauge Choice.

(working within gauge theories without the explicit use of a gauge)

§1 Introduction

In this work a gauge free formalism is developed and used to calculate the differential cross section for scattering of non-relativistic charged scalar particles from a classical Aharonov-Bohm solenoid without the explicit choice of a gauge. The result is found to agree with that obtained through a gauge choice.

In the classical theory of electromagnetic interactions (Electrodynamics), as consolidated by Maxwell, one has physical fields. There is the electrostatic ($\mathbf{E}$) field and the magnetic ($\mathbf{B}$) field, which although a relativistic manifestation of the $\mathbf{E}$ field, turns out to be useful to consider in its own right. At this level (classical) it is calculationally convenient to introduce potentials from which the $\mathbf{E}$ and $\mathbf{B}$ fields are obtained. The problem is complicated in that although a field of potentials uniquely describes a particular electromagnetic ($\mathbf{E}$ and $\mathbf{B}$) field, the converse is not true. This leads to freedom of choice as to which potential description one chooses to work with (any one of a family giving the same physical predictions). Naturally a gauge is chosen so as to make the computation as simple or illuminating as possible. But since any one of the family are in principle equally good, one might suspect that a technique exists whereby a computation could be performed without the explicit choice of a particular gauge. In classical electromagnetism the use of a potential field is entirely mathematical and in principle it need not have been introduced (although it was for calculational convenience); and so such oddities as gauge freedom (and the associated need to gauge fix) might not seem objectionable. The big surprise arrives with the introduction of

quantum mechanics, where the potentials are introduced as a part of the formalism describing charged particles, rather than on an optional basis as before. The potentials here are no longer a mathematical option, but they retain their gauge freedom; i.e. entire families continue to describe individual physical configurations (This relates through Noether's theorem to the conservation of electric charge). This inclusion of the potentials leads to philosophical problems as to whether the potentials are physical fields or not. In classical electromagnetism they were not directly responsible for any physically detectable effect; as is clear from recalling that this theory can be formulated in terms of the electric and magnetic fields with no reference to the potentials. This is not the case for quantum mechanics, where it was shown (by Aharonov and Bohm in their influential paper *[Aharonov and Bohm, 1959; see also Kretzschmar, 1965]*) that the potential has a physically detectable influence. It is in this sense that the potential field is a physical field (it gives rise to physical effects). Yet the potential field has an arbitrariness (gauge freedom); and this might lead one to believe that it was still a mathematical artifact even in the quantum theory.

The so called Aharonov-Bohm effect *[Feynman, 1963]* has been experimentally confirmed and shows that the potential contains some physical reality, although gauge freedom speaks against it being the physical field itself.

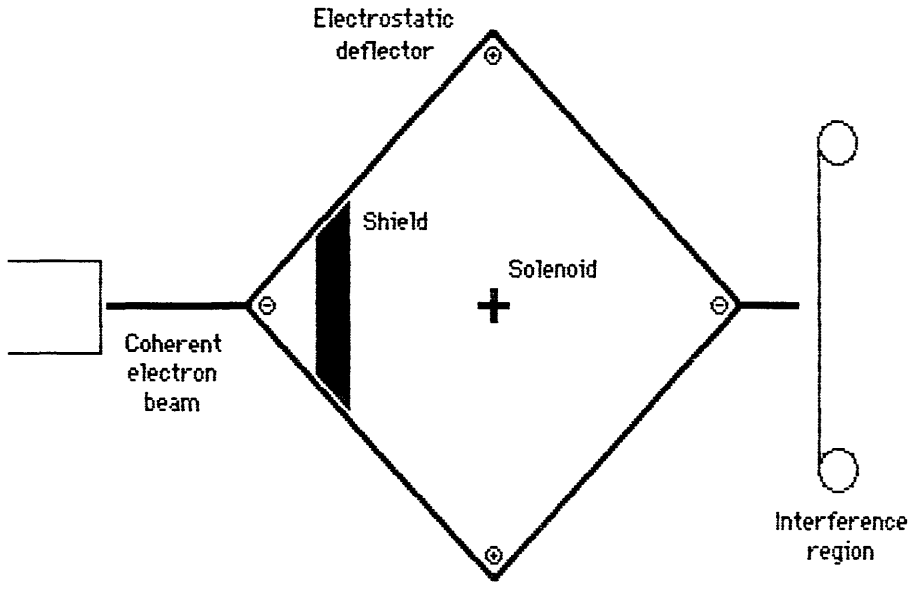
At present, most calculations are done having selected a particular gauge to work in. These procedures, although valid, are not without associated problems. In practice it seems that no particular gauge wins outright, one with certain desirable advantages tends to have associated with it disadvantages. Further it has been found by Feynman that the perturbation

expansion can be expressed in diagrammatic form with the possible interpretation of particles interacting in different ways. The contribution of a particular diagram can be gauge dependent, which brings the above interpretation into question. For these and other reasons it would be nice (and should be possible in principle) to formulate a description of the physics which, although still possessing gauge freedom (as it must), does not require an explicit choice of gauge in making a prediction.

An excellent and extensive review of the Aharonov-Bohm phenomena has recently been published *[Olariu and Popescu, 1985]* and discusses in detail the conceptual and experimental problems it broaches.

§II The Aharonov-Bohm effect

Particular attention has been paid to the Aharonov-Bohm effect, as this phenomena isolates the physical influence of the vector potential (A) field. To understand this effect consider the schematic experimental configuration illustrated below.



Schematic experiment to demonstrate interference with a time-independent vector potential

For calculational simplicity we shall work with non-relativistic charged scalar particles, to which non-relativistic unpolarized electrons approximate well. We shall refer to such particles simply as 'electrons'. In this experiment a coherent beam is split and deflected around a neutral 'infinite' solenoid via two 'well defined' paths; the beams then being recombined to interfere on the other side. The solenoid, which is shielded

from the electron beam carries a constant current. For such a solenoid the magnetic field is contained within the coils. However, the vector potential A cannot be zero everywhere outside the solenoid because the total flux through every loop is equal to the penetrating flux (#):

$$\oint A.dl = \int (\nabla \wedge A).dS = \int B.dS = \#$$

(by Stokes' law and the definition of A)

So in this configuration the electrons pass through regions occupied by the A field only. This clarifies the situation by removing the influence of the electric and magnetic fields on the electrons. We should now like to calculate the detectable influence of this A field (if any) upon the electron beam. Consider the motion of non-relativistic scalar particles which are described by the Schrödinger equation:

$$[(i\hbar\partial_x)^2/2M - i\hbar\partial_t]\,\psi = 0 \qquad (P^2/2M = E)$$

If, to describe charged particles, we then demand that the global gauge invariance becomes local, we introduce the covariant derivative (minimal coupling) into the equation of motion:

$$i\hbar\partial_\mu \rightarrow i\hbar\partial_\mu + eA_\mu$$

where c = 1 in these units

$$[(i\hbar\partial_x + eA_x)^2/2M - (i\hbar\partial_t + eA_t)]\,\phi = 0$$

which as pointed out by Dirac, has the solution for the contribution from the path p:

$$\phi = \psi \exp[iS/\hbar]$$

where

$$S = e\int_p A.dl$$

ψ being the uncoupled (free field) solution.

this is in fact a result of the covariant derivative and does not depend on the particular equation of motion

The integral being evaluated along the path p. This phase shift has a physical consequence when the two symmetric paths interfere; for then, adding amplitudes:

$$\Phi = \psi\exp(iS_1/\hbar) + \psi\exp(iS_2/\hbar)$$

$$= \psi \exp[ie/\hbar \int_{p1} A.dl] \{1 + \exp[-ie\#/\hbar]\}$$

where # is the flux contained within the path loop. Then the (experimentally observable) probability density is then given by:

$$|\Phi|^2 = 4\,|\psi|^2 \cos^2(e\#/2\hbar)$$

which predicts an observable effect upon the interference pattern due to the flux within the solenoid. This derivation is along the lines of that performed by Aharonov and Bohm *[1959]* in their original paper, and it should be noted that the solution has been obtained without the explicit use of a gauge.

Two further things are worth noting:

i) the effect is 'lost' if the flux is an integer multiple of h/e; the Dirac quantized magnetic flux (remembering that c=1 in this analysis).

ii) the gauge invariant quantity $\oint A.dl$ is acting as the physically invariant quantity. This quantity does not suffer from the same arbitrariness as A itself, since it is not dependent upon the choice of gauge (one need not be

made for its determination).

This analysis serves to suggest important quantities and motivates the procedure adopted in the gauge free approach that follows. This work is based upon a paper by the author *[Shiekh, 1986]*

§III The Gauge free approach

In an attempt to clarify the mechanism at work in the previous analysis; the same result has been rederived from a slightly different perspective: The following notation is adopted for clarity:

A lower case Greek character symbolizes the contribution to the field from a particular path; while the upper case is used for the complete field at that point; i.e. the sum of the contributions from all paths to that point.

Starting from the field equation for non-relativistic charged scalar particles:

$$[(i\hbar\partial_x + eA_x)^2/2M - (i\hbar\partial_t + eA_t)]\,\Phi(x) = 0$$

The use of a gauge choice might be avoided if one could formulate the above in terms of gauge invariant variables. For this reason Mandelstam *//962/* introduces the covariant variables:

$$\psi(p) \equiv \phi(p)\,\exp[-ie/\hbar \int_p A.dl]$$

since such variables do not require a gauge choice for their determination. The introduction of this path dependent integral is motivated by the previous analysis.

It should be made clear at this point that the Feynman path integral outlook *[Feynman, 1948; Feynman and Hibbs, 1965]* is being taken, where the field at a point $\Phi(x)$ is the sum of contributions $\phi(p)$ from all possible paths to the point x (see appendix I for a heuristic derivation of the path integral technique).

That is:

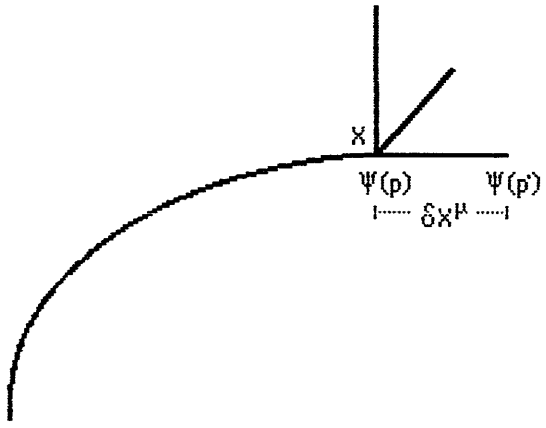
$$\Phi(x) = \sum_p \phi(p)$$

(Having specified the path p, the end point is redundant.)

The derivatives on the path dependent Mandelstam variables are defined in a natural way and are themselves covariant:

$$D_\mu \Psi(p) \equiv \mathrm{Lim}_{\delta x^\mu \to 0}\{\Psi(p') - \Psi(p)\}/\delta x^\mu$$

where the path p' is obtained from the path p by giving it an extension of magnitude δx in the μ direction (see figure below).



The path extension as used in the definition of the covariant derivative on the Mandelstam variables

It should be noted that, like the usual covariant derivatives, the operators D_μ and D_ν do not commute if there is an electromagnetic field present; explicit calculation yields:

$$[D_\mu, D_\nu]\,\Psi(p) = -ie/\hbar\, \Psi(p)\, F_{\mu\nu}$$

where

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu$$

Under Mandelstam's transformation, the field equations become

$$[(i\hbar D_x)^2/2M - i\hbar D_t]\,\psi(p) = 0$$

the advantage of this procedure is that the Mandelstam variable ψ obeys a 'free field' equation of motion. The problem then breaks down into solving for the free field contributions, and then inverting the Mandelstam transformation in order to determine the original field contributions.

Because the result of any measurement involves only closed loops of paths, the inversion procedure might be expected to involve only the gauge invariant quantity:

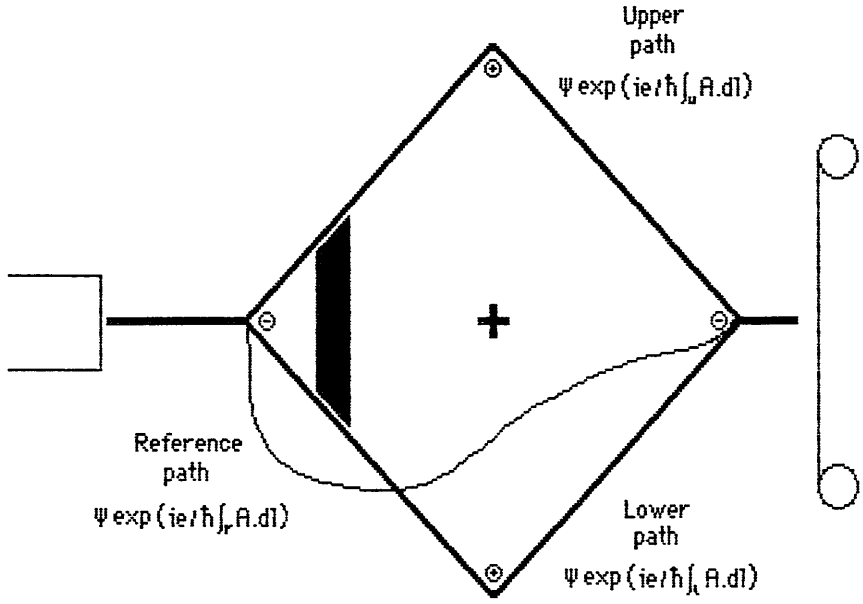
$$\oint A.dl$$

It is hoped therefore, by this procedure, to find the probability density of the field without the necessity of specifying a particular gauge.

This technique is illustrated in the calculation of the Aharonov-Bohm effect, as described previously.

The concept of a reference path will be introduced at this stage, although in this particular case it is not necessary; but becomes convenient for less symmetric configurations. When many paths are involved it is possible to compare each against a chosen one, but in general none is naturally selected. The use of a separate reference path avoids this dilemma.

The configuration of interest (with reference path) is illustrated in the figure below.



The use of a reference path against which to compare phases

The Mandelstam variable Ψ obeys the 'free field' equation:

$$[(i\hbar D_x)^2/2M - i\hbar D_t]\,\Psi(p) = 0$$

Having solved for Ψ one then has the task of reverting back to ϕ; this procedure being path dependent.

For the upper path:

$$\phi_u = \Psi_u \exp\,[ie/\hbar \int_u A.dl]$$

u representing the upper path; similarly for the lower path:

$$\phi_l = \Psi_l \exp\,[ie/\hbar \int_l A.dl]$$

but $\Psi_u = \Psi_l$ ($\equiv \Psi$) from symmetry.

Now multiplying the field at each point by a **unique** phase factor does not alter the physics (but completes the loops as desired).

It would not be admissible to multiply by a **multivalued** phase factor

(each loop to a given point must be compared against the same phase at that point).

So, re-define:

$$\phi_u = \psi \exp [ie/\hbar \int_u A.dl] U_r^*$$

$$\phi_l = \psi \exp [ie/\hbar \int_l A.dl] U_r^*$$

where U_r^* is the (fixed) phase change along the reference path (see previous figure):

$$U_r = \exp [ie/\hbar \int_r A.dl]$$

this is analogous to a choice of gauge; but this choice is arbitrary and so unspecified i.e. an explicit gauge choice has not been made.

So:

$$\phi_u = \psi \exp [ie/\hbar \oint_{u,\bar{r}} A.dl]$$

(the bar symbolizing the path reversed)

where this is the loop integral over the upper and reference paths.

Although these path contributions are themselves multivalued, the total kernel should be single valued.

Similiarly:

$$\phi_l = \psi \exp [ie/\hbar \oint_{l,\bar{r}} A.dl]$$

then adding path contributions:

$$\Phi = \phi_u + \phi_l$$

$$\Phi = \psi \left(\exp [ie/\hbar \oint_{u,\bar{r}} A.dl] + \exp [ie/\hbar \oint_{l,\bar{r}} A.dl] \right)$$

This kernel is not single valued (although its magnitude is). This is because we have modeled a situation that cannot be set up even in

principle, since it is not possible to eliminate contributions from paths that loop the solenoid many times. In this derivation, such contributions have been neglected (which is a valid approximation if the path length is much greater than the De-Broglie wave length). If account is taken of all possible paths; then the total kernel becomes single valued. This is clear because, on looping the origin with the detector (by any path), each contributing path is modified; but we still perform the same sum over all possible paths.

The probability density is given by:

$$|\Phi|^2 = |\psi|^2 \ (\ 2 + \exp [ie/\hbar \oint_{u,l} A.dl] + \exp [-ie/\hbar \oint_{u,l} A.dl] \ )$$

where the integrals now loop over the upper and lower path and the arbitrary reference path has dropped out of the formalism. Note that we have not had to actually specify this reference path (which is equivalent to not explicitly making a gauge choice).

$$|\Phi|^2 = |\psi|^2 \cos^2(e\#/2\hbar)$$

as before, where # is the flux looped

All this work seems to indicate the adoption of the Feynman path integral formalism *[Feynman, 1948; Feynman and Hibbs, 1965]* and it is hoped that within this context one might be able to continue in general to avoid the explicit use of a gauge.

The work set out above suggests a natural extension. The original Aharonov-Bohm paper *[1959]* and a recent paper by Aharonov et al *[1984]* are concerned with plane wave scattering by an Aharonov-Bohm solenoid (see also *[Kretzschmar, 1965]*). Both calculations make use of traditional techniques with the associated need to make a gauge choice. It would seem natural to try and rederive their result for the differential cross section

using the formalism presented above in the desire to perform the calculation without the use of an explicit gauge choice.

It should be noted that the path integral formalism seems to be naturally adopted by this technique.

§IV Notes on Scattering by an Aharonov-Bohm Solenoid

Using the gauge free formalism (explained previously) the scalar field amplitude is given by:

$$\Phi(x) = \sum_p \psi(p) \exp\left[ie/\hbar \oint A.dl\right]$$

(summing over all paths)

where $\psi(p)$ is the free field amplitude contribution from the path p and

$$ie/\hbar \oint A.dl$$

is the phase change due to the field A along the closed loop formed by this and the reference path.

(These are in fact the Wilson loops of lattice gauge theory, which is also a formalism that does not require an explicit gauge choice.)

It might be supposed that this phase change is path independent (for the 'Aharonov-Bohm case') since:

$$\oint A.dl = \#$$

where # is the flux enclosed. But it must be remembered that all paths must be considered i.e. paths that loop more than once are included. The phase change actually depends upon the number of loops performed by the path around the solenoid i.e.:

$$\oint A.dl = m\#$$

where m is the winding number.

So it seems natural to divide the above into families of paths according to the total number of loops made. It can in fact be shown *[Laidlaw and DeWitt-Morette, 1971]* that the kernel must factorize in this manner i.e.:

$$\Phi(x) = \sum_1 \psi(p_1) \exp[ie/\hbar \oint_1 A.dl] \quad \text{(summing over one loop paths)}$$

$$+ \sum_2 \psi(p_2) \exp[ie/\hbar \oint_2 A.dl] \quad \text{(summing over two loop paths)}$$

$$+ \text{etc.} \quad \text{(including counter looping)}$$

Then for each individual sum over paths the phase change is constant and can be taken out:

$$\Phi = e^{ie\#/\hbar} \sum_1 \psi(p_1)$$

$$+ e^{i2e\#/\hbar} \sum_2 \psi(p_2)$$

$$+ \text{etc.}$$

leaving a set of path integrals, each of which is now a partial sum of paths over the free field *[Dowker, 1977]*.

It seems that drawing the distinction between n loop paths is very difficult in Cartesian coordinates and calls for the use of cylindrical polars *[Edwards and Gulyaev, 1964]* with their associated complications. Then if the end point is at an angular coordinate ϕ; the one loop paths end at $\phi+2\pi$ etc.

§V Calculating the Differential Cross Section for Plane Wave Scattering from an Aharonov-Bohm Solenoid in the Gauge Free Formalism

The calculation is performed for non-relativistic charged scalar particles within a classical potential field.

The two dimensional, non-relativistic, free particle Feynman Kernel in Cartesian coordinates is given by (see appendix I):

$$K = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\prod_{k=1,n-1} dx(k)\, dy(k)$$

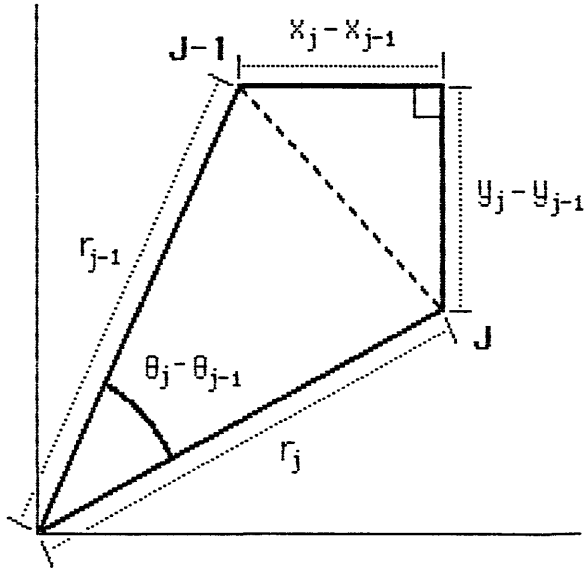
$$\exp\Big[\, i\rho \sum_{j=1,n}\{\, (x(j) - x(j-1))^2/\Delta t + (y(j) - y(j-1))^2/\Delta t \,\}\Big]$$

where:

$$\rho \equiv M/2\hbar$$

$$\Delta t \equiv \tau/n \qquad \tau = \text{'time of flight'}$$

Transforming this to cylindrical polar coordinates (see figure below):



The Conversion between Cartesian and cylindrical polar Coordinates

$$K = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\prod_{k=1,n-1} r(k)dr(k)\,d\theta(k)$$

$$\exp\Big[\, i\rho \sum_{j=1,n}\Big\{ \big(r^2(j) + r^2(j-1) - 2\, r(j)\, r(j-1)\cos(\theta(j)-\theta(j-1)) \big)/\Delta t \Big\}\Big]$$

Now there are certain subtleties here, in that if one wishes to expand and truncate the cosine, one need retain the argument up to the fourth power and not just the second, in order to get all the contributions to the first order in Δt. In some treatments this is approached by the introduction of an effective potential. These problems are avoided here, in that it is found unnecessary to expand the cosine, since it is possible to proceed directly.

Now comes the problem of distinguishing between θ and $\theta+2\pi$ etc.; i.e. the separation into winding number families. This is achieved by introducing a constraint on the angle *[Gerry and Singh, 1979; Peak and Inomata, 1969]*, which separates the contributions of the paths winding around the solenoid a definite number of times. Had the cosine been expanded (with the adoption of the problems mentioned above), then the looping distinction implicitly exists, since the angle is not periodic; whereas the cosine is.

$$K_m = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\prod_{k=1,n-1} r(k)dr(k)\,d\theta(k)$$

$$\delta\big(\phi + 2\pi m - \textstyle\sum_{j=1,n}(\theta(j)-\theta(j-1))\big)$$

$$\exp\Big[\, i\rho \sum_{j=1,n}\Big\{ \big(r^2(j) + r^2(j-1) - 2\, r(j)\, r(j-1)\cos(\theta(j)-\theta(j-1)) \big)/\Delta t \Big\}\Big]$$

$$-\pi \le \phi < \pi$$

If ϕ is not restricted to a 2π interval, the constraint will be incorrectly applied.

A 'trick' is used to place the constraint into the exponential *[Edwards, 1967]* with the Lagrangian by using the relation (which follows from Fourier expanding):

$$2\pi\delta(x) = \int_{-\infty,\infty} e^{i\lambda x}\, d\lambda$$

So:

$$K_m = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty}\int_{-\infty,\infty}\cdots\int_{-\infty,\infty}\prod_{k=1,n-1} r(k)dr(k)\, d\theta(k)$$

$$1/2\pi \int_{-\infty,\infty} e^{i\lambda(\phi + 2\pi m)}\, d\lambda$$

$$\prod_{j=1,n} \exp\left[i\rho \left(r^2(j) + r^2(j-1) - 2\, r(j)\, r(j-1)\cos(\theta(j)-\theta(j-1))\right)/\Delta t - i\lambda(\theta(j)-\theta(j-1))\right]$$

$$-\pi \le \phi \le \pi$$

Using the transformation:

$$\chi(j) \equiv \theta(j) - \theta(j-1)$$

for which the Jacobian is unity.

$$K_m = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty}\prod_{k=1,n-1} r(k)dr(k)$$

$$1/2\pi \int_{-\infty,\infty} e^{i\lambda(\phi + 2\pi m)}\, d\lambda \prod_{j=1,n} \exp[i\rho(r^2(j) + r^2(j-1))/\Delta t]$$

$$\int_{-\pi,\pi}\cdots\int_{-\pi,\pi}\prod_{l=1,n-1} d\chi(l)\, \exp[-2i\rho(\, r(j)\, r(j-1)\cos(\chi(j))\,)/\Delta t - i\lambda\chi(j)\,]$$

Asymmetric angular limits 0-2π are incorrect, since they compel the path to circle in one direction, but not circle back.

The angular integrals may be performed using the asymptotic relation (for $|z|\to\infty$) *[Gradshteyn and Ryzhik; P958 from 8.451(5)]*:

$$\int_{-\pi,\pi} e^{i\lambda\chi + z\cos(\chi)}\, d\chi \to 2\pi I_{|\lambda|}(z)$$

$$|\arg z| \leq \pi/2$$

It should be noted that this limit is achieved when going to the continuum ($\Delta t \to 0$), and so an approximation is not being made at this point.

It is this step that allows us to proceed without expanding and truncating the cosine.

$$K_m = \mathrm{Lim}_{n\to\infty}(\rho/i\pi\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty} \prod_{k=1,n-1} r(k)dr(k)$$

$$1/2\pi \int_{-\infty,\infty} e^{i\lambda(\phi + 2\pi m)}\, d\lambda$$

$$\prod_{j=1,n} \exp[i\rho(r^2(j) + r^2(j-1))/\Delta t]\, 2\pi i_{|\lambda|}(-i\rho 2r(j)r(j-1)/\Delta t)$$

Looking at the r integrals:

$$I \equiv \mathrm{Lim}_{n\to\infty}(2\rho/i\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty} \prod_{k=1,n-1} r(k)dr(k)$$

$$\prod_{j=1,n} \exp[i\rho(r^2(j) + r^2(j-1))/\Delta t]\, I_{|\lambda|}(-i\rho 2r(j)r(j-1)/\Delta t)$$

Explicitly

$$I = \mathrm{Lim}_{n\to\infty}(2\rho/i\Delta t)^n \int_{0,\infty}\cdots\int_{0,\infty} r_1(k)dr_1(k)\, r_2(k)dr_2(k) \ldots r_{n-1}(k)dr_{n-1}(k)$$

$$\exp[i\rho R'^2/\Delta t]\, \exp[i\rho 2r_1^2/\Delta t]\, \exp[i\rho 2r_2^2/\Delta t] \ldots \exp[i\rho R^2/\Delta t]$$

$$I_{|\lambda|}(-i\rho 2R'r_1/\Delta t)\, I_{|\lambda|}(-i\rho 2r_2r_1/\Delta t)\, I_{|\lambda|}(-i\rho 2r_3r_2/\Delta t) \ldots I_{|\lambda|}(-i\rho 2r_{n-1}R/\Delta t)$$

It is now possible to proceed using the identity *[Gradshteyn and Ryzhik, P710 from 6.611]*:

$$\int_{0,\infty} \exp[i\alpha r^2]\, I_\lambda(-iar)\, I_\lambda(-ibr)\, r\, dr = i/2\alpha\, \exp[-i(a^2+b^2)/4\alpha]\, I_\lambda(iab/2\alpha)$$

$$(\mathrm{Re}\,\lambda > -1)$$

by which the r integrals may be successively performed to yield:

$$K_m = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau] \int_{-\infty,\infty} d\lambda\, e^{i\lambda(\phi + 2\pi m)}\, I_{|\lambda|}(-2iR'R\rho/\tau)$$

where τ = 'time of flight'

Applying the gauge free technique as described previously we sum over all possible winding numbers before doing the λ integration:

$$K = \sum_{m=-\infty,\infty} e^{iem\#/\hbar}\, K_m$$

$$K = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau] \int_{-\infty,\infty} d\lambda \sum_{m=-\infty,\infty} e^{2\pi i m\alpha}\, e^{i\lambda(\phi + 2\pi m)}\, I_{|\lambda|}(-2iR'R\rho/\tau)$$

where $\alpha \equiv e\#/h$

Using the identity:

$$\sum_{m=-\infty,\infty} e^{im\theta} = 2\pi \sum_{n=-\infty,\infty} \delta(\theta + 2\pi n)$$

which follows from the Poisson sum formula, which itself derives from Fourier analysis.

$$K = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau] \sum_{n=-\infty,\infty} e^{-i(n+\alpha)\phi}\, I_{|n+\alpha|}(-2iR'R\rho/\tau)$$

Now note that:

$$I_\nu(-ix) = (-i)^\nu J_\nu(x)$$

Leading to:

$$K = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau] \sum_{n=-\infty,\infty} e^{-i(n+\alpha)\phi}\, (-i)^{|n+\alpha|}\, J_{|n+\alpha|}(2R'R\rho/\tau)$$

where:

$$\rho \equiv M/2\hbar \quad \alpha \equiv e\#/h \quad (c=1)$$

$$-\pi \le \phi < \pi$$

The non-relativistic scalar kernel for the needle solenoid

This kernel *[Dowker, 1977]*, although single valued, as it must be, is

discontinuous in phase. This is due to an implicit insistence that on looping the origin with the detector, the reference path must be restored to that originally used to that point. (i.e. only a single gauge be used at each point). This requires that the solenoid be cut by the reference path and leads to the discontinuity. Since this discontinuity exists only in phase, it is not reflected in the physical predictions.

We have here linked up with the solution to the differential equation, but what takes a few lines for that technique *[Aharonov and Bohm, 1959, Kretzschmar, 1965]* has taken us longer.

So:

$$K = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau]\, S(2R'R\rho/\tau)\, e^{-i\alpha\phi}$$

where:

$$S(s) \equiv \sum_{n=-\infty,\infty} (-i)^{|n+\alpha|} J_{|n+\alpha|}(s)\, e^{-in\phi}$$

Now we are at liberty to multiply by an overall **single valued** phase factor (for the reasons expanded upon previously):

$$e^{ik\phi}$$

where k is an integer, in order to work with a new α that lies in the range $0 \le \alpha < 1$. This is a matter of convenience and illustrates the periodic behavior in α (the rescaled flux strength).

Following the work of Aharonov and Bohm *[1959]* we choose to split S into three parts; so that the absolute value sign may be removed:

$$S = S_1 + S_2 + S_3$$

where:

$$S_1 = \sum_{n=1,\infty} (-i)^{n+\alpha} J_{n+\alpha}(s)\, e^{-in\phi}$$

$$S_2 = \sum_{n=-\infty,-1} (-i)^{|n+\alpha|} J_{|n+\alpha|}(s)\, e^{-in\phi}$$

$$= \sum_{n=1,\infty} (-i)^{n-\alpha} J_{n-\alpha}(s)\, e^{+in\phi}$$

$$S_3 = (-i)^{\alpha} J_{\alpha}(s)$$

We now construct and solve for a partial differential equation satisfied by S_1 *[Aharonov and Bohm, 1959]* in this way we evaluate the sum for S_1 (S_2 follows from $\phi \rightarrow -\phi$; $\alpha \rightarrow -\alpha$):

$$\partial S_1/\partial s = 1/2 \sum_{n=1,\infty} (-i)^{n+\alpha} \left(J_{n+\alpha-1}(s) - J_{n+\alpha+1}(s) \right) e^{-in\phi}$$

having used

$$dJ_{\nu}(s)/ds = 1/2 \left(J_{\nu-1}(s) - J_{\nu+1}(s) \right)$$

$$\nu = 0$$

yielding a finite term partial differential equation:

$$\partial S_1/\partial s = -i \cos\phi\, S_1 + 1/2\,(-i)^{\alpha} \left(J_{\alpha+1}(s) - i\, J_{\alpha}(s)\, e^{-i\phi} \right)$$

which is of the form:

$$\partial S(s,\phi)/\partial s = p(s,\phi)\, S(s,\phi) + q(s,\phi)$$

and has the solution:

$$S(s,\phi) = \exp\left[\int (s,\phi)\, ds \right] \left\{ \int_s q(u,f) \exp\left[-\int_u p(v,\phi)\, dv \right] du + f(\phi) \right\}$$

where $f(\phi)$ is an arbitrary function. Hence:

$$S_1 = 1/2\,(-i)^{\alpha} e^{-is\cos\phi} \int_{0,s} e^{iu\cos\phi} \left(J_{\alpha+1}(u) - i\, J_{\alpha}(u)\, e^{-i\phi} \right) du$$

The lower limit (and arbitrary function of ϕ) being determined by the requirement that when s goes to zero, S_1 also goes to zero because S_1 includes Bessel functions of positive order only. This form for S_1 is superior for numerical evaluation than the infinite sum, which suffers from slow convergence for large Bessel function argument.

This leads to an exact finite term expression for **K** as:

$$\mathbf{K} = \rho/i\pi\tau \exp[i\rho(R'^2+R^2)/\tau]\, S(2R'R\rho/\tau)\, e^{-i\alpha\phi}$$

where:

$$S(s) = (-i)^{\alpha} J_{\alpha}(s)$$

$$+ 1/2\,(-i)^{\alpha}\left\{e^{-is\cos\phi}\int_{0,s} e^{iu\cos\phi}\left(J_{\alpha+1}(u) + i\,J_{\alpha}(u)\,e^{-i\phi}\right)du + (\phi\rightarrow-\phi,\ \alpha\rightarrow-\alpha)\right\}$$

In order to deduce the differential cross-section, consider the special case of plane wave scattering ($R'\rightarrow\infty$); then

$$2R'\rho/\tau = 2R'/\tau\, M/2\hbar = Mv/\hbar = p/\hbar = k$$

the wave number. Then:

$$\mathbf{K} = k/2i\pi R'\, e^{ik.x}\, e^{-i\alpha\phi}\, S(kR)$$

where:

$$S(s) = (-i)^{\alpha} J_{\alpha}(s)$$

$$+ 1/2\,(-i)^{\alpha}\left\{e^{-is\cos\phi}\int_{0,s} e^{iu\cos\phi}\left(J_{\alpha+1}(u) + i\,J_{\alpha}(u)\,e^{-i\phi}\right)du + (\phi\rightarrow-\phi,\ \alpha\rightarrow-\alpha)\right\}$$

Dividing the limits on these integrals; i.e. define:

$$I_1 = \int_{0,\infty} e^{iu\cos\phi}\left[\,J_{\alpha+1}(u) - i\,e^{-i\phi}\,J_{\alpha}(u)\,\right]du$$

$$I_2 = \int_{s,\infty} e^{iu\cos\phi}\left[\,J_{\alpha+1}(u) - i\,e^{-i\phi}\,J_{\alpha}(u)\,\right]du$$

the first integral is known *[Gradshteyn and Ryzhik; P 707 from 6.611(1)]*:

$$\int_{0,\infty} e^{iu\cos\phi}\,J_{\alpha}(u)\,du = e^{i\alpha(\pi/2\,-\,|\phi|)}/|\sin\phi|$$

so that:

$$I_1 = 0 \qquad \text{for } \phi < 0$$

$$I_1 = \exp[i\alpha\phi]\,2i^{\alpha} \qquad \text{for } \phi > 0$$

where $-\pi \le \phi < \pi$

Now looking at I_2:

$$I_2 = \int_{s,\infty} e^{iu\cos\phi} \left[J_{\alpha+1}(u) - i\, e^{-i\phi} J_\alpha(u) \right] du$$

In the asymptotic limit ($z \to \infty$):

$$J_\alpha(z) \to \sqrt{(2/\pi z)} \cos(z - \pi\alpha/2 - \pi/4)$$

Then:

$$I_2 \to \sqrt{(2/\pi)} \left[1 + e^{-i\phi} \right] (-i)^{\alpha+3/2} / \sqrt{(1 + \cos\phi)} \int_{\sqrt{[s(1+\cos\phi)]},\infty} \exp[+iz^2]\, dz$$

$$+ \sqrt{(2/\pi)} \left[1 - e^{-i\phi} \right] (+i)^{\alpha+3/2} / \sqrt{(1 - \cos\phi)} \int_{\sqrt{[s(1-\cos\phi)]},\infty} \exp[-iz^2]\, dz$$

where we have put:

$$z = \sqrt{[u(1 + \cos\phi)]} \quad \text{in the first integral}$$

$$z = \sqrt{[u(1 - \cos\phi)]} \quad \text{in the second integral}$$

Using the asymptotic behavior for the Fresnel Integrals *[Gradshteyn and Ryzhik; P 932 from 8.255]*:

$$\int_{a,\infty} \exp[+iz^2]\, dz \to +i/2a \exp[+ia^2]$$

$$\int_{a,\infty} \exp[-iz^2]\, dz \to -i/2a \exp[-ia^2]$$

Putting this together:

$S_1 + S_2 \to$

$$-\sqrt{(-i/2\pi)} \left\{ i\, e^{-is}/\sqrt{s} + e^{is}/\sqrt{s} \cos(\pi\alpha + \phi/2)/\cos(\phi/2) \right\} + e^{i(\alpha\phi - s\cos\phi)}$$

There remains the contribution of S_3, whose asymptotic behavior is:

$$(-i)^\alpha J_\alpha(s) \to (-i)^\alpha \sqrt{(2/\pi s)} \cos(s - \pi\alpha/2 - \pi/4)$$

Hence:

$$S \rightarrow e^{i(\alpha\phi - s\cos\phi)} - \sqrt{(i/2\pi s)}\, e^{is} \sin(\pi\alpha)\, e^{+i\phi/2}/\cos(\phi/2)$$

So finally:

$K \rightarrow$

$$k/2i\pi R'\, e^{ik.x}\, e^{-i\alpha\phi} \left\{ e^{i(\alpha\phi - kR\cos\phi)} - \sqrt{(i/2\pi kR)}\, e^{ikR} \sin(\pi\alpha)\, e^{+i\phi/2}/\cos(\phi/2) \right\}$$

the second term representing the scattered wave, from which we can deduce the differential cross section:

$$\partial\sigma/\partial\phi = 1/2\pi k \sin^2(\pi\alpha)/\cos^2(\phi/2)$$

$\alpha \equiv e\#/h$

\# = flux in solenoid

k = wave number

It should be noted that this yields an infinite total cross section. This reflects the fact that the effect is not dependent on loop size (which is true only for the infinitely long solenoid).

Conclusion

Through the development of a gauge free technique, and the use of the Feynman path integral method *[Feynman, 1948; Feynman and Hibbs, 1965]*, the differential cross-section for scattering of non-relativistic charged scalar particles from a classical Aharonov-Bohm solenoid has been determined. The result agrees with that obtained by Aharonov and Bohm *[1959]*, but the calculation differs in principle, in that, it was no longer necessary to make an **explicit** choice of gauge; although one was **implicitly** made in the use of an arbitrary, but fixed, reference path.

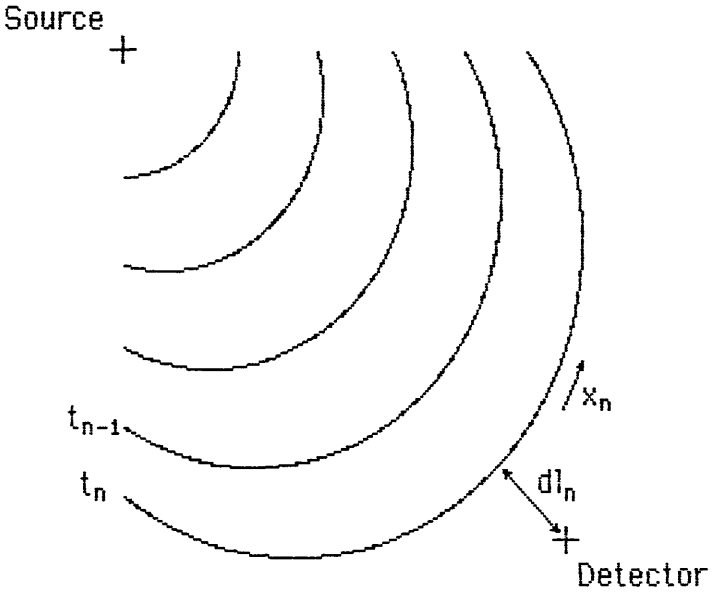
The gauge free approach adopted here obliges one to use the path integral formalism, since there is not an explicit potential for which to state Schrödinger 's equation.

Appendix I

Deducing the Feynman Path Integral formalism directly from the Probabilistic Wave description.

(a heuristic approach)

Divicing the wave propagation into discrete time slots, then the amplitude at each point is determined by the field at an earlier time. If the evolution time is small then the point of interest is causally connected only to the region directly behind, see figure below, and Huygens' principle (contributions from any but around the closest sources mutually cancelling) becomes asymptotically true for $\Delta t \to 0$.



Time evolution of the wave, each successive field being determined by an earlier field

Expressing this fact that each point evolves from those previously, which

are themselves determined by their own previous field:

$$\Phi \propto \int dx_1 \exp[ik_1.dl_1] \int dx_2 \exp[ik_2.dl_2] \ldots \int dx_n \exp[ik_n.dl_n]$$

This procedure is nothing more than summing over all possible paths.

$$\Phi = 1/Z \sum_p \exp[i \int_p k.dl]$$

It is not suggested that a particle follows these paths, but rather the paths should be considered only within the mathematical framework as an alternative description of wave propagation. Invoking the correspondence principle, which tells us how a particle's properties are related to its wave nature gives:

$$\Phi = 1/Z \sum_p \exp[i/\hbar \, (\int p.dx - \int E \, dt)]$$

$$\Phi = 1/Z \sum_p \exp[i/\hbar \int (p.\dot{x} - H) dt]$$

with suitable provisos for when the Hamiltonian equals the energy.

$$\Phi = 1/Z \sum_p \exp[iS/\hbar]$$

where S is the Action

The path integral technique of Feynman

For non-relativistic particles in free field the action is simply:

$$S = M/2 \int (v_x^2 + v_y^2) \, dt$$

which is used in discrete form in the text:

$$K = \mathrm{Lim}_{n \to \infty} \, 1/Z \int_{-\infty,\infty} \ldots \int_{-\infty,\infty} \int_{-\infty,\infty} \ldots \int_{-\infty,\infty} \prod_{k=1,n-1} dx(k) \, dy(k)$$

$$\exp\left[i\rho \sum_{j=1,n} \{ (x(j) - x(j-1))^2/\Delta t + (y(j) - y(j-1))^2/\Delta t \} \right]$$

where $\rho \equiv M/2\hbar$

The normalization constant (Z) may be determined (up to an overall phase

factor) by the requirement that the particle be detectable somewhere. i.e.

$$\left| \int_{-\infty,\infty} \int_{-\infty,\infty} K \, dx_n dy_n \right|^2 = 1$$

This is so since the possibility exists of bringing together the dispersed wave such that the magnitude and relative phases from each point are maintained. This 'lensing' allows the amplitudes to interfere **before** the act of localized interaction. That this is different from the usual is explained by the fact that the kernel gives the amplitude for the particle to be found at a **point** and not the amplitude density usual to the wave function. Performing the Gaussian integrals leads to:

$$1/Z = (i\pi\Delta t/\rho)^{-n}$$

$$K = Lim_{n\to\infty} (\rho/i\pi\Delta t)^n \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \int_{-\infty,\infty} \cdots \int_{-\infty,\infty} \prod_{k=1,n-1} dx(k)\, dy(k)$$

$$\exp\left[i\rho \sum_{j=1,n} \left\{ (x(j) - x(j-1))^2/\Delta t + (y(j) - y(j-1))^2/\Delta t \right\} \right]$$

where $\rho \equiv M/2\hbar$

The free field non-relativistic scalar kernel

It has been implicitly assumed that we are working in flat space without a velocity dependent 'potential' term. In general the normalization factor is path dependent *[DeWitt-Morette, 1951]*.

Appendix II

A look at the controlling function (regulator) for indefinite integrals

Many of the identities quoted depend on the evaluation of oscillating integrands, which are made well defined by regulating the integrand and then removing the regulator at the ends.

For example:

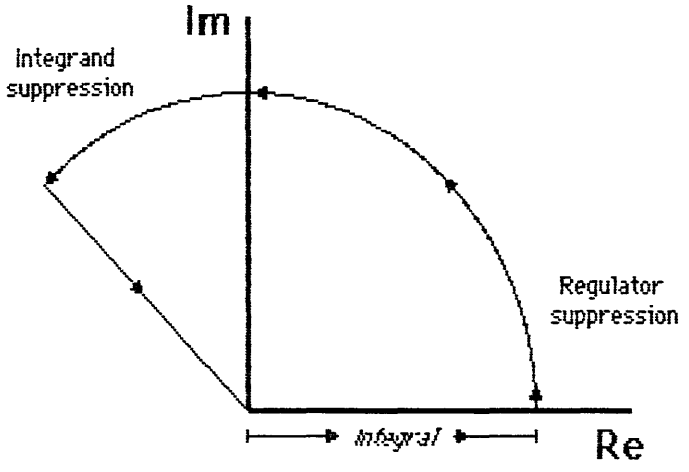
$$I = \mathrm{Lim}_{\alpha \to 0^+} \int_{0,\infty} e^{it} e^{-\alpha t} \, dt$$

(α positive)

$$= i$$

This procedure can only be reasonable if the result is independent of the choice of regulator. Although expected on physical grounds this is not altogether obvious and is investigated below.

Consider integrating such a function along a closed path in the complex plane. The first section of the contour is taken as the path (along the real axis) of the original indefinite integral and extends to infinity. The contour is then continued off the real axis 'at infinity' to any point in the complex plane where the unregulated integrand is itself suppressed to zero. The contour is then completed from this point, by a return path, back to the starting place.



Evaluation of an oscillatory integral by means of a general regulator

Now if any regulator is chosen such that the contribution of the path section at infinity is zero (such a regulator being referred to as 'good' and being determined by Jordan's Lemma), and if no poles are enclosed by the closed contour; then by Cauchy's theorem, the integral back along the return path is equal to the original integral. Since this new integral is independent of the choice of 'good' regulator (the integrand itself now achieving regulation and the regulator not contributing); so it becomes clear that without obstructing poles the result of regularization is regulator independent.

Chapter Two

Path Integral approach to exact scalar Diffraction from an Impenetrable Wedge

(a systematic approach)

Based on a paper by:

C.DeWitt-Morette, S.Low, L.Schulman and A.Shiekh, *Found. of Phys.*, **16**, (1986), 311-.

(contributions by DeWitt-Morette, Low and Schulman stand independently and have not been included)

§1 Introduction

In this work the path integral technique is used to calculate the diffraction patterns from an impenetrable (perfectly absorbing or perfectly reflecting) wedge for non-relativistic scalar particles and light. An interesting connection with the Aharonov-Bohm effect is used to help obtain these solutions. Time dependent kernels are developed for non-relativistic particles, but only time independent kernels are found for light. New forms of the solution are also presented, which overcome the slow convergence problems of former exact solutions.

Sommerfeld in 1896 solved exactly the problem of the diffraction of light from a perfectly reflecting wedge.

The same problem had been solved in electrostatics by solving Laplace's equation:

$$\nabla^2 u = 0$$

for a point charge outside of a two dimensional wedge. For a conducting wedge of external angle π/ν (ν being a positive integer) the boundary conditions u=0 may be implemented by the usual method of images. Images being placed such that the boundary conditions are achieved by symmetry. This technique fails for a general angle, as the images then infringe upon the physical region outside of the wedge.

This difficulty may be overcome by means of a conformal transformation, a technique developed by Riemann in his doctoral thesis.

Since any analytic function:

$$W(z) \equiv U(z) + i\, V(z)$$

$$z = x + i\, y$$

satisfies Laplace's equation by virtue of the Cauchy-Riemann conditions i.e.

$$\partial u/\partial x = \partial v/\partial y \qquad \partial v/\partial x = -\partial u/\partial y$$

One may transform the original configuration by the map:

$$Z = f(z)$$

to another that will automatically satisfy Laplace's equation

$$\partial^2 W/\partial X^2 + \partial^2 W/\partial Y^2 = 0$$

$$W(Z) \equiv U(Z) + i\, V(Z)$$

wherever the map is analytic.

Then solve this new electrostatic configuration for U (V follows from the Cauchy-Riemann conditions) and transform back to determine the potential that is a solution to the original problem.

The transformation:

$$Z = z^{1/\mu}$$

may be used to turn a wedge of external angle $\mu\pi/\nu$ (μ,ν being positive integers), into the tractable wedge problem of angle π/ν.

Transforming back yields a many-valued solution which is understood to be interpreted in the physical region outside of the wedge.

The analytic difficulties of many-valued functions may be overcome by introducing the idea of a Riemannian surface (described in appendix I). In this picture it becomes clear that the images do not lie in the physical space, but are 'hidden' in the lower folds and act only to implement boundary conditions.

From the analogy with such problems in electrostatics; Sommerfeld *[1896]* proposed a many-valued anzatz, which satisfied the Helmholtz equation:

$$[\partial^2/\partial R^2 + 1/R\ \partial/\partial R + 1/R^2\ \partial^2/\partial\phi^2 + k^2]\ G = -\delta(R-R')\ \delta(\phi-\phi')$$

as well as the condition of no incoming wave from infinity. Here we have converted to rationalized units and continue to do so. in this way he deduced the (free relativistic massless time independent scalar) Green's function on a μ sheeted Riemannian surface as:

$$G = 1/2\pi \sum_{n=0,\infty} \gamma_n\ J_{n/\mu}(kR)\ e^{-i\pi n/2\mu}\ K_{n/\mu}(-ikR')\ \cos(n(\phi-\phi')/\mu)$$

$$\gamma_n = 2/\mu \text{ for } n>0$$

$$\gamma_n = 1/\mu \text{ for } n=0$$

for $R < R'$; (if $R' < R$ interchange R and R')

where:

$$K_\nu(-ix) = \pi/2\ e^{i\pi\nu/2}\ \{ J_{-\nu}(x) - e^{-i\nu\pi}\ J_\nu(x)\ \}/\sin(\nu\pi)$$

k wave number

This, with the addition of suitable image contributions, satisfies the wedge boundary conditions. In this way it is possible to describe diffraction from an impenetrable wedge; be it reflecting (with Dirichlet or Neumann boundary conditions), or perfectly absorbing.

Sommerfeld in his original paper fully develops the solution for the reflecting infinite half plane. Carslaw *//919/* under his guidance completed this task for the wedge, having earlier *//910/* solved the diffusion equation (and so Schrödinger's equation) for the wedge of any angle.

MacDonald*//902/* in his Adams prize essay, developed the same results for the Dirichlet wedge by finding a solution that obeyed the Helmholtz equation and the desired boundary conditions. He obtained the Green's function (here rationalized):

$$G_w^- = 2/\theta \sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(kR)\, K_{n\pi/\theta}(-ikR')\, \sin(n\pi\phi/\theta)\, \sin(n\pi\phi'/\theta)$$

for $R < R'$; (if $R > R'$ interchange R and R')

That for the Neumann wedge is:

$$G_w^+ = 1/\theta \left\{ J_0(kR)\, K_0(-ikR') + \right.$$

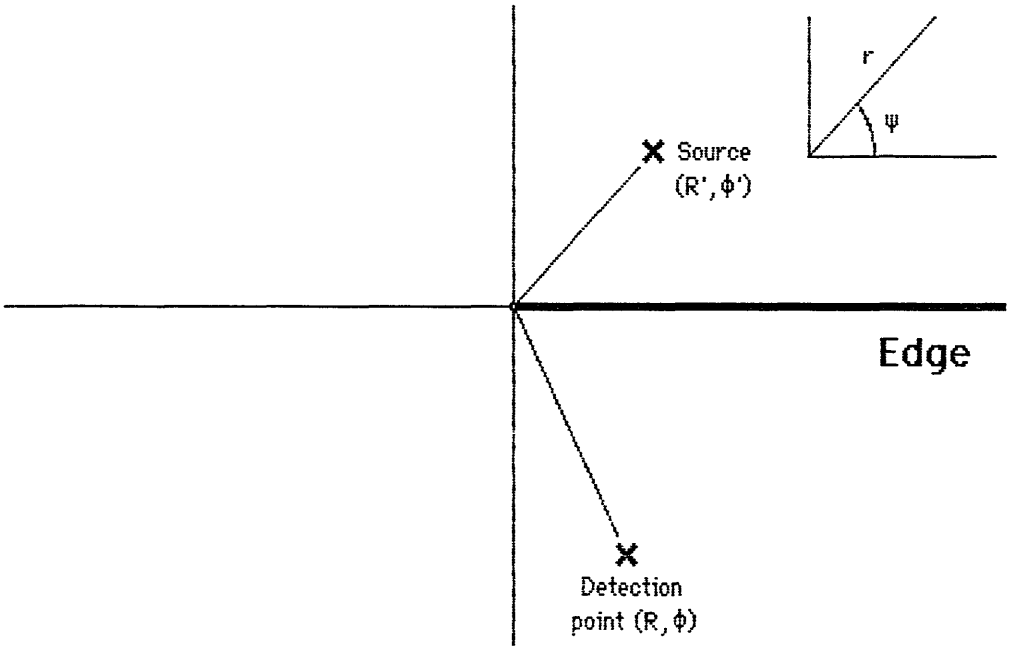
$$\left. 2 \sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(kR)\, K_{n\pi/\theta}(-ikR')\, \cos(n\pi\phi/\theta)\, \cos(n\pi\phi'/\theta) \right\}$$

for $R < R'$; (if $R > R'$ interchange R and R')

these results are rederived here, in a constructive fashion, using the path integral technique of Feynman *[Feynman, 1948; Feynman and Hibbs, 1965].*

§II Path Integral Approach

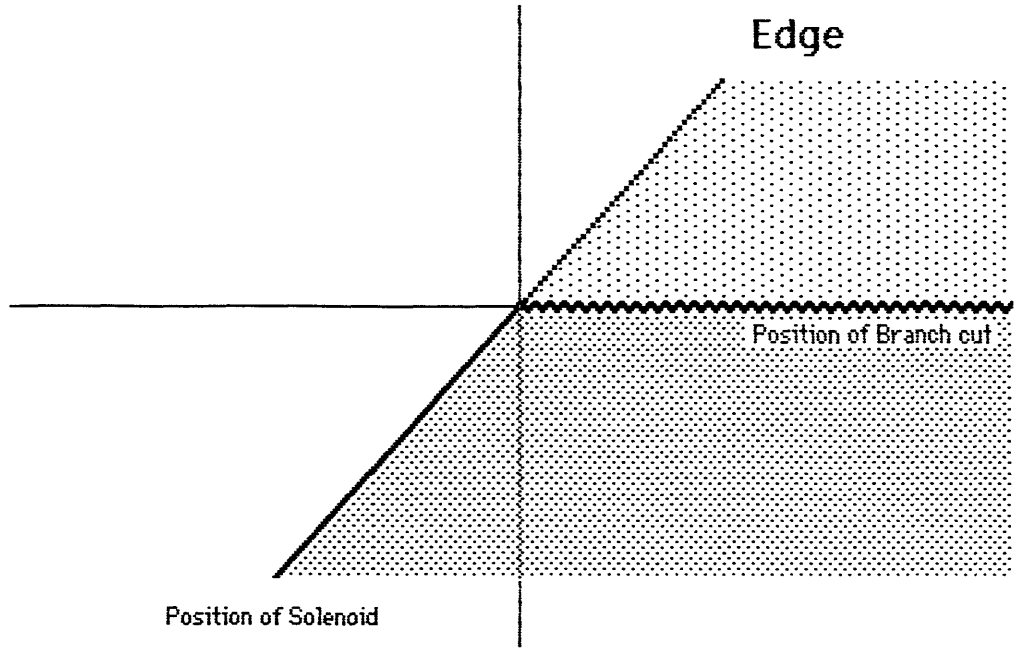
It has been realized by L.S.Schulman and C.M.Newman (private communication) that diffraction from an infinite half plane (see figure below)



Diffraction from a half Plane

can be related to the Aharonov-Bohm effect for a needle (infinitely narrow) solenoid of infinite extent.

To see this unobvious connection consider scattering from a needle solenoid with strength α=1/2 (α the rescaled flux ≡ e#/h; where # = flux within the solenoid). Now one can gauge away the potential A at all points except for a branch cut and so have a zero field except along this line (see figure below).



Location of Solenoid and associated Branch cut

The probability amplitude $K_{(\alpha=1/2)}$ to detect a particle changes by a phase factor $\exp(i\pi)$ when the detector crosses the line of non-zero potential. If one then adds the kernel $K_{(\alpha=1/2)}$ to $K_{(\alpha=0)}$, one achieves mimicing of a system with no penetration through the line, since the detector on passing this line has half the total amplitude change sign, which kills the total kernel.

The complete normalized kernel for the edge, K_e, is thus given by:

$$K_e = 1/2 \left(K_{(\alpha=1/2)} + K_{(\alpha=0)}\right)$$

Since the combined solution satisfies the free field equation, except on the line, and does not allow penetration of this line; one is in this way modeling a perfectly absorbing half plane barrier in free field. It should be noted that a path that passes through the barrier and returns, has its influence restored. This is a weaker condition than demanding that any path that passes through the barrier should not contribute.

Image sources may then be introduced to model a perfectly reflecting barrier. This is an extension of the normal method of images and is discussed in more detail later.

Although use was made of a special gauge to conceive this technique, the solution itself, being gauge independent, tells us that, given a fixed source and a fixed detector on each side of the barrier, the orientation or dispersion of the barrier is irrelevant.

The complete non-relativistic scalar kernel can be readily deduced from the expression *[Morandi and Menossi, 1984]* for the kernel for the Aharonov-Bohm solenoid in two dimensions; namely from:

$$K(\alpha) = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} e^{-i(n+\alpha)(\phi-\phi')} (-i)^{|n+\alpha|} J_{|n+\alpha|}(2R'R\rho/\tau)$$

$$-\pi \leq \phi < \pi$$

(or any 2π interval)

where $\rho \equiv M/2\hbar$

- M scalar particle mass
- τ time of flight
- R distance from solenoid to detector
- R' distance from solenoid to source
- α rescaled flux = e#/h; # = flux within the solenoid
- e scalar particle charge
- ϕ angle to detector
- ϕ' angle to source

and c=1 in the chosen units

yielding

$$K_e = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau]$$

$$\{ 1/2\, J_0(2R'R\rho/\tau) + \sum_{n=1,\infty} (-i)^{n/2} J_{n/2}(2R'R\rho/\tau) \cos(n(\phi-\phi')/2) \}$$

Now using the identity *[Gradshteyn and Ryzhik, 1980; P973 from 8.511(5)]*,

(a particular case of the identity developed in appendix III)

$$1/2\, J_0(z) + \sum_{n=1,\infty} (-i)^{n/2}\, J_{n/2}(z) \cos(n\theta)$$

$$= \sqrt{(1/i\pi)}\, e^{-iz\cos(2\theta)} \int_{-\infty,\sqrt{(2z)}\cos(\theta)} \exp[is^2]\, ds$$

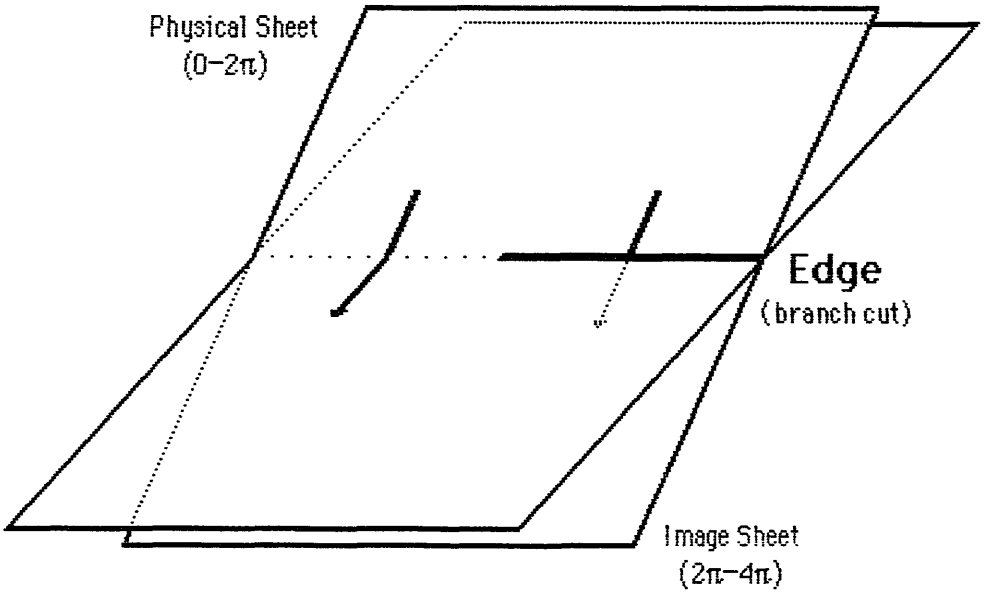
and recalling that $\rho \equiv M/2\hbar$ (M=scalar particle mass)

$$K_e = M/2i\pi\hbar\tau \exp[iM(R^2+R'^2)/2\hbar\tau]$$

$$\sqrt{(1/i\pi)}\, e^{-i(R'RM/\hbar\tau)\cos(\phi-\phi')} \int_{-\infty,\sqrt{(2R'RM/\hbar\tau)}\cos((\phi-\phi')/2)} \exp[is^2]\, ds$$

$$-\pi \leq \phi < \pi$$

The kernel is divalued if we consider all ϕ. To construct the probability amplitude in the presence of a perfectly reflecting barrier it is enlightening to consider this extended (analytically continued) kernel on a two sheeted Riemannian surface (see figure below).



Two Sheeted Riemannian Surface

A short discussion of the use of Riemannian sheeting instead of branch cuts is given in appendix I. In this description the kernel is again single-valued, and one of the sheets is taken to represent the physical space. On such a surface the absorbed wave descends into the second sheet, rather than terminating upon crossing the barrier (as before).

Boundary conditions are implemented using the method of images *[Sommerfeld, 1954]*. The physical configuration may for convenience be considered to dwell upon the top (0-2π) sheet, while the image is 'hidden' on the lower (2π-4π) sheet, which only influences the physical space in implementing boundary conditions. In this way it is understood that the solution is to be interpreted only upon the physical sheet.

To model a perfectly reflecting edge an image is introduced at the position, on the other sheet, obtained by reflecting the source in the boundary wall. Dirichlet boundary conditions (the total field $\mathbf{K}$=0 on the boundary) may be achieved by adding an image of equal amplitude, but in antiphase with the source; while Neumann conditions ($\partial\mathbf{K}/\partial n$=0; where n is the normal to the boundary) are achieved by having the image run in phase with the source.

From this one may deduce the non-relativistic scalar kernel for a half plane barrier (edge), with Dirichlet(-) or Neumann(+) boundary conditions; respectively, as:

$$\mathbf{K}_e^{\pm} = M/2i\pi\hbar\tau \exp[iM(R^2+R'^2)/2\hbar\tau]\sqrt{(1/i\pi)}$$

$$\left\{ e^{-i(R'RM/\hbar\tau)\cos(\phi-\phi')} \int_{-\infty,\sqrt{(2R'RM/\hbar\tau)}\cos((\phi-\phi')/2)} \exp[is^2]\, ds \pm (\phi'\rightarrow-\phi') \right\}$$

where ϕ' is the angle to the source and ϕ is the angle to the point of detection.

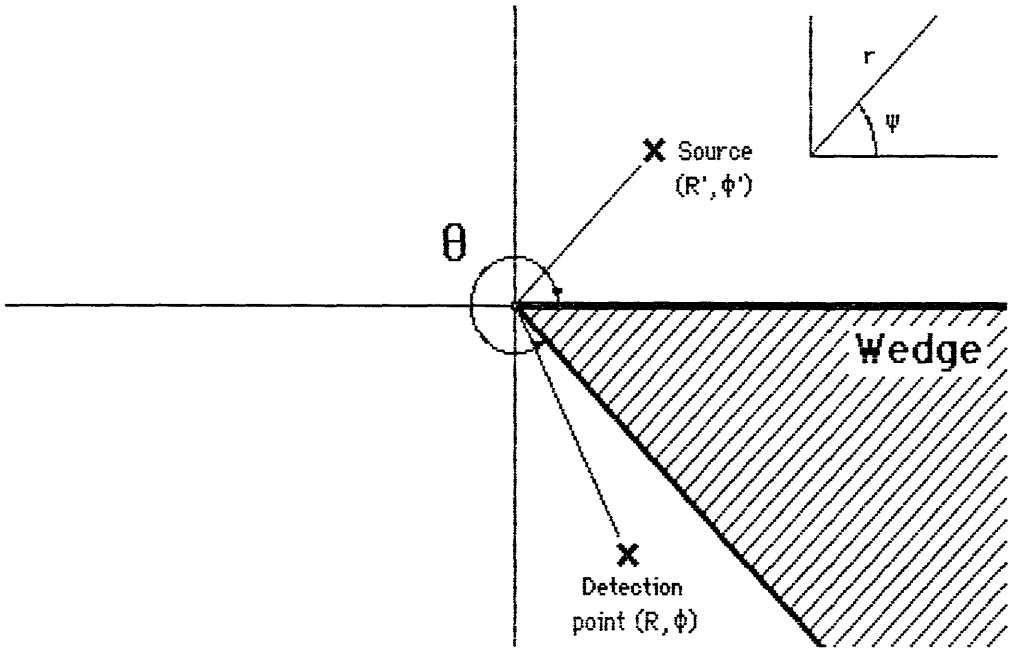
Note that the barrier has been placed at zero angle.

Note also that the kernel for the **reflecting** barrier does depend upon the location of the barrier, since this determines the image positions.

The above results agree with that obtained by Schulman *[1982, 1982]*

§III Generalization

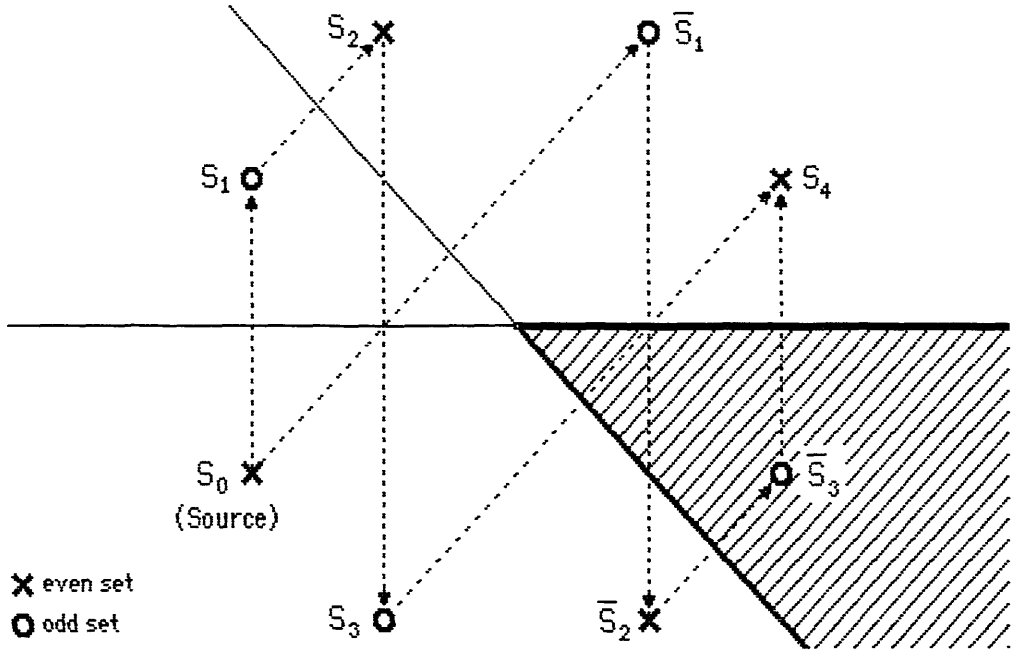
A natural progression of this work is to model an impenetrable wedge of external angle θ (see figure below).



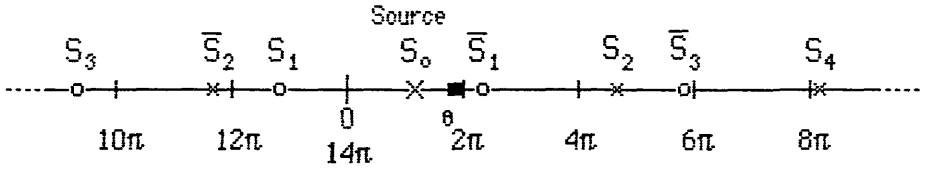
Diffraction from a Wedge

In order to do this, one would again like to use the method of images to implement the desired boundary conditions upon the two edges. This suggests the introduction of image sources at the two positions obtained by reflecting the source in each boundary wall. However, this does not quite achieve the desired result, since an image placed to achieve a boundary condition for one of the faces will disturb that of the second. One can correct for this by adding further images to restore these conditions. This leads to images standing at $\phi = \pm \phi' \pm 2k\phi$; k an integer (see figure

below).



The use of images to implement boundary conditions
(for a wedge of external angle $\theta = 7\pi/4$ and source at $\phi' = 7\pi/6$)



x even set
o odd set
Wedge

Image Positions
(for a wedge of external angle $\theta = 7\pi/4$ and source at $\phi' = 7\pi/6$)

Such a sequence of images will close upon itself if the external wedge

angle is a rational number times π i.e.:

$$\theta = \pi\mu/\nu$$

μ,ν positive integers

The image positions, which are conveniently grouped as those obtained after an even number of reflections and those for an odd number (see figure), are then given respectively by:

$$R = R'$$
$$\phi = \phi' + 2\pi k\ \mu/\nu$$

and

$$R = R'$$
$$\phi = -\phi' + 2\pi k\ \mu/\nu$$

$k = 1...\nu$

This use of images, with the need to hide them, requires the consideration of a μ sheeted Riemannian surface; μ sheeted since the images close upon themselves after μ turns.

It is these considerations that motivate us to consider amplitudes defined upon a μ sheeted configuration space; in the manner of Sommerfeld *[1896, 1954]*. So a wedge of external angle $\pi\mu/\nu$ lives on a μ sheeted surface with 2ν sources.

In such a configuration space, paths are constrained to loop a multiple of μ times from the source in order to reach the detector, which must also lie in the physical Riemannian sheet. The complete non-relativistic scalar kernel for free field on the μ sheeted Riemannian surface is then given by *[Morandi and Menossi, 1984]*, as was also derived independently and differently in the previous chapter:

$$K = p/i\pi\tau\mu\ \exp[ip(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} e^{-in(\phi-\phi')/\mu}\ (-i)^{|n/\mu|}\ J_{|n/\mu|}(2R'Rp/\tau)$$

Note that this result can also be obtained by generalizing the method of superposing solenoids as used previously. This approach is presented in appendix II for completeness.

The image amplitudes are chosen so as to implement the desired boundary conditions, namely:

$$K = 0 \text{ at } \phi = 0 \text{ and } \phi = \theta$$

for Dirichlet conditions

or

$$\partial K/\partial\phi = 0 \text{ at } \phi = 0 \text{ and } \phi = \theta$$

for Neumann conditions

The perfectly absorbing wedge is not a boundary condition problem and is considered later.

Dirichlet boundary conditions are achieved by having the two sets run at equal strength but in antiphase, while Neumann conditions are achieved by having them run in phase.

The first set of images leads to a combined kernel:

$K_w =$

$$\rho/i\pi\tau\mu \exp[i\rho(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} \sum_{k=1,\nu} e^{-in(\phi-\phi')/\mu - 2\pi k\mu/\nu} (-i)^{|n/\mu|} J_{|n/\mu|}(2R'R\rho/\tau)$$

each term yields zero unless n is a multiple of ν, since the factor:

$$\sum_{k=1,\nu} e^{in2\pi k/\nu}$$

= ν if n is a multiple of ν

= 0 if not

This is most easily seen by noticing that this is the sum of evenly spaced unit vectors in the complex plane. So:

$$K_w = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau] \nu/\mu$$

$$\{ J_0(2R'R\rho/\tau) + 2\sum_{n=1,\infty} e^{-in\nu\pi/2\mu} J_{n\nu/\mu}(2R'R\rho/\tau) \cos(n\nu(\phi-\phi')/\mu) \}$$

It is in fact possible to re-express these infinite series, which have slow convergence for large Bessel function argument, by a finite sum (for a wedge that is a rational multiple of π) using the identity (developed in the appendix III):

$$1/2\, J_0(z) + \sum_{n=1,\infty} e^{-in\pi\nu/2\mu} J_{n\nu/\mu}(z) \cos(n\nu\phi/\mu)$$

$$= 1/2\nu \sum_{k=1,\nu} \{ e^{-iz\cos(\phi+2\pi k\mu/\nu)} \{ -i \sum_{n=1,\mu-1} \cos[((\mu-n)/\mu)(\phi+2\pi k\mu/\nu)]$$

$$\int_{0,z} [e^{in\pi/2\mu} J_{-n/\mu}(u) - e^{-in\pi/2\mu} J_{n/\mu}(u)]\, e^{iu\cos(\phi+2\pi k\mu/\nu)}\, du + 1 \} \}$$

This is useful for numerical evaluation, but for clarity will not be implemented here.

The contribution of the second image set is realized by ($\phi' \rightarrow -\phi'$), leading to the final non-relativistic reflecting wedge.

$$K_w^- = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau]\, 4\nu/\mu$$

$$\sum_{n=1,\infty} e^{-in\nu\pi/2\mu} J_{n\nu/\mu}(2R'R\rho/\tau) \sin(n\nu\phi/\mu) \sin(n\nu\phi'/\mu)$$

and

$$K_w^+ = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau]\, 2\nu/\mu$$

$$\{ J_0(2R'R\rho/\tau) + 2\sum_{n=1,\infty} e^{-in\nu\pi/2\mu} J_{n\nu/\mu}(2R'R\rho/\tau) \cos(n\nu\phi/\mu) \cos(n\nu\phi'/\mu) \}$$

where $\rho \equiv M/2\hbar$ (M = scalar particle mass)

which can be seen to satisfy the required Dirichlet(-) or Neumann(+) conditions respectively at the angle θ given by:

$$\pi/\theta = \nu/\mu$$

as they were so constructed to do.

In this way we have modeled non-relativistic diffraction from a perfectly conducting wedge in free field; yielding kernels, for Dirichlet(-) or Neumann(+) boundary conditions respectively, as:

$$K_w^- = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau]\, 4\pi/\theta$$

$$\sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(2R'R\rho/\tau)\, \sin(n\pi\phi/\theta)\, \sin(n\pi\phi'/\theta)$$

and

$$K_w^+ = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau]\, 2\pi/\theta$$

$$\{\, J_0(2R'R\rho/\tau) + 2\sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(2R'R\rho/\tau)\, \cos(n\pi\phi/\theta)\, \cos(n\pi\phi'/\theta)\, \}$$

where $\rho \equiv M/2\hbar$ (M = scalar particle mass)

That these are the required solutions may be verified by confirming that they satisfy Schrödinger's free field equation as well as the desired boundary conditions.

Namely:

i) there should be no ingoing wave from infinity

ii) the desired conditions should be satisfied upon the wedge faces

iii) the short time kernel should, in the physical sheet, be a delta function source (this is effectively done in appendix II).

The perfectly absorbing wedge *[MacDonald, 1904]*, although not a boundary value problem, may be obtained from the two reflecting solutions obtained above. Dirichlet boundary conditions give rise to a reflected wave that, at

a wedge boundary, runs in antiphase with the incoming wave; while the reflected wave of the Neumann condition runs in phase. This is clear from considering the images used to implement these conditions.

Thus, by superposing these two solutions, the reflected wave is eliminated and the normalized non-relativistic scalar kernel for the perfectly absorbing wedge obtained as:

$$K_w = 1/2\,(K_w^{-} + K_w^{+})$$

$$K_w = \rho/i\pi\tau\, \exp[i\rho(R^2 + R'^2)/\tau]\, \pi/\theta$$

$$\{\, J_0(2R'R\rho/\tau) + 2\sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(2R'R\rho/\tau)\, \cos\{n\pi(\phi-\phi')/\theta\} \,\}$$

Once again the kernel for an absorbing barrier is independent of the orientation between the source and detector.

§IV Diffraction of Light

It is shown in appendix IV how an electromagnetic wave incident upon a perfectly plane conductor can be decomposed into two component wave, each of which obeys the scalar Helmholtz equation. One component has Dirichlet boundary conditions, and the other Neumann conditions. In this way, solving Maxwell's equations reduces to solving scalar wave equations.

By means of a suitable Fourier transform it is possible to convert the time dependent Schrödinger equation into the time independent Klein-Gordon equation (Helmholtz equation). In fact this technique may be used to convert a parameterized Schrödinger equation into a time dependent Klein-Gordon equation.

Starting from Schrödinger's time dependent equation for the Feynman kernel *[Feynman, 1948; Feynman and Hibbs, 1965]*:

$$i\hbar\partial_\tau \mathbf{K} - (i\hbar)^2/2M\ \nabla^2\mathbf{K} = i\hbar\ \delta(x - x_0)\ \delta(\tau)$$

One can Fourier transform to obtain the Helmholtz equation with a point source:

$$-k^2\mathbf{G} - \nabla^2\mathbf{G} = \delta(x - x_0) \qquad (c = 1)$$

using the Fourier transform pair:

$$\mathbf{G} = i\hbar/2M \int_{-\infty,\infty} \mathbf{K}\, e^{+i\omega\tau}\, d\tau$$

and

$$\mathbf{K} = 1/2\pi\ 2M/i\hbar \int_{-\infty,\infty} \mathbf{G}\, e^{-i\omega\tau}\, d\omega$$

where:

$$\omega \equiv \hbar k^2/2M$$

In this way the time independent relativistic massless kernel ($\mathbf{G}_w$) may

be obtained by Fourier transforming the time dependent non-relativistic kernel (K_w); i.e.:

$$G_w = i/4\rho \int_{0,\infty} K_w \exp[ik^2\tau/4\rho]\, d\tau$$

$$\rho \equiv M/2\hbar$$

since $K_w = 0$ for $\tau < 0$.

Using the expression for the non-relativistic scalar kernel, namely from:

$K_w(\alpha;R,\phi;R',\phi') =$

$$\rho/i\pi\tau\mu \exp[i\rho(R'^2+R^2)/\tau] \sum_{n=-\infty,\infty} e^{-i(n(\phi-\phi')/\mu)} (-i)^{|n/\mu|} J_{|n/\mu|}(2R'R\rho/\tau)$$

leads to:

$$G_w = i/4\pi\mu \sum_{n=-\infty,\infty} e^{-i(n(\phi-\phi')/\mu)} (-i)^{|n/\mu|}$$

$$\int_{0,\infty} 1/\chi \exp[ik^2\chi/4] \exp[i(R'^2+R^2)/\chi] J_{|n/\mu|}(2R'R/\chi)\, d\chi$$

where $\chi \equiv \tau/\rho$

Which may be evaluated using the identity *[Gradshteyn and Ryzhik, 1980, P719 from 6.635(3)]*:

$$\int_\nu \equiv \int_{0,\infty} 1/\chi\, e^{-\alpha\chi - \beta/\chi} J_\nu(\gamma/\chi)\, d\chi = 2\, J_\nu\{\sqrt{(2\alpha[\sqrt{(\beta^2+\gamma^2)}-\beta])}\}$$

$$K_\nu\{\sqrt{(2\alpha[\sqrt{(\beta^2+\gamma^2)}+\beta])}\}$$

where: $\mathrm{Re}\,\alpha > 0$; $\mathrm{Re}\,\beta > 0$; $\gamma > 0$

(K_ν being the modified Bessel function)

In order to make our integral well defined, and so use the above identity, we must regulate it by adding, to the now imaginary quantities α and β, small positive real parts (δ and ε respectively) which are to be reduced to

zero at the end.

The arguments:

$$\sqrt{\{\ 2(\alpha+\delta)[\ \sqrt{((\beta+\varepsilon)^2+\gamma^2)} \pm (\beta+\varepsilon)]\ \}}$$

then become, to first order in δ and ε:

$$\sqrt{\{\ 2\alpha[\ \sqrt{(\beta^2+\gamma^2)} \pm \beta]\ \}}\ [\ 1 + (1/2\alpha)\,\delta \pm (1/\sqrt{(\beta^2+\gamma^2)})\,\varepsilon/2\ ]$$

identifying:

$$\alpha = -ik^2/4;\ \beta = -i(R^2+R'^2);\ \gamma = 2R'R$$

a unique **convergent** solution is obtained for the integral:

$$\int_\nu =$$

$$2J_\nu\{kR + i(2R/k)\delta + ikR/(R^2-R'^2)\,\varepsilon/2\}\ K_\nu\{-ikR' + (2R'/k)\delta - (kR'/(R^2-R'^2))\,\varepsilon/2\}$$

for $R' > R$

$$2J_\nu\{kR' + i(2R'/k)\delta - ikR'/(R^2-R'^2)\,\varepsilon/2\}\ K_\nu\{-ikR + (2R/k)\delta + (kR/(R^2-R'^2))\,\varepsilon/2\}$$

for $R' < R$

These solutions can be seen to be well behaved at infinity from the asymptotic relations (as $|z|$ tends to ∞):

$$J_\nu(z) \to \sqrt{(2/\pi z)}\cos(z - \nu\pi/2 - \pi/4) \qquad |\arg| < \pi$$

$$K_\nu(z) \to \sqrt{(\pi/2z)}\,e^{-z} \qquad |\arg| < 3\pi/2$$

In the limit $\delta \to 0^+$ and $\varepsilon \to 0^+$, this leads to:

$$G_w(\alpha;R,\phi;R',\phi') = 1/2\pi\mu \sum_{n=-\infty,\infty} e^{-i(n(\phi-\phi')/\mu)}\,(-i)^{|n/\mu|}\,J_{|n/\mu|}(kR)\,K_{|n/\mu|}(-ikR')$$

when $R < R'$; while for $R > R'$ interchange R and R'

The time independent relativistic massless kernel

(Green's function for the Helmholtz equation)

This agrees with the anzatz of Sommerfeld *//896/* up to a factor of 2π due to our use of rationalized units.

The solution has the required R, R' symmetry. The convergence requirement is equivalent to ensuring no incoming waves from infinity.

Then, by introducing images as before, we may model the impenetrable wedge. This yields for the first set of images, the relativistic time independent scalar kernel for the perfectly absorbing wedge as:

$$G_w(\alpha;R,\phi;R',\phi') = 1/2\theta$$

$$\{ J_0(kR)\, K_0(-ikR')$$

$$+ 2\sum_{n=1,\infty} \exp[-in\pi^2/2\theta]\, J_{n\pi/\theta}(kR)\, K_{n\pi/\theta}(-ikR')\cos(n\pi(\phi-\phi')/\theta) \}$$

when R < R'; while for R > R' interchange R and R'

This agrees with the result obtained by Carslaw *//919/* when account is taken of his now non-standard definition of K_ν and the overall factor of $1/2\pi$ due to our use of rationalized units.

Used previously was an identity, developed in appendix III, for the non-relativistic case. This reduced the infinite sum (which suffers slow convergence for large Bessel function argument) to a finite sum (for a wedge angle that is a rational multiple of π). The same Fourier transformation that converted solutions will generate a finite term solution for nis case. For analytic clarity the infinite term form is retained. Sommerfeld *//896/* presented asymptotic solutions that were good approximations in the far field except along certain lines. Pauli later *//938/* found improved asymptotic forms that overcame this shortcoming.

As before, we may model the perfectly reflecting wedge by introducing the second set of images in antiphase for Dirichlet(-) boundary conditions,

or in phase for Neumann(+) conditions. To yield:

$$G_w^-(\alpha;R,\phi;R',\phi') = 2/\theta$$

$$\{ \sum_{n=1,\infty} \exp[-in\pi^2/2\theta] J_{n\pi/\theta}(kR) K_{n\pi/\theta}(-ikR') \sin(n\pi\phi/\theta) \sin(n\pi\phi'/\theta) \}$$

$$G_w^+(\alpha;R,\phi;R',\phi') = 1/\theta \{ J_0(kR) K_0(-ikR') +$$

$$2\sum_{n=1,\infty} \exp[-in\pi^2/2\theta] J_{n\pi/\theta}(kR) K_{n\pi/\theta}(-ikR') \cos(n\pi\phi/\theta) \cos(n\pi\phi'/\theta) \}$$

when $R < R'$; while for $R > R'$ interchange R and R'

In agreement with the Dirichlet(-) result of MacDonald *[1902]*

Remark

Throughout this analysis we have continued to sum over all paths, and have avoided the introduction of path constraints to implement boundary conditions.

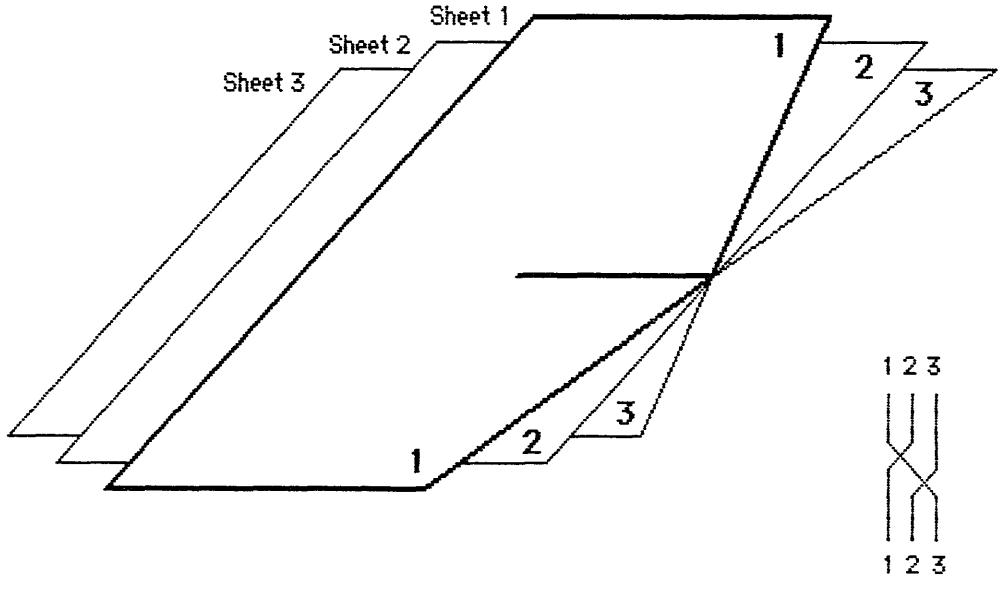
The use of a superposition of solenoids in fact replaced a constraint condition (impenetrable surface) by a suitable use of potentials.

Appendix I

Riemannian Sheeting

A multivalued function may be made single-valued by considering it to live upon a many sheeted surface. This description is a substitute for the use of branch cuts.

For example; the cube root of a complex number is trivalued and would live upon a three sheeted Riemannian surface. These sheets connect where the branch cut once lay. Upon crossing this connection, transfer is made to another sheet in the manner indicated in the figure below.



The use of Riemannian sheeting in making a multivalued function single-valued

This picture generalizes in a natural way for multivalued functions.

Riemannian sheeting is more than just an alternative to the use of branch cuts, in that it makes clear the distinction between positions on different sheets. This is an important feature in the use of such functions here.

Appendix II

Solenoid Superpositions

Following the procedure of before, we choose to superpose combinations of needle solenoids to achieve a free field kernel satisfying the desired boundary conditions.

As discussed previously, our use of images to implement boundary conditions leads us to consider a μ sheeted Riemannian surface. Only solenoids whose strength (α) are a multiple of $1/\mu$ exist upon such a surface. So choose combinations of these solutions such that the source lies within the physical sheet.

Namely that:

$$\mathrm{Lim}_{\tau\to 0^+} K = \delta(R-R') \sum_{n=-\infty,\infty} \delta\{(\phi-\phi') - 2\pi\mu n\}$$

Starting from the arbitrary linear combination:

$$K = \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} a_n e^{-in(\phi-\phi')/\mu} (-i)^{|n/\mu|} J_{|n/\mu|}(2R'R\rho/\tau)$$

$$= \rho/i\pi\tau \exp[i\rho(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} a_n e^{-in(\phi-\phi')/\mu} I_{|n/\mu|}(-i2R'R\rho/\tau)$$

but for $|z|\to\infty$:

$$I_\nu(z) \to e^z/\sqrt{(2\pi z)}$$
$$|\arg z| < \pi/2$$

(regularization is implicitly used throughout)

So:

$\mathrm{Lim}_{\tau\to 0^+} K =$

$$\text{Lim}_{\tau\to 0+}\ \rho/i\pi\tau\ \exp[i\rho(R^2+R'^2)/\tau]\ \sqrt{(i\tau/4\pi R'R\rho)}\ e^{-i2R'R\rho/\tau}\sum_{n=-\infty,\infty} a_n\ e^{-in(\phi-\phi')/\mu}$$

The angular factor:

$$\sum_{n=-\infty,\infty} a_n\ e^{-in(\phi-\phi')/\mu}$$

is required to be a series of delta functions lying at $\phi-\phi'=2\pi\mu$ x integer. The a_n's are in fact nothing but the Fourier coefficients of a Fourier series for such a periodic delta function. Fourier analysis yields the Poisson sum:

$$\sum_{n=-\infty,\infty} e^{im\theta} = 2\pi\sum_{n=-\infty,\infty}\delta(\theta+2\pi n)$$

from which one can deduce that the a_n's are in fact equal (a); and this leads to:

$$\text{Lim}_{\tau\to 0+}K = \text{Lim}_{\tau\to 0+}\ a\mu\ \sqrt{(\rho/i\pi R'R\tau)}\ \exp[i\rho(R-R')^2/\tau]\sum_{n=-\infty,\infty}\delta((\phi-\phi')-2\pi\mu n)$$

Look at:

$$\text{Lim}_{\tau\to 0+}\int_{0,\infty}\sqrt{(\rho/i\pi R'R\tau)}\ \exp[i\rho(R-R')^2/\tau]\ R\ dR$$

The integrand contributes only around R=R'

$$= \sqrt{(\rho/i\pi\tau)}\int_{-\infty,\infty}\exp[i\rho(R-R')^2/\tau]\ dR$$

$$= 1$$

i.e. the integrand = $\delta(R-R')$

Hence:

$$\text{Lim}_{\tau\to 0+}K = a\mu\ \delta(R-R')\sum_{n=-\infty,\infty}\delta((\phi-\phi')-2\pi\mu n)$$

i.e. $a = 1/\mu$

Yielding the complete kernel of before, namely:

$$K = \rho/i\pi\tau\mu \exp[i\rho(R^2+R'^2)/\tau] \sum_{n=-\infty,\infty} e^{-in(\phi-\phi')/\mu} (-i)^{|n/\mu|} J_{|n/\mu|}(2R'R\rho/\tau)$$

from which we proceed as previously.

Appendix III

Finite sum expressions

To evaluate a finite sum form for:

$$S(z,\phi) = 1/2\, J_0(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, \cos(n\phi/\mu)$$

where μ is a positive integer.

The approach taken is to develop a finite term partial differential equation (w.r.t. z) satisfied by S, which is then integrated to yield an integral form for S.

Look at:

$$S_\phi(z,\phi) \equiv 1/2\, J_0(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, e^{in\phi/\mu}$$

$$S = 1/2\,(S_\phi + S_{-\phi})$$

$$\partial S_\phi(z,\phi)/\partial z = -1/2\, J_1(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu}\, 1/2\,[\, J_{(n/\mu)-1}(z) - J_{(n/\mu)+1}(z)\,]\, e^{in\phi/\mu}$$

having used:

$$J_\nu' = 1/2\,(J_{\nu-1} - J_{\nu+1}) \qquad \nu \neq 0$$

and

$$J_0' = -J_1$$

After considerable manipulation:

$$\partial S_\phi(z,\phi)/\partial z = -\,i/2\, e^{i\phi} J_0(z) - i/2 \sum_{n=1,\mu-1} e^{in\pi/2\mu}\, J_{-n/\mu}(z)\, e^{i(\mu-n)\phi/\mu}$$

$$+\, i/2 \sum_{n=1,\mu-1} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, e^{-i(\mu-n)\phi/\mu} - i\cos\phi \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, e^{in\phi/\mu}$$

recall:

$$\partial S/\partial z = 1/2\ \partial(S_{\phi} + S_{-\phi})/\partial z$$

$$= -i/2\ \cos\phi\, J_0(z) - i/2 \sum_{n=1,\mu-1} \left\{ e^{in\pi/2\mu}\, J_{-n/\mu}(z) - e^{-in\pi/2\mu}\, J_{n/\mu}(z) \right\} \cos((\mu-n)\phi/\mu)$$

$$- i\ \cos\phi \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, \cos(n\phi/\mu)$$

Leading to the finite term partial differential equation for S:

$$\partial S(z,\phi)/\partial z$$

$$= -i/2 \sum_{n=1,\mu-1} \left\{ e^{in\pi/2\mu}\, J_{-n/\mu}(z) - e^{-in\pi/2\mu}\, J_{n/\mu}(z) \right\} \cos((\mu-n)\phi/\mu) - i\ \cos\phi\ S(z,\phi)$$

which is of the form:

$$\partial S(z,\phi)/\partial z = p(z,\phi)\ S(z,\phi) + q(z,\phi)$$

and has the solution:

$$S(z,\phi) = \exp\left[\int p(z,\phi)\, dz\right] \left\{ \int_z q(u,\phi)\, \exp\left[-\int_u p(v,\phi)\, dv\right] du + f(\phi) \right\}$$

where f is an arbitrary function of ϕ.

Hence:

$$S(z,\phi) = e^{-iz\cos\phi} \left\{ -i/2 \sum_{n=1,\mu-1} \cos((\mu-n)\phi/\mu) \right.$$

$$\left. \int_{0,z} \left[e^{in\pi/2\mu}\, J_{-n/\mu}(u) - e^{-in\pi/2\mu}\, J_{n/\mu}(u) \right] e^{iu\cos\phi}\, du + f(\phi) \right\}$$

put z=0 to find $f(\phi)$. This gives $f(\phi)=1/2$.

Having used the fact that:

$$J_{\nu}(0) = 0 \qquad \nu>0$$

and

$$J_0(0) = 1$$

Finally the identity is obtained as:

$$1/2\ J_0(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n/\mu}(z)\, \cos(n\phi/\mu)$$

$$= e^{-iz\cos\phi}\left\{ -i/2 \sum_{n=1,\mu-1} \cos((\mu-n)\phi/\mu) \right.$$

$$\left. \int_{0,z} \left[e^{in\pi/2\mu} J_{-n/\mu}(u) - e^{-in\pi/2\mu} J_{n/\mu}(u) \right] e^{iu\cos\phi}\, du + 1/2 \right\}$$

This reduces to the known result for $\mu=2$ *[Gradshteyn and Ryzhik, P973 from 8.511(5)]*, namely:

$$1/2\, J_0(z) + \sum_{n=1,\infty} e^{-in\pi/4} J_{n/2}(z) \cos(n\phi/2)$$

$$= \sqrt{(1/i\pi)}\, e^{-iz\cos\phi} \int_{-\infty,\sqrt{(2z)}\cos(\phi/2)} \exp[is^2]\, ds$$

by using:

$$J_{-1/2}(z) = \sqrt{(2/\pi z)}\cos(z)$$

and

$$J_{1/2}(z) = \sqrt{(2/\pi z)}\sin(z)$$

the equation:

$$1/2 = \sqrt{(1/i\pi)} \int_{-\infty,0} \exp[is^2]\, ds$$

and the variable change:

$$s = \sqrt{(2u)}\cos(\phi/2)$$

One may **further** generalize this identity by adding together this expression for angles given by:

$$\phi + 2\pi k\mu/\nu \qquad k = 1 \ldots \nu$$

where ν is a positive integer

The left hand side of the identity developed becomes:

$$1/2 \sum_{k=1,\nu} \left\{ J_0(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu} J_{n/\mu}(z) \left[e^{-in(\phi+2\pi k\mu/\nu)/\mu} + e^{in(\phi+2\pi k\mu/\nu)/\mu} \right] \right\}$$

but:

$$= \nu \text{ if } n \text{ is a multiple of } \nu$$

$$\sum_{k=1,\nu} e^{-i2\pi kn/\nu}$$

= 0 if not

This is most easily seen by noticing that this is the sum of evenly spaced unit vectors in the complex plane.

So the left hand side becomes:

$$1/2\, J_0(z) + \sum_{n=1,\infty} e^{-in\pi/2\mu}\, J_{n\nu/\mu}(z)\, \cos(n\nu\phi/\mu)$$

$$= 1/2\nu \sum_{k=1,\nu} \Big\{ e^{-iz\cos(\phi+2\pi k\mu/\nu)} \Big\{ -i \sum_{n=1,\mu-1} \cos\big((\mu-n)(\phi+2\pi k\mu/\nu)/\mu\big)$$

$$\int_{0,z} \left[e^{in\pi/2\mu}\, J_{-n/\mu}(u) - e^{-in\pi/2\mu}\, J_{n/\mu}(u) \right] e^{iu\cos(\phi+2\pi k\mu/\nu)}\, du + 1 \Big\} \Big\}$$

These results are useful in that they convert an infinite series which suffers from slow convergence (for large Bessel function argument) into an expression with a finite number of terms (for μ,ν finite).

Appendix IV

Decomposition of the electromagnetic wave

[Jackson, 1975]

Inside a perfect conductor, the electric and magnetic fields are zero.

Using Maxwell's equations to see what this implies just outside of the surface.

$$\nabla.B = 0 \qquad\qquad \nabla \wedge E = -\partial B/\partial t$$

$$\downarrow \qquad\qquad \downarrow$$

Gauss — Stokes

$$\downarrow \qquad\qquad \downarrow$$

$$\oint B.dS = 0 \qquad\qquad \oint E.dl = -\partial/\partial t \int B.dS$$

(the 'loop' integral symbolizing the use of a closed 'surface')

$$(B_n)_S = 0 \qquad\qquad (E_t)_S = 0$$

n: normal
t: tangent

Similar deductions cannot be made from the remaining equations, since the current and charge densities are infinite on the surface.

A more convenient form of the first condition is obtained from Maxwell's equation for free space.

$$\nabla \wedge B = 1/c^2 \, \partial E/\partial t$$

$$(\nabla \wedge B)_t = 0$$

$$B_n = 0$$

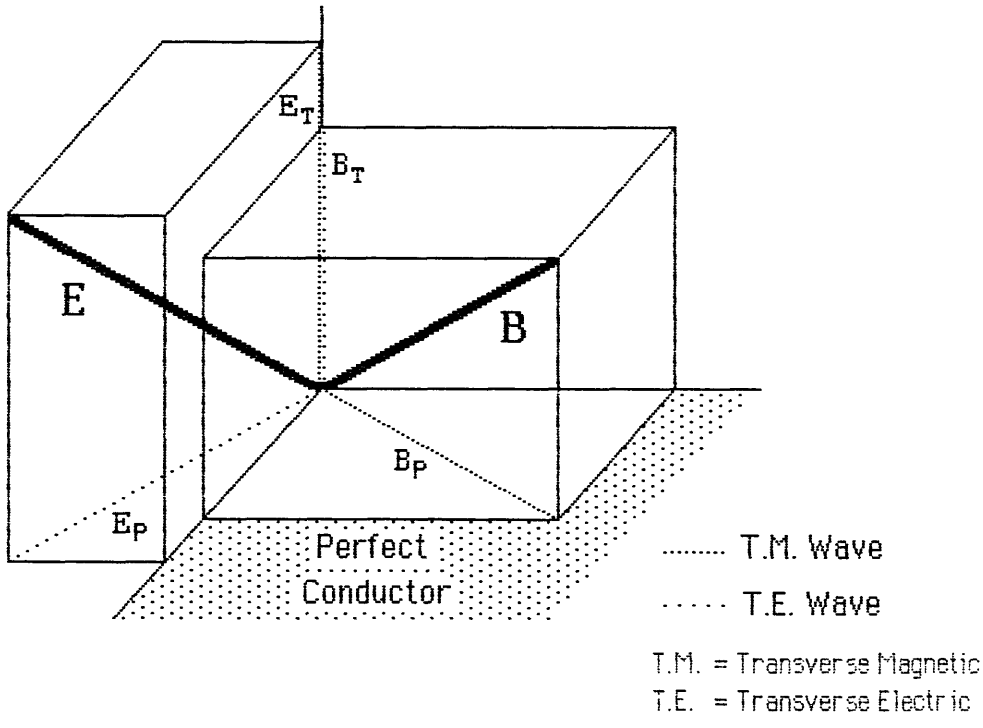
Yielding two alternative, independent boundary conditions:

$$(E_t)_S = 0$$

$$(\partial B_t/\partial n)_S = 0$$

$((B_n)_S = 0$ follows by virtue of Maxwell's equations$)$

It is convenient to decompose the wave into two components (see diagram below)



Decomposition of an Electromagnetic Wave

i) Transverse magnetic (T.M.) wave (B perpendicular to plane)

$B_t = 0$ everywhere; remaining boundary condition $(E_t)_S = 0$

ii) Transverse electric (T.E.) wave (E perpendicular to plane)

$E_t = 0$ everywhere; remaining boundary condition $(\partial B_t/\partial n)_S = 0$

Each component obeys the scalar wave equation. T.M. waves being subject to Dirichlet conditions on the electric field, and T.E. waves having

Neumann conditions on the magnetic field. (These boundary conditions induce reflected waves).

Chapter Three

Canonical Transformations in Quantum Mechanics

(a canonically invariant discretization prescription for the path integral)

§1 Introduction

In this preliminary work canonical transformations for the path integral are identified to be those of classical mechanics, and a time discretization scheme found that allows the transformation to a trivial Hamiltonian, as well as a consistent quantization of a classical system.

Traditional quantization through operators *[Dirac, 1958; Chernoff, 1981,* does not generate a unique quantum theory. Equivalent classical systems (related by a canonical transformation) in general yield differing quantum systems *[Kapoor, 1984]* Also, in the operator formalism, it is not clear how to implement a canonical transformation due to the use of non-commuting variables. The ambiguities in quantizing the classical theory means that one cannot fall back on the classical theory to perform the canonical transformation. The path integral description of quantum mechanics *[Feynman, 1948; Feynman and Hibbs, 1965]* offers an alternative method of quantization and poses a possible way out of this dilemma, since it uses commuting variables in its structure.

Starting from the classical action, one can form the path integral expression:

$$\int\int e^{i/\hbar \int (pq - H)dt}\, Dq\, Dp$$

This formal expression is deceptive in that it employs commuting variables, but is supposed to be equivalent to the traditional operator formalism. The above formal expression is in fact ill defined. In order to evaluate it one can discretize it in time; but the answer is in fact dependent upon the finite difference scheme adopted. Factor ordering is carried within the prescription *[Schulman, 1980; Mayes and Dowker, 1972].*

In general, however, the prescription will change under a canonical transformation *[Klauder, 1980]*, so a quantization scheme based on a particular prescription will in general generate inequivalent quantum systems from equivalent classical ones. These features have been dealt with in more detail in the introduction. However, a particular discretization scheme has been found that is invariant under general canonical transformations, and opens the way to a consistent quantization scheme, as well as a quantum mechanical application of the Hamilton-Jacobi theory of classical mechanics *[Goldstein, 1980, Schulman, 1980]*.

§II Canonical Transformations in the Path Integral

In classical mechanics a canonical transformation is one that preserves the least action principle *[Goldstein, 1980]*. For the path integral one might analogously require that there be a path integral representation in the new variables (Q,P,t), if one existed in the old ones (q,p,t). Such a transformation should be system independent, that is to say, the transformation should be canonical not only for some specific system, but for all problems with the same degrees of freedom. The amplitude may alter under such a transformation by at most a phase factor.

i.e. **formally**, with end points (a,b) in phase space held fixed:

$$\int\int e^{i/\hbar \int(p\dot{q} - \mathbf{H})dt}\, Dq\, Dp = e^{i/\hbar (F_b - F_a)} \int\int e^{i/\hbar \int(P\dot{Q} - \mathbf{K})dt}\, DQ\, DP \qquad \forall\, \mathbf{H}(q,p,t)$$

F being an arbitrary smooth function. Assuming that a canonically invariant discretization prescription exists (just such a scheme being sought), then this formal statement becomes true for that scheme. Any other expression should be manipulated into this form with the resulting $O(\hbar^2)$ term additions to the Hamiltonian. These terms may be replaced by 'potential like' terms of the same effect *[McLaughlin and Schulman, 1976]*, the technique for achieving this being illustrated later. It is being claimed that the quantum canonical transformation is a cleaner object when used with an invariant path integral scheme.

Since the above equation is to be true for all Hamiltonians, the integrands must be equal. This is perhaps most easily seen by choosing Hamiltonians that are highly localized in phase space. The integrands must then be equal at the 'localization point'. By choosing Hamiltonians localized at each point, it follows that the integrands must be equal

everywhere. This implies that:

$$p\dot{q} - \mathbf{H} = P\dot{Q} - \mathbf{K} + dF/dt$$

if the end points in phase space are fixed. i.e. we should work with a coherent state type path integral *[Klauder, 1980]*. This is the same requirement as in classical mechanics *[Goldstein, 1980]*; as well as the further condition that the Jacobian of the transformation be unity.

Suppose $F = F(q,Q,t)$; then because:

$$p\dot{q} - \mathbf{H} = P\dot{Q} - \mathbf{K} + (\partial F/\partial q)_{Qt}\dot{q} + (\partial F/\partial Q)_{qt}\dot{Q} + (\partial F/\partial t)_{qQ}$$

and by the independence of q and Q:

$$p = (\partial F/\partial q)_{Qt} \qquad P = -(\partial F/\partial Q)_{qt} \qquad \mathbf{K} = \mathbf{H} + (\partial F/\partial t)_{qQ}$$

F being now seen to be the generating function of the canonical transformation. It follows automatically that the Jacobian is unity *[Goldstein, 1980]*. One concludes from this that the quantum canonical transformations are the same as those for classical mechanics, excepting that scaling transformations are excluded.

If one could perform general canonical transformations in quantum mechanics, then one might consider emulating the Hamilton-Jacobi philosophy of classical mechanics. In this approach *[Goldstein, 1980, Schulman, 1980]*, rather than directly solve the equations of motion following from a given Hamiltonian $\mathbf{H}(q,p,t)$, a canonical transformation is implemented that renders the transformed Hamiltonian (Kamiltonian $\mathbf{K}(Q,P,t)$) equal to zero. The work then lies in finding this transformation, the generator of which is determined by the Hamilton-Jacobi equation. For this purpose it is convenient to work with an alternative generating function given by:

$$\mathcal{F}(q,P,t) \equiv F(q,Q,t) + QP$$

so:

$$p\dot{q} - \mathbf{H} = P\dot{Q} - \mathbf{K} + dF/dt$$

$$= -Q\dot{P} - \mathbf{K} + (\partial \boldsymbol{F}/\partial q)_{Pt}\,\dot{q} + (\partial \boldsymbol{F}/\partial P)_{qt}\,\dot{P} + (\partial \boldsymbol{F}/\partial t)_{qP}$$

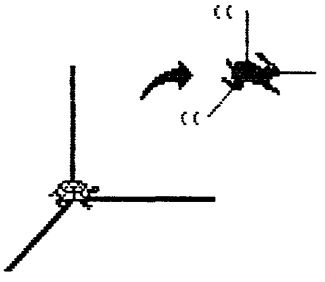
from which follows, by the independence of q and P:

$$Q = (\partial \boldsymbol{F}/\partial P)_{qt} \qquad p = (\partial \boldsymbol{F}/\partial q)_{Pt} \qquad \mathbf{K} = \mathbf{H} + (\partial \boldsymbol{F}/\partial t)_{qP}$$

leading to the Hamiiton-Jacobi equation:

$$\mathbf{H}(q,(\partial \boldsymbol{F}/\partial q)_{Pt},t) + (\partial \boldsymbol{F}/\partial t)_{qP} = 0$$

Classically one has transformed into a frame that 'tracks' the system so that it then has trivial motion (constant phase space coordinates). The transformation then carries the motion (see figure below):



The Hamilton-Jacobi transformation

§III The Symmetric Path Integral

Due to the higher order sensitivities of the path integral *[Schulman, 1980]*, in order to correctly transform the path integral one can start from some time discretized version. An especially convenient scheme for the propagator is the 'symmetric' prescription given by:

$$K(q_b,p_b,t_b|q_a,p_a,t_a) \equiv$$
$$Lim_{N\to\infty} \int..\int \prod_{j=1,N-1} (dq(j)dp_m(j)/2\pi\hbar)$$
$$\exp[i/\hbar \sum_{k=1,N} \{ p_m(k)(q(k)-q(k-1)) - H(q_m(k),p_m(k),k-1/2)\,\Delta t \}]$$

where:

$$q_m(k) \equiv 1/2\,(q(k) + q(k-1))$$
$$p_m(k) \equiv 1/2\,(p(k) + p(k-1))$$
$$\Delta t \equiv T/N$$

The end points not being integrated over, allowing them to be held constant. This is most closely related to the coherent state path integral *[Klauder, 1980]* where end points are naturally not integrated over and there are an equal number of coordinate and conjugate momenta integrations. In general a given phase space path integral (with fixed end points) must be kneaded into this form with the corresponding $\hbar^2$ additions to the Hamiltonian, which is then highly quantum mechanical in nature. What has been achieved is an 'exposure' of all stochastic terms. The use of the symmetric (mid-point) finite difference expressions was discussed and motivated in the introduction to path integrals. By considering p_m as a dummy variable, this mid-point ordering can be seen to correspond to 'Weyl ordering' in the operator formalism *[Gervais and*

Jevicki, 1980]. The properties of mid-point investigated earlier suggest that the proposed discretization might be the canonical invariant sought.

The end conditions are not always independent, since if one wishes to recover the classical limit as $\hbar \to 0$, the end points must then be connected by a classical path. Any two end conditions are then sufficient to determine the other two.

> *There are in fact pairs of points in configuration space that cannot be joined by a least action principle, for any Hamiltonian [Landau and Lifshitz, 1982]. Motions between such points would not have an 'action description'. It is assumed that coordinate systems leading to this dilemma are not adopted.*

This manner of path integral has been investigated by Klauder *[1980]* and would seem to be the starting point for making the path integral a well defined mathematical object *[Daubechies and Klauder, 1985].*

§IV Transforming the Path Integral

Consider a general canonical transformation of the p and q implemented by a generating function F(q,Q,t).

$$p = (\partial F/\partial q)_{Qt} \qquad P = -(\partial F/\partial Q)_{qt} \qquad \mathbf{K} = \mathbf{H} + (\partial F/\partial t)_{qQ}$$

(could use any other generating function)

or equivalentiy:

$$q = q(Q,P,t) \qquad Q = Q(q,p,t)$$

$$p = p(Q,P,t) \qquad P = P(q,p,t)$$

such that

$$(\partial Q/\partial q)_{pt} = (\partial p/\partial P)_{Qt} \qquad (\partial Q/\partial p)_{qt} = -(\partial q/\partial P)_{Qt}$$

$$(\partial P/\partial q)_{pt} = -(\partial p/\partial Q)_{Pt} \qquad (\partial P/\partial p)_{qt} = (\partial q/\partial Q)_{Pt}$$

It is useful to first consider the **formal** canonical transformation of the path integral with no consideration of stochastic terms.

Formally, with all end points fixed:

$$\iint e^{i/\hbar \int (p\dot{q} - \mathbf{H})dt}\, Dq\, Dp \Rightarrow e^{i/\hbar (F_b - F_a)} \iint e^{i/\hbar \int (P\dot{Q} - \mathbf{K})dt}\, DQ\, DP$$

where:

$$\mathbf{K}(Q,P,t) = \mathbf{H}(q,p,t) + (\partial F/\partial t)_{qQ}$$

so that using the symmetric expansion scheme this is interpreted as:

$$e^{i/\hbar (F_b - F_a)} \operatorname{Lim}_{N\to\infty} \int \cdots \int \prod_{j=1,N-1} (dQ(j)\, dP_M(j)/2\pi\hbar)$$

$$\exp[i/\hbar \sum_{k=1,N} \{ P_M(k)(Q(k)-Q(k-1)) - \mathbf{K}(Q_M(k),P_M(k),k-1/2)\, \Delta t \}]$$

where:

$$\mathbf{K}(Q_M(k),P_M(k),k-1/2) = \mathbf{H}(q_M(k),p_M(k),k-1/2) + (\partial F_M/\partial t)_{qQ}$$

$$Q_M(k) \equiv 1/2\, (Q(k) + Q(k-1))$$

$$P_M(k) \equiv 1/2\,(P(k) + P(k-1))$$
$$q_M(k) = q(Q_M(k), P_M(k), k-1/2)$$
$$p_M(k) = p(Q_M(k), P_M(k), k-1/2)$$

Under this notation an m subscript means at the q,p mid-point, while an M subscript means at the Q,P mid-point.

In general the naively transformed expression is not equal to its parent, due to the generation of extra (stochastic) terms in the process. That is to say, a general discretization prescription is not canonically invariant *[Klauder, 1980]*. The task ahead is to correctly perform a canonical transformation and determine the stochastic terms so generated in the hope that they sum to zero, as required of a canonically invariant scheme.

§V Mid-point Expansions

Of use are mid-point expansions, since in the symmetric prescription all functions are evaluated at the mid-point.

Adopting the following notation:

$$f_m(k) \equiv f(q_m(k),p_m(k),k-1/2)$$

$$f_M(k) \equiv f(q(Q_M(k),P_M(k),k-1/2),p(Q_M(k),P_M(k),t-1/2),k-1/2)$$

$$f_{,Q} \equiv (\partial F/\partial Q)_{Pt} \quad f_{,}{}^{P} \equiv (\partial F/\partial P)_{Qt} \quad f_{,t} \equiv (\partial F/\partial t)_{QP}$$

$$\Delta f(k) \equiv f(q(k),p(k),k) - f(q(k-1),p(k-1),k-1)$$

Note that this implies that:

$$q_m(k) \equiv 1/2\,(q(k) + q(k-1)) \quad Q_M(k) \equiv 1/2\,(Q(k) + Q(k-1))$$

whereas $$q_M(k) \equiv q(Q_M(k),P_M(k),k-1/2)$$

similarly for p, P.

Then by Taylor expansion:

$$\begin{aligned} f_m = f_M &+ 1/8\, f_{M,QQ} && \Delta Q\,\Delta Q \\ &+ 1/8\, f_{M,}{}^{PP} && \Delta P\,\Delta P \\ &+ 1/8\, f_{M,tt} && \Delta t\,\Delta t \\ &+ 1/4\, f_{M,Q}{}^{P} && \Delta Q\,\Delta P \\ &- 1/4\, f_{M,Qt} && \Delta Q\,\Delta t \\ &+ 1/4\, f_{M,}{}^{P}{}_{t} && \Delta P\,\Delta t \\ &+ \ldots \end{aligned}$$

$$\begin{aligned} \Delta f = &\quad f_{M,Q} && \Delta Q \\ &+ f_{M,}{}^{P} && \Delta P \\ &+ f_{M,t} && \Delta t \\ &+ 1/24\, f_{M,QQQ} && \Delta Q\,\Delta Q\,\Delta Q \end{aligned}$$

$$
\begin{aligned}
&+ 1/24\ f_{M,}{}^{PPP}\ \Delta P\,\Delta P\,\Delta P \\
&+ 1/24\ f_{M,ttt}\ \Delta t\,\Delta t\,\Delta t \\
&+ 1/8\ f_{M,QQ}{}^{P}\ \Delta Q\,\Delta Q\,\Delta P \\
&+ 1/8\ f_{M,QQt}\ \Delta Q\,\Delta Q\,\Delta t \\
&+ 1/8\ f_{M,}{}^{PP}{}_{t}\ \Delta P\,\Delta P\,\Delta t \\
&+ 1/8\ f_{M,Q}{}^{PP}\ \Delta Q\,\Delta P\,\Delta P \\
&+ 1/8\ f_{M,Qtt}\ \Delta Q\,\Delta t\,\Delta t \\
&+ 1/4\ f_{M,Q}{}^{P}{}_{t}\ \Delta Q\,\Delta P\,\Delta t \\
&+ \ldots
\end{aligned}
$$

By considering F as a function of Q,P and t, as opposed to q,Q and t, we may develop:

$$
\begin{aligned}
\Delta F = \quad & F_{M,Q}\ \Delta Q \\
&+ F_{M,}{}^{P}\ \Delta P \\
&+ F_{M,t}\ \Delta t \\
&+ 1/24\ F_{M,QQQ}\ \Delta Q\,\Delta Q\,\Delta Q \\
&+ 1/24\ F_{M,}{}^{PPP}\ \Delta P\,\Delta P\,\Delta P \\
&+ 1/24\ F_{M,ttt}\ \Delta t\,\Delta t\,\Delta t \\
&+ 1/8\ F_{M,QQ}{}^{P}\ \Delta Q\,\Delta Q\,\Delta P \\
&+ 1/8\ F_{M,QQt}\ \Delta Q\,\Delta Q\,\Delta t \\
&+ 1/8\ F_{M,}{}^{PP}{}_{t}\ \Delta P\,\Delta P\,\Delta t \\
&+ 1/8\ F_{M,Q}{}^{PP}\ \Delta Q\,\Delta P\,\Delta P \\
&+ 1/8\ F_{M,Qtt}\ \Delta Q\,\Delta t\,\Delta t \\
&+ 1/4\ F_{M,Q}{}^{P}{}_{t}\ \Delta Q\,\Delta P\,\Delta t \\
&+ \ldots
\end{aligned}
$$

The generating function derivatives may be converted to p,q derivatives by starting from:

$$\delta F = (\partial F/\partial Q)_{qt}\,\delta Q + (\partial F/\partial q)_{Qt}\,\delta q + (\partial F/\partial t)_{qQ}\,\delta t$$

$$= -P\,\delta Q + p\,\delta q + (\partial F/\partial t)_{qQ}\,\delta t$$

leading to:

$$
\begin{aligned}
F_{,Q} &= -P + q_{,Q}\, p \\
F_{,}{}^{P} &= q_{,}{}^{P}\, p \\
F_{,t} &= q_{,t}\, p + (\partial F/\partial t)_{qQ} \\
F_{,QQ} &= q_{,QQ}\, p + 2q_{,Q}\, p_{,Q} + q_{,Q}\, p_{,QQ} \\
F_{,Q}{}^{P} &= q_{,Q}{}^{P}\, p + 2q_{,Q}{}^{P}\, p_{,Q} + q_{,}{}^{P}\, p_{,QQ} \\
F_{,Q}{}^{PP} &= q_{,Q}{}^{PP}\, p + 2q_{,Q}{}^{P}\, p_{,}{}^{P} + q_{,Q}\, p_{,}{}^{PP} \\
F_{,}{}^{PPP} &= q_{,}{}^{PPP}\, p + 2q_{,}{}^{PP}\, p_{,}{}^{P} + q_{,}{}^{P}\, p_{,}{}^{PP} \\
F_{,Qt} &= q_{,Qt}\, p + 2q_{,Qt}\, p_{,t} + q_{,Q}\, p_{,tt} \\
F_{,}{}^{P}{}_{tt} &= q_{,}{}^{P}{}_{tt}\, p + 2q_{,}{}^{P}{}_{t}\, p_{,t} + q_{,}{}^{P}\, p_{,tt}
\end{aligned}
$$

Having used the necessary and sufficient condition for a canonical transformation *[Goldstein 1980]*:

$$q_{,Q}\, p_{,}{}^{P} - q_{,}{}^{P}\, p_{,Q} = 1$$

which follows from the canonical conditions given earlier. Care should be taken of which variables are being held constant.

We may now convert the path integral in the search for additional contributions beyond the formal conversion. These additional stochastic terms will stem from both the Jacobian and Action.

Look for stochastic contributions from the Jacobian. Since:

$$\int\!\!\ldots\!\int \prod_{j=1,N-1} (dq(j)dp_m(j)/2\pi\hbar) = \int\!\!\ldots\!\int \prod_{j=1,N-1} (dq_m(j)dp_m(j)/\pi\hbar)$$

and

$$\int\!\!\ldots\!\int \prod_{j=1,N-1} (dQ(j)dP_M(j)/2\pi\hbar) = \int\!\!\ldots\!\int \prod_{j=1,N-1} (dQ_M(j)dP_M(j)/\pi\hbar)$$

the Jacobian of interest arises from:

$$dq_m(j)\, dp_m(j) \;\rightarrow\; dQ_M(j)\, dP_M(j)$$

This is not unity because $q_m(j),p_m(j)$ and $Q_M(j),P_M(j)$ are based at different points in phase space (recalling that we are transforming q and p as opposed to q_m and p_m).

Jacobian:

$$J = (\partial q_m/\partial Q_M)_{Pt}\,(\partial p_m/\partial P_M)_{Qt} - (\partial q_m/\partial P_M)_{Qt}\,(\partial p_m/\partial Q_M)_{Pt}$$

which leads to:

$$\begin{aligned}
J = \;& q_{M,Q}\,p_M{}^{,P} - q_M{}^{,P}\,p_{M,Q} \\
& + 1/8\,(q_{M,QQQ}\,p_M{}^{,P} + q_{M,Q}\,p_{M,QQ}{}^{P} - q_M{}^{,P}\,p_{M,QQQ} - q_{M,QQ}{}^{P}\,p_{M,Q})\,\Delta Q\,\Delta Q \\
& + 1/8\,(q_{M,Q}{}^{PP}\,p_M{}^{,P} + q_{M,Q}\,p_M{}^{,PPP} - q_M{}^{,P}\,p_{M,Q}{}^{PP} - q_M{}^{,PPP}\,p_{M,Q})\,\Delta P\,\Delta P \\
& + 1/8\,(q_{M,Qtt}\,p_M{}^{,P} + q_{M,Q}\,p_M{}^{,P}{}_{tt} - q_M{}^{,P}\,p_{M,Qtt} - q_M{}^{,P}{}_{tt}\,p_{M,Q})\,\Delta t\,\Delta t \\
& + 1/8\,(q_{M,QQ}{}^{P}\,p_M{}^{,P} + q_{M,Q}\,p_{M,Q}{}^{PP} - q_M{}^{,P}\,p_{M,QQ}{}^{P} - q_{M,Q}{}^{PP}\,p_{M,Q})\,\Delta Q\,\Delta P \\
& + 1/8\,(q_{M,QQt}\,p_M{}^{,P} + q_{M,Q}\,p_{M,Q}{}^{P}{}_{t} - q_M{}^{,P}\,p_{M,QQt} - q_{M,Q}{}^{P}{}_{t}\,p_{M,Q})\,\Delta Q\,\Delta t \\
& + 1/8\,(q_{M,Q}{}^{P}{}_{t}\,p_M{}^{,P} + q_{M,Q}\,p_M{}^{,PP}{}_{t} - q_M{}^{,P}\,p_{M,Q}{}^{P}{}_{t} - q_M{}^{,PP}{}_{t}\,p_{M,Q})\,\Delta P\,\Delta t \\
& + \ldots
\end{aligned}$$

but, for a canonical transformation:

$$q_{,Q}\,p_{,}{}^{P} - q_{,}{}^{P}\,p_{,Q} = 1$$

By applying this at the **M** mid-point yields:

$$\begin{aligned}
J = 1 \;& + 1/4\,(q_{M,Q}{}^{P}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}{}^{P}) && \Delta Q\,\Delta Q \\
& + 1/4\,(q_M{}^{,PP}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_M{}^{,PP}) && \Delta P\,\Delta P \\
& + 1/4\,(q_M{}^{,P}{}_{t}\,p_{M,Qt} - q_{M,Qt}\,p_M{}^{,P}{}_{t}) && \Delta t\,\Delta t \\
& + 1/8\,(q_M{}^{,PP}\,p_{M,QQ} - q_{M,QQ}\,p_M{}^{,PP}) && \Delta Q\,\Delta P \\
& + 1/8\,(q_M{}^{,P}{}_{t}\,p_{M,QQ} + q_{M,Q}{}^{P}\,p_{M,Qt} - q_{M,QQ}\,p_M{}^{,P}{}_{t} - q_{M,Qt}\,p_{M,Q}{}^{P})\,\Delta Q\,\Delta t \\
& + 1/8\,(q_M{}^{,P}{}_{t}\,p_{M,Q}{}^{P} + q_M{}^{,PP}\,p_{M,Qt} - q_{M,Q}{}^{P}\,p_M{}^{,P}{}_{t} - q_{M,Qt}\,p_M{}^{,PP})\,\Delta P\,\Delta t \\
& + \ldots
\end{aligned}$$

Continue by looking at the Action term $p_{m(k)}\,\Delta q_{(k)}$ and comparing it to $P_{M(k)}\,\Delta Q_{(k)} + \Delta F_{(k)} - (\partial F_{M(k)}/\partial t)_{qQ}\,\Delta t$; its formal counterpart.

This leads to:

$$\mathbf{p_m\,\Delta q = \Delta F + P_M\,\Delta Q - (\partial F_M/\partial t)_{qQ}\,\Delta t}$$

$$+ 1/12\,(q_{M,Q}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}) \qquad \Delta Q\,\Delta Q\,\Delta Q$$

$$
\begin{aligned}
&+ 1/12\,(q_{M,}{}^{P}\,p_{M,}{}^{PP} - q_{M,}{}^{PP}\,p_{M,}{}^{P}) && \Delta P\,\Delta P\,\Delta P\\
&+ 1/24\,(q_{M,ttt}\,p_{M} + 3q_{M,t}\,p_{M,tt} - F_{M,ttt}) && \Delta t\,\Delta t\,\Delta t\\
&+ 1/4\,(q_{M,Q}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,Q}) && \Delta Q\,\Delta Q\,\Delta P\\
&+ 1/8\,(q_{M,QQt}\,p_{M} + q_{M,t}\,p_{M,QQ} + 2q_{M,Q}\,p_{M,Qt} - F_{M,QQt}) && \Delta Q\,\Delta Q\,\Delta t\\
&+ 1/8\,(q_{M,}{}^{PP}{}_{t}\,p_{M} + q_{M,t}\,p_{M,}{}^{PP} + 2q_{M,}{}^{P}\,p_{M,}{}^{P}{}_{t} - F_{M,}{}^{PP}{}_{t}) && \Delta P\,\Delta P\,\Delta t\\
&+ 1/4\,(q_{M,Q}{}^{P}{}_{t}\,p_{M} + q_{M,t}\,p_{M,Q}{}^{P} + q_{M,}{}^{P}\,p_{M,Qt} + q_{M,Q}\,p_{M,}{}^{P}{}_{t} - F_{M,Q}{}^{P}{}_{t}) && \Delta Q\,\Delta P\,\Delta t\\
&+ 1/4\,(q_{M,}{}^{P}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}) && \Delta Q\,\Delta P\,\Delta P\\
&+ 1/8\,(q_{M,Q}\,p_{M,tt} + 2q_{M,t}\,p_{M,Qt} + q_{M,Qtt}\,p_{M} - F_{M,Qtt}) && \Delta Q\,\Delta t\,\Delta t\\
&+ 1/8\,(q_{M,}{}^{P}\,p_{M,tt} + 2q_{M,t}\,p_{M,}{}^{P}{}_{t} + q_{M,}{}^{P}{}_{tt}\,p_{M} - F_{M,}{}^{P}{}_{tt}) && \Delta P\,\Delta t\,\Delta t\\
&+ \ldots
\end{aligned}
$$

Finally, determining stochastic contributions from the Hamiltonian. By again applying the canonical transformation at the **M** mid-point:

$$K_M = H_M + (\partial F_M/\partial t)_{qQ}$$

the original Hamiltonian becomes:

$$
\begin{aligned}
H_m = {} & K_M - (\partial F_M/\partial t)_{qQ}\\
&+ 1/8\,H_{M,QQ}\,\Delta Q\,\Delta Q\\
&+ 1/8\,H_{M,}{}^{PP}\,\Delta P\,\Delta P\\
&+ 1/8\,H_{M,tt}\,\Delta t\,\Delta t\\
&+ 1/4\,H_{M,Q}{}^{P}\,\Delta Q\,\Delta P\\
&+ 1/4\,H_{M,Qt}\,\Delta Q\,\Delta t\\
&+ 1/4\,H_{M,}{}^{P}{}_{t}\,\Delta P\,\Delta t\\
&+ \ldots
\end{aligned}
$$

Collecting up the stochastic terms:

$$
\begin{aligned}
&1/4\,(q_{M,Q}{}^{P}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}{}^{P}) && \Delta Q\,\Delta Q\\
&- 1/4\,(q_{M,}{}^{PP}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{PP}) && \Delta P\,\Delta P\\
&+ 1/4\,(q_{M,}{}^{P}{}_{t}\,p_{M,Qt} - q_{M,Qt}\,p_{M,}{}^{P}{}_{t}) && \Delta t\,\Delta t \quad \textit{Jacobian}\\
&+ 1/8\,(q_{M,}{}^{PP}\,p_{M,QQ} - q_{M,QQ}\,p_{M,}{}^{PP}) && \Delta Q\,\Delta P \quad \textit{contribution}\\
&+ 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,QQ} + q_{M,Q}{}^{P}\,p_{M,Qt} - q_{M,QQ}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,Q}{}^{P}) && \Delta Q\,\Delta t
\end{aligned}
$$

$$+ 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,Q}{}^{P} + q_{M,}{}^{PP}\,p_{M,Qt} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,}{}^{PP}) \qquad \Delta P\,\Delta t$$
$$+ \ldots$$

$$i/\hbar\,\{$$
$$1/12\,(q_{M,Q}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}) \qquad \Delta Q\,\Delta Q\,\Delta Q$$
$$+ 1/12\,(q_{M,}{}^{P}\,p_{M,}{}^{PP} - q_{M,}{}^{PP}\,p_{M,}{}^{P}) \qquad \Delta P\,\Delta P\,\Delta P$$
$$+ 1/24\,(q_{M,ttt}\,p_{M} + 3q_{M,t}\,p_{M,tt} - F_{M,ttt}) \qquad \Delta t\,\Delta t\,\Delta t$$
$$+ 1/4\,(q_{M,Q}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,Q}) \qquad \Delta Q\,\Delta Q\,\Delta P$$
$$+ 1/8\,(q_{M,Qt}\,p_{M} + q_{M,t}\,p_{M,Q} + 2q_{M,Q}\,p_{M,t} - F_{M,Qt}) \qquad \Delta Q\,\Delta Q\,\Delta t \qquad \textit{pq̇}$$
$$+ 1/8\,(q_{M,}{}^{PP}{}_{t}\,p_{M} + q_{M,t}\,p_{M,}{}^{PP} + 2q_{M,}{}^{P}\,p_{M,}{}^{P}{}_{t} - F_{M,}{}^{PP}{}_{t}) \qquad \Delta P\,\Delta P\,\Delta t \quad \textit{contribution}$$
$$+ 1/4\,(q_{M,Q}{}^{P}{}_{t}\,p_{M} + q_{M,t}\,p_{M,Q}{}^{P} + q_{M,}{}^{P}\,p_{M,Qt} + q_{M,Q}\,p_{M,}{}^{P}{}_{t} - F_{M,Q}{}^{P}{}_{t}) \qquad \Delta Q\,\Delta P\,\Delta t$$
$$+ 1/4\,(q_{M,}{}^{P}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}) \qquad \Delta Q\,\Delta P\,\Delta P$$
$$+ 1/8\,(q_{M,Q}\,p_{M,tt} + 2q_{M,t}\,p_{M,Qt} + q_{M,Qtt}\,p_{M} - F_{M,Qtt}) \qquad \Delta Q\,\Delta t\,\Delta t$$
$$+ 1/8\,(q_{M,}{}^{P}\,p_{M,tt} + 2q_{M,t}\,p_{M,}{}^{P}{}_{t} + q_{M,}{}^{P}{}_{tt}\,p_{M} - F_{M,}{}^{P}{}_{tt}) \qquad \Delta P\,\Delta t\,\Delta t$$
$$+ \ldots$$

$$- 1/8\,H_{M,QQ} \qquad \Delta Q\,\Delta Q\,\Delta t$$
$$- 1/8\,H_{M,}{}^{PP} \qquad \Delta P\,\Delta P\,\Delta t$$
$$- 1/8\,H_{M,tt} \qquad \Delta t\,\Delta t\,\Delta t \qquad \textit{Hamiltonian}$$
$$- 1/4\,H_{M,Q}{}^{P} \qquad \Delta Q\,\Delta P\,\Delta t \quad \textit{contribution}$$
$$- 1/4\,H_{M,Qt} \qquad \Delta Q\,\Delta t\,\Delta t$$
$$- 1/4\,H_{M,}{}^{P}{}_{t} \qquad \Delta P\,\Delta t\,\Delta t$$
$$+ \ldots \qquad \}$$

Since the path integral is only sensitive to order Δt, we need only work to this order. The sensitivity to order Δt follows from the fact that there are N such integrals where $\Delta t \equiv T/N$. So in the limit $N \to \infty$; $\Delta t \to 0$, but $N\Delta t = T$ (the 'time of flight').

The correctly transformed path integral then has the form:

$$I \equiv e^{i/\hbar\,(F_b - F_a)}\,\mathrm{Lim}_{N\to\infty} \int\!\!\ldots\!\int \prod_{j=1,N-1} (dQ(j)\,dP_M(j)/2\pi\hbar)$$

$$\Pi_{k=1,N}(1 + \text{Jacobian stochastic terms})$$

$$\exp[i/\hbar\{P_M(k)(Q(k)-Q(k-1)) + \mathbf{K}(Q_M(k),P_M(k),k-1/2)\,\Delta t + \text{Action stochastic terms}\}]$$

Now work to replace the stochastic terms by a potential like term *[McLaughlin and Schulman, 1976]*,

$$\boldsymbol{V}(Q_M)\,\Delta t$$

of the same effect (to order Δt).

So further define:

$$J \equiv e^{i/\hbar\,(F_b - F_a)}\,\mathrm{Lim}_{N\to\infty}\int..\int\Pi_{j=1,N-1}(dQ(j)dP_M(j)/2\pi\hbar)$$

$$\exp[i/\hbar\,\Sigma_{k=1,N}\{\,P_M(k)(Q(k)-Q(k-1)) + \mathbf{K}(Q_M(k),P_M(k),k-1/2)\,\Delta t + \boldsymbol{V}(Q_M(k))\,\Delta t\,\}]$$

Working to order Δt:

$$I = e^{i/\hbar\,(F_b - F_a)}\,\mathrm{Lim}_{N\to\infty}\int..\int\Pi_{j=1,N-1}(dQ(j)dP_M(j)/2\pi\hbar)$$

$$\Pi_{k=1,N}(1 + \text{Jacobian stochastic terms} + i/\hbar\ \text{Action stochastic terms})$$

$$\exp[i/\hbar\,\{\,P_M(k)(Q(k)-Q(k-1)) + \mathbf{K}(Q_M(k),P_M(k),k-1/2)\,\Delta t\,\}]$$

and

$$J = e^{i/\hbar\,(F_b - F_a)}\,\mathrm{Lim}_{N\to\infty}\int..\int\Pi_{j=1,N-1}(dQ(j)dP_M(j)/2\pi\hbar)$$

$$\Pi_{k=1,N}(1 + i/\hbar\ \boldsymbol{V}(Q_M(k))\,\Delta t\,)$$

$$\exp[i/\hbar\,\{\,P_M(k)(Q(k)-Q(k-1)) + \mathbf{K}(Q_M(k),P_M(k),k-1/2)\,\Delta t\,\}]$$

Consider now the particular cases of:

i) a Hamilton-Jacobi transformation,

ii) a point canonical transformation.

§VI Hamilton-Jacobi Transformations

The Hamilton-Jacobi transformation is the special case where the canonical transformed Hamiltonian (Kamiltonian) given by:

$$K = H + (\partial F/\partial t)_{qQ}$$

is null. i.e.

$$H(q,p,t) + (\partial F/\partial t)_{qQ} = 0$$

but recall:

$$p = (\partial F/\partial q)_{Qt}$$

so that the generator (Γ) of the required transformation is given by:

$$H(q,(\partial \Gamma/\partial q)_{Qt},t) + (\partial \Gamma/\partial t)_{qQ} = 0$$

the Hamilton-Jacobi equation. It should be recalled that the Hamiltonian will in general look 'quantum mechanical' due to the adoption of $\hbar$ terms in 'Weyl ordering' the path integral. In this special case of a Hamilton-Jacobi transformation:

$$I = e^{i/\hbar (\Gamma_b - \Gamma_a)} \mathrm{Lim}_{N\to\infty} \int..\int \prod_{j=1,N-1} (dQ(j)dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + \text{Jacobian stochastic terms} + i/\hbar \text{ Action stochastic terms})$$

$$\exp[i/\hbar \{ P_M(k)(Q(k)-Q(k-1)) \}]$$

to be compared with:

$$J = e^{i/\hbar (\Gamma_b - \Gamma_a)} \mathrm{Lim}_{N\to\infty} \int..\int \prod_{j=1,N-1} (dQ(j)dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + i/\hbar \, V(Q_M(k)) \, \Delta t)$$

$$\exp[i/\hbar \{ P_M(k)(Q(k)-Q(k-1)) \}]$$

The 'loss' of Δt with the Kamiltonian is ultimately responsible for the null contribution from stochastic terms.

These integrals are ill defined and may be made tractable by the inclusion of a 'mass' term:

$$I = \mathrm{Lim}_{N,\Lambda\to\infty}\, e^{i/\hbar\,(r_b - r_a)} \int\!\!\int \prod_{j=1,N-1} (dQ(j)\,dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + \text{Jacobian stochastic terms} + i/\hbar \text{ Action stochastic terms})$$

$$\exp[i/\hbar\,\{\, P_M(k)(Q(k)-Q(k-1)) + \mathbf{P_M^2(k)\,\Delta t/2\Lambda}\,\}]$$

$$J = \mathrm{Lim}_{N,\Lambda\to\infty}\, e^{i/\hbar\,(r_b - r_a)} \int\!\!\int \prod_{j=1,N-1} (dQ(j)\,dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + i/\hbar\, \boldsymbol{V}(q_M(k))\,\Delta t\,)$$

$$\exp[i/\hbar\,\{\, P_M(k)(Q(k)-Q(k-1)) + \mathbf{P_M^2(k)\,\Delta t/2\Lambda}\,\}]$$

where the stochastic terms are:

$1/4\,(q_{M,Q}{}^{P}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}{}^{P})$	$\Delta Q\,\Delta Q$
$+\ 1/4\,(q_{M,}{}^{PP}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{PP})$	$\Delta P\,\Delta P$
$+\ 1/4\,(q_{M,}{}^{P}{}_{t}\,p_{M,Qt} - q_{M,Qt}\,p_{M,}{}^{P}{}_{t})$	$\Delta t\,\Delta t$ *Jacobian*
$+\ 1/8\,(q_{M,}{}^{PP}\,p_{M,QQ} - q_{M,QQ}\,p_{M,}{}^{PP})$	$\Delta Q\,\Delta P$ *contribution*
$+\ 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,QQ} + q_{M,Q}{}^{P}\,p_{M,Qt} - q_{M,QQ}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,Q}{}^{P})$	$\Delta Q\,\Delta t$
$+\ 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,Q}{}^{P} + q_{M,}{}^{PP}\,p_{M,Qt} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,}{}^{PP})$	$\Delta P\,\Delta t$
$+\ \ldots$	
$i/\hbar\,\{$	
$1/12\,(q_{M,Q}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q})$	$\Delta Q\,\Delta Q\,\Delta Q$
$+\ 1/12\,(q_{M,}{}^{P}\,p_{M,}{}^{PP} - q_{M,}{}^{PP}\,p_{M,}{}^{P})$	$\Delta P\,\Delta P\,\Delta P$
$+\ 1/24\,(q_{M,ttt}\,p_{M} + 3q_{M,t}\,p_{M,tt} - \Gamma_{M,ttt})$	$\Delta t\,\Delta t\,\Delta t$

$$
\begin{aligned}
&+ 1/4\ (q_{M,Q}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,Q}) && \Delta Q\,\Delta Q\,\Delta P \\
&+ 1/8\ (q_{M,QQt}\,p_M + q_{M,t}\,p_{M,QQ} + 2q_{M,Q}\,p_{M,Qt} - \Gamma_{M,QQt}) && \Delta Q\,\Delta Q\,\Delta t \quad \dot{pq} \\
&- 1/8\ (q_{M,}{}^{PP}{}_{t}\,p_M + q_{M,t}\,p_{M,}{}^{PP} + 2q_{M,}{}^{P}\,p_{M,}{}^{P}{}_{t} - \Gamma_{M,}{}^{PP}{}_{t}) && \Delta P\,\Delta P\,\Delta t \ \textit{contribution} \\
&+ 1/4\ (q_{M,Q}{}^{P}{}_{t}\,p_M + q_{M,t}\,p_{M,Q}{}^{P} + q_{M,}{}^{P}\,p_{M,Qt} + q_{M,Q}\,p_{M,}{}^{P}{}_{t} - \Gamma_{M,Q}{}^{P}{}_{t}) && \Delta Q\,\Delta P\,\Delta t \\
&+ 1/4\ (q_{M,}{}^{P}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}) && \Delta Q\,\Delta P\,\Delta P \\
&+ 1/8\ (q_{M,Q}\,p_{M,tt} + 2q_{M,t}\,p_{M,Qt} + q_{M,Qtt}\,p_M - \Gamma_{M,Qtt}) && \Delta Q\,\Delta t\,\Delta t \\
&+ 1/8\ (q_{M,}{}^{P}\,p_{M,tt} + 2q_{M,t}\,p_{M,}{}^{P}{}_{t} + q_{M,}{}^{P}{}_{tt}\,p_M - \Gamma_{M,}{}^{P}{}_{tt}) && \Delta P\,\Delta t\,\Delta t \\
&+ \ldots
\end{aligned}
$$

$$
\begin{aligned}
&- 1/8\ \mathbf{H}_{M,QQ} && \Delta Q\,\Delta Q\,\Delta t \\
&- 1/8\ \mathbf{H}_{M,}{}^{PP} && \Delta P\,\Delta P\,\Delta t \\
&- 1/8\ \mathbf{H}_{M,tt} && \Delta t\,\Delta t\,\Delta t \quad \textit{Hamiltonian} \\
&- 1/4\ \mathbf{H}_{M,Q}{}^{P} && \Delta Q\,\Delta P\,\Delta t \ \textit{contribution} \\
&- 1/4\ \mathbf{H}_{M,Qt} && \Delta Q\,\Delta t\,\Delta t \\
&- 1/4\ \mathbf{H}_{M,}{}^{P}{}_{t} && \Delta P\,\Delta t\,\Delta t \\
&+ \ldots && \}
\end{aligned}
$$

In this **special case** of a Hamilton-Jacobi transformation **K**=0, so:

$$
\begin{aligned}
\mathbf{H} &= -(\partial\Gamma/\partial t)_{qQ} \\
&= -\Gamma_{,t} + p\,q_{,t}
\end{aligned}
$$

as was shown previously.

This leads to the Hamilton stochastic terms cancelling many of their $\dot{pq}$ counterparts, since the Hamilton stochastic contribution:

$$
\begin{aligned}
&= i/\hbar\ \{ \\
&\quad - 1/8\ (-\Gamma_{M,QQt} + q_{M,QQt}\,p_M + 2q_{M,Qt}\,p_{M,Q} + q_{M,t}\,p_{M,QQ}) && \Delta Q\,\Delta Q\,\Delta t \\
&\quad - 1/8\ (-\Gamma_{M,}{}^{PP}{}_{t} + q_{M,}{}^{PP}{}_{t}\,p_M + 2q_{M,}{}^{P}{}_{t}\,p_{M,}{}^{P} + q_{M,t}\,p_{M,}{}^{PP}) && \Delta P\,\Delta P\,\Delta t \\
&\quad - 1/8\ (-\Gamma_{M,tt} + q_{M,ttt}\,p_M + 2q_{M,tt}\,p_{M,t} + q_{M,t}\,p_{M,tt}) && \Delta t\,\Delta t\,\Delta t \\
&\quad - 1/4\ (-\Gamma_{M,Q}{}^{P}{}_{t} + q_{M,Q}{}^{P}{}_{t}\,p_M + q_{M,Qt}\,p_{M,}{}^{P} + q_{M,}{}^{P}{}_{t}\,p_{M,Q} + q_{M,t}\,p_{M,Q}{}^{P}) && \Delta Q\,\Delta P\,\Delta t \\
&\quad - 1/4\ (-\Gamma_{M,Qtt} + q_{M,Qtt}\,p_M + q_{M,Qt}\,p_{M,t} + q_{M,tt}\,p_{M,Q} + q_{M,t}\,p_{M,Qt}) && \Delta Q\,\Delta t\,\Delta t \\
&\quad - 1/4\ (-\Gamma_{M,}{}^{P}{}_{tt} + q_{M,}{}^{P}{}_{tt}\,p_M + q_{M,}{}^{P}{}_{t}\,p_{M,t} + q_{M,tt}\,p_{M,}{}^{P} + q_{M,t}\,p_{M,}{}^{P}{}_{t}) && \Delta P\,\Delta t\,\Delta t
\end{aligned}
$$

$+ \ldots$ }

Yielding the set of stochastic terms:

$$
\begin{aligned}
& 1/4\,(q_{M,Q}{}^{P}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}{}^{P}) && \mathbf{\Delta Q\ \Delta Q} \\
+\ & 1/4\,(q_{M,}{}^{PP}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{PP}) && \Delta P\ \Delta P \\
+\ & 1/4\,(q_{M,}{}^{P}{}_{t}\,p_{M,Qt} - q_{M,Qt}\,p_{M,}{}^{P}{}_{t}) && \Delta t\ \Delta t \quad \textit{Jacobian} \\
+\ & 1/8\,(q_{M,}{}^{PP}\,p_{M,QQ} - q_{M,QQ}\,p_{M,}{}^{PP}) && \Delta Q\ \Delta P \quad \textit{contribution} \\
+\ & 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,QQ} + q_{M,Q}{}^{P}\,p_{M,Qt} - q_{M,QQ}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,Q}{}^{P}) && \mathbf{\Delta Q\ \Delta t} \\
+\ & 1/8\,(q_{M,}{}^{P}{}_{t}\,p_{M,Q}{}^{P} + q_{M,}{}^{PP}\,p_{M,Qt} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,}{}^{PP}) && \Delta P\ \Delta t \\
+\ & \ldots
\end{aligned}
$$

$i/\hbar$ {

$$
\begin{aligned}
& 1/12\,(q_{M,Q}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}) && \mathbf{\Delta Q\ \Delta Q\ \Delta Q} \\
+\ & 1/12\,(q_{M,}{}^{P}\,p_{M,}{}^{PP} - q_{M,}{}^{PP}\,p_{M,}{}^{P}) && \Delta P\ \Delta P\ \Delta P \\
+\ & 1/12\,(\Gamma_{M,ttt} - q_{M,ttt}\,p_{M} - 3q_{M,tt}\,p_{M,t}) && \Delta t\ \Delta t\ \Delta t \\
+\ & 1/4\,(q_{M,Q}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,Q}) && \Delta Q\ \Delta Q\ \Delta P \\
+\ & 1/4\,(q_{M,Q}\,p_{M,Qt} - q_{M,Qt}\,p_{M,Q}) && \mathbf{\Delta Q\ \Delta Q\ \Delta t} \quad \textit{Action} \\
+\ & 1/4\,(q_{M,}{}^{P}\,p_{M,}{}^{P}{}_{t} - q_{M,}{}^{P}{}_{t}\,p_{M,}{}^{P}) && \Delta P\ \Delta P\ \Delta t \quad \textit{contribution} \\
+\ & 1/4\,(q_{M,}{}^{P}\,p_{M,Qt} + q_{M,Q}\,p_{M,}{}^{P}{}_{t} - q_{M,Qt}\,p_{M,}{}^{P} - q_{M,}{}^{P}{}_{t}\,p_{M,Q}) && \Delta Q\ \Delta P\ \Delta t \\
+\ & 1/4\,(q_{M,}{}^{P}\,p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\,p_{M,}{}^{P}) && \Delta Q\ \Delta P\ \Delta P \\
+\ & 1/4\,(q_{M,Q}\,p_{M,tt} - q_{M,tt}\,p_{M,Q}) && \Delta Q\ \Delta t\ \Delta t \\
+\ & 1/4\,(q_{M,}{}^{P}\,p_{M,tt} - q_{M,tt}\,p_{M,}{}^{P}) && \Delta P\ \Delta t\ \Delta t \\
+\ & \ldots && \}
\end{aligned}
$$

having used:

$$\Gamma_{M,Qtt} = q_{M,Qtt}\,p_{M} + 2q_{M,Qt}\,p_{M,t} + q_{M,Q}\,p_{M,tt}$$

$$\Gamma_{M,}{}^{P}{}_{tt} = q_{M,}{}^{P}{}_{tt}\,p_{M} + 2q_{M,}{}^{P}{}_{t}\,p_{M,t} + q_{M,}{}^{P}\,p_{M,tt}$$

which were developed earlier.

From the appendix it follows that only the highlighted terms contribute, namely:

$$1/4\,(q_{M,Q}{}^{P}\,p_{M,QQ} - q_{M,QQ}\,p_{M,Q}{}^{P})\ \mathbf{\Delta Q\ \Delta Q}$$

$$1/8\ (q_{M,Q}{}^{P}{}_{t}\ p_{M,QQ} + q_{M,Q}{}^{P}\ p_{M,Qt} - q_{M,QQ}\ p_{M,}{}^{P}{}_{t} - q_{M,Qt}\ p_{M,Q}{}^{P})\ \mathbf{\Delta Q\ \Delta t}$$

$$1/12\ i/\hbar\ (q_{M,Q}\ p_{M,QQ} - q_{M,QQ}\ p_{M,Q})\ \mathbf{\Delta Q\ \Delta Q\ \Delta Q}$$

$$1/4\ i/\hbar\ (q_{M,Q}\ p_{M,Qt} - q_{M,Qt}\ p_{M,Q})\ \mathbf{\Delta Q\ \Delta Q\ \Delta t}$$

Their nature can be discovered from recalling that (in the limit $\Delta t \to 0$) $p \sim (\Delta t)^{-1/2}$ as does P, which informs us that the leading stochastic terms contribute respectively like: Δt, $(\Delta t)^{3/2}$, Δt, $(\Delta t)^{3/2}$. This is because differentiating w.r.t. P induces a $(\Delta t)^{1/2}$. Considering the two remaining terms, namely:

$$1/4\ (q_{M,Q}{}^{P}\ p_{M,QQ} - q_{M,QQ}\ p_{M,Q}{}^{P})\ \mathbf{\Delta Q\ \Delta Q}$$

$$1/12\ i/\hbar\ (q_{M,Q}\ p_{M,QQ} - q_{M,QQ}\ p_{M,Q})\ \mathbf{\Delta Q\ \Delta Q\ \Delta Q}$$

which have leading behaviour that must then be of the form:

$$1/4\ F(Q,t)\ \mathbf{\Delta Q\ \Delta Q}$$

$$1/12\ i/\hbar\ G(Q,t)\ \mathbf{P\ \Delta Q\ \Delta Q\ \Delta Q}$$

i.e. order Δt.

Performing these integrals (see appendix) leads to leading contributions:

$$-1/4\ (\hbar/i)\ F(Q,t)\ \Delta t/\Lambda$$

$$1/4\ (\hbar/i)\ G(Q,t)\ \Delta t/\Lambda$$

where $1/2\Lambda$ is the coefficient preceding the p^2 term in the Hamiltonian. A distinction is then made between the case when this term is present, and as here when not (tackled as Lim $\Lambda \to \infty$). In the latter case the terms are lost trivially; while the former is contained in the example of a point canonical transformation, considered next. In this case the stochastic terms mutually cancel.

In actual fact we have allowed rather too many canonical

transformations; as those generating terms containing p^n $(n>2)$ are unphysical and lead to infinite contributions.

§VII Point Canonical Transformations

(an explicit example)

It is possible, in the special case of a point canonical transformation, *[Gervais and Jevicki, 1980]* to explicitly calculate the stochastic contributions. According to the previous results, these should sum to zero.

In the case of the point canonical transformation, only the $p_m^2\Delta t/2m(q_m)$ 'term' of the Hamiltonian need be considered, since this is the strongest term permissible (order Δt^0) and the only one that is active in the calculation of the order Δt effective potential V.

So look at:

$$-p_m^2\Delta t/2m(q_m) = -\Delta t/2m(q_M)\,[p_M^2$$
$$+ 1/4\; p_M\, p_{M,QQ}\; \mathbf{\Delta Q\,\Delta Q}$$
$$+ 1/2\; p_M\, p_{M,Q}{}^{P}\; \Delta Q\,\Delta P$$
$$+ 1/4\; p_M\, p_{M,}{}^{PP}\; \Delta P\,\Delta P$$
$$+ \ldots\quad]$$

Collecting all stochastic terms to be converted:

$$1/4\,(q_{M,Q}{}^{P}\, p_{M,QQ} - q_{M,QQ}\, p_{M,Q}{}^{P})\;\; \mathbf{\Delta Q\,\Delta Q}$$
$$+ 1/4\,(q_{M,}{}^{PP}\, p_{M,QQ} - q_{M,QQ}\, p_{M,}{}^{PP})\;\; \Delta Q\,\Delta P \qquad \textit{Jacobian}$$
$$+ 1/4\,(q_{M,}{}^{PP}\, p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\, p_{M,}{}^{PP})\;\; \Delta P\,\Delta P \qquad \textit{contribution}$$
$$+ \ldots$$

$$i/\hbar\,\{\;\; 1/12\,(q_{M,Q}\, p_{M,QQ} - q_{M,QQ}\, p_{M,Q})\;\; \mathbf{\Delta Q\,\Delta Q\,\Delta Q}$$
$$+ 1/4\;\; (q_{M,Q}\, p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\, p_{M,Q})\;\; \Delta Q\,\Delta Q\,\Delta P \qquad \dot{pq}$$
$$+ 1/4\;\; (q_{M,}{}^{P}\, p_{M,Q}{}^{P} - q_{M,Q}{}^{P}\, p_{M,}{}^{P})\;\; \Delta Q\,\Delta P\,\Delta P \qquad \textit{contribution}$$
$$+ 1/12\,(q_{M,}{}^{P}\, p_{M,}{}^{PP} - q_{M,}{}^{PP}\, p_{M,}{}^{P})\;\; \Delta P\,\Delta P\,\Delta P$$
$$+ \ldots$$

$$-\Delta t/2m(q_M)\,[\;\; 1/4\; p_M\, p_{M,QQ} \qquad \mathbf{\Delta Q\ \Delta Q}$$
$$+\; 1/2\; p_M\, p_{M,Q}{}^{P} \qquad \Delta Q\ \Delta P \qquad \textit{Hamiltonian}$$
$$+\; 1/4\; p_M\, p_{M,}{}^{PP} \qquad \Delta P\ \Delta P \qquad \textit{contribution}$$
$$+\ldots \qquad \;]\;\}$$

For the case of a point canonical transformation, consider the generating function $\boldsymbol{F}(q,P,t) \equiv F(q,Q,t) + QP$. So as shown earlier:

$$Q = (\partial \boldsymbol{F}/\partial P)_{qt} \qquad p = (\partial \boldsymbol{F}/\partial q)_{Pt} \qquad \mathbf{K = H + (\partial \boldsymbol{F}/\partial t)_{qP}}$$

leading to a general point canonical transformation generated by:

$$\boldsymbol{F}(q,P,t) = Q(q,t)\,P + G(q,t)$$

i.e.:

$$q = q(Q,t)$$

$$p = q_{,Q}{}^{-1}(Q,t)\,P + g(Q,t)$$

g being the inverse of G. Then:

$$q_{M,Q}{}^{P}\, p_{M,QQ} = 0$$
$$q_{M,QQ}\, p_{M,Q}{}^{P} = -\, q_{M,Q}{}^{-2}\, q_{M,QQ}{}^{2}$$
$$q_{M,Q}\;\; p_{M,QQ} = [2q_{M,Q}{}^{-2}\, q_{M,QQ}{}^{2} - q_{M,Q}{}^{-1}\, q_{M,QQQ}]\, P_M + q_{M,Q}\, g_{M,QQ}$$
$$q_{M,QQ}\, p_{M,Q} = -\, q_{M,Q}{}^{-2}\, q_{M,QQ}{}^{2}\, P_M + q_{M,QQ}\, g_{M,Q}$$
$$p_M \quad p_{M,QQ} = (q_{M,Q}{}^{-1}\, P_M + g_M)\,[(2q_{M,Q}{}^{-3}\, q_{M,QQ}{}^{2} - q_{M,Q}{}^{-2}\, q_{M,QQQ})\, P_M + g_{M,QQ}]$$

$$p_M{}^{2}/2m(q_M) \rightarrow (q_{M,Q}{}^{-1}\, P_M + g_M)^{2}/2m(q_M)$$

Carrying only contributing (order Δt) terms $\Longrightarrow$

$$i/\hbar\, \boldsymbol{V}(q_M)\,\Delta t = \quad 1/4 \qquad q_{M,Q}{}^{-2}\, q_{M,QQ}{}^{2} \qquad \mathbf{\Delta Q\ \Delta Q}$$
$$+\; i/12\hbar \qquad [3q_{M,Q}{}^{-2}\, q_{M,QQ}{}^{2} - q_{M,Q}{}^{-1}\, q_{M,QQQ}]\, P_M \qquad \mathbf{\Delta Q\ \Delta Q\ \Delta Q}$$
$$-\; i\Delta t/8m(q_M)\hbar \qquad [2q_{M,Q}{}^{-4}\, q_{M,QQ}{}^{2} - q_{M,Q}{}^{-3}\, q_{M,QQQ}]\, P_M{}^{2} \qquad \mathbf{\Delta Q\ \Delta Q}$$

In this case:

$$I = e^{i/\hbar (F_b - F_a)} \mathrm{Lim}_{N\to\infty} \int..\int \prod_{j=1,N-1} (dQ(j) dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + \text{Jacobian stochastic terms} + i/\hbar \text{ Action stochastic terms})$$

$$\exp[i/\hbar \{ P_M(k)(Q(k)-Q(k-1)) + (q_{M,Q}^{-2}(k) P_M^2(k)/2m(q_M) + \ldots)\Delta t \}]$$

to be compared against:

$$J = e^{i/\hbar (F_b - F_a)} \mathrm{Lim}_{N\to\infty} \int..\int \prod_{j=1,N-1} (dQ(j) dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} (1 + i/\hbar \, V(q_M(k)) \, \Delta t)$$

$$\exp[i/\hbar \{ P_M(k)(Q(k)-Q(k-1)) + (q_{M,Q}^{-2}(k) P_M^2(k)/2m(q_M) + \ldots)\Delta t \}]$$

evaluating the integrals to order Δt (see appendix, with $\alpha = m(q_M) q_{M,Q}^2$, a function of Q,t only) yields:

$$i\hbar \, \Delta t/4m(q_M) \{ \quad q_{M,Q}^{-4} \, q_{M,QQ}^2 - [3 q_{M,Q}^{-4} \, q_{M,QQ}^2 - q_{M,Q}^{-3} \, q_{M,QQQ}] + [2 q_{M,Q}^{-4} \, q_{M,QQ}^2 - q_{M,Q}^{-3} \, q_{M,QQQ}^{-1}] \}$$

$$= \emptyset$$

One might argue, in fact, that this constitutes a proof of invariance of the mid-point prescription under a **general** canonical transformation. This is because, by the group property, a general canonical transformation may be decomposed into successive q and p transformations. The general p transformation is obtained from the general q (point) transformation by

following it with an exchange transformation ($q \rightarrow P$, $p \rightarrow -Q$) which generates no additional stochastic terms.

§VIII General Canonical Transformations

Since no extra potential term is generated for the symmetric scheme in the transformation between the Hamiltonian and trivial Kamiltonian coherent state path integral; using the fact that canonical transformations form a group, one can make a general canonical transformation via the Hamilton-Jacobi transformation. In this way we see indirectly that there is no contribution generated by a general canonical transformation.

The argument leading to this point assumed the use of a physical Hamiltonian (one for which $H\Delta t$ is of order $(\Delta t)^p$, $(p\geq 0)$ in the path integral), and here it is understood that only canonical transformations that generate such Hamiltonians are considered.

Having achieved a Hamilton-Jacobi transformation one is lead to the path integral:

$$K(q_b,p_b,t_b|q_a,p_a,t_a) = e^{i/\hbar\,(\Gamma_b - \Gamma_a)}\,K(Q_b,P_b,t_b|Q_a,P_a,t_a)$$

where:

$$K(Q_b,P_b,t_b|Q_a,P_a,t_a) = \int\!\!\ldots\!\!\int \prod_{j=1,N-1} (dQ(j)dP_M(j)/2\pi\hbar)$$

$$\prod_{k=1,N} \exp[i/\hbar\,\{\,P_M(k)(Q(k)-Q(k-1))\,\}]$$

$$= \delta(Q_b - Q_a)\,\delta(P_b - P_a)$$

so that the amplitude becomes simply:

$$e^{i/\hbar\,(\Gamma_b - \Gamma_a)}$$

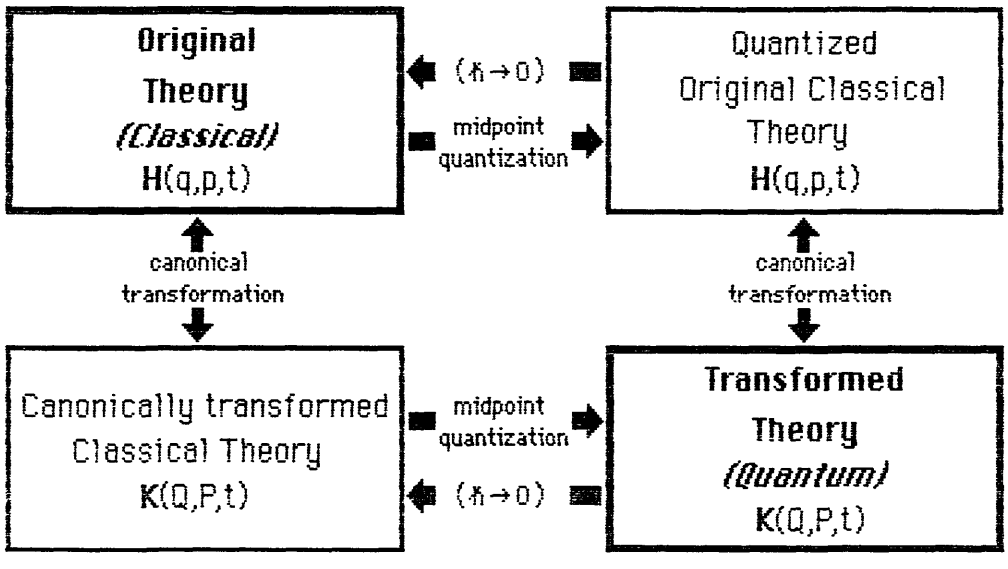
where Γ is a generating function of the Hamilton-Jacobi transformation, and the new coordinates (Q,P) are constant (determined from the end conditions of q,p). This is not a physical quantity (c.f. coherent states) and

has still to be converted to an amplitude between physical states.

§IX Conclusion

It would seem that within the symmetric scheme, no additional terms are generated by a general canonical transformation. This was explicitly demonstrated in the case of a point canonical transformation.

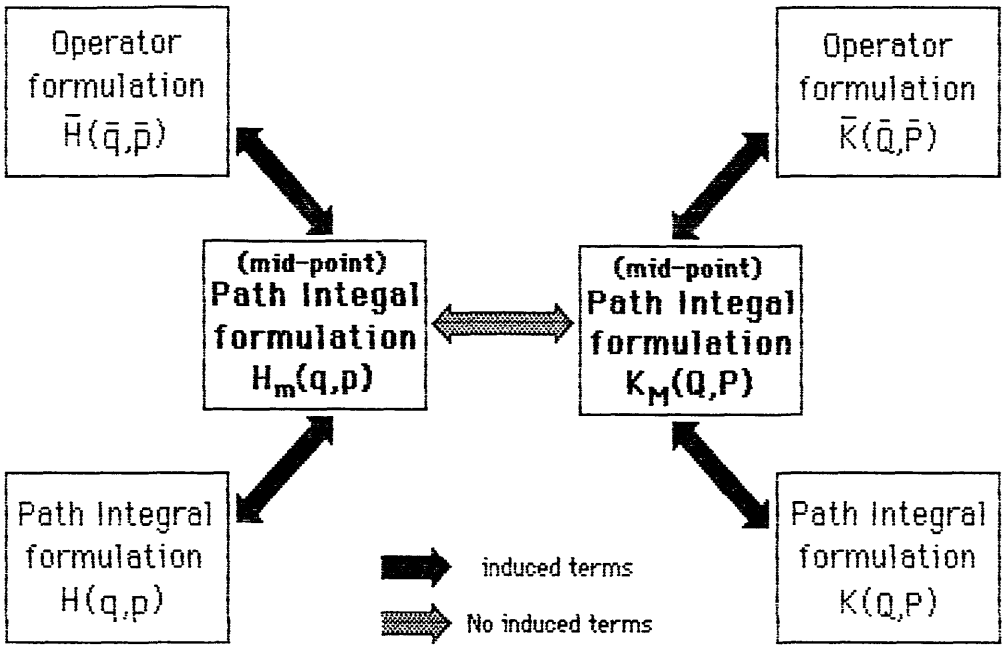
This suggests that the symmetric scheme is a canonically invariant prescription i.e. pictorially.



This allows a consistent quantization of a classical system regardless of which canonical variables are used in its description, as well as the use of the trivializing Hamilton-Jacobi transformation in quantum mechanics.

It should perhaps be remarked that the mid-point rule is favoured (not compelled) over others, in that it generates no additional terms during the canonical transformation. Note however, that to get into and from the mid-point scheme, stochastic $\hbar^2$ terms appear. The virtue of no terms occurring during the transformation is that the Hamiltonian is then

trivialized by the Hamilton-Jacobi transformation. The appearance of stochastic terms during the transformation would spoil this attempt (see figure below).



The Mid-Point Crossing

It is also not clear what a canonical transformation is outside of the mid-point scheme.

That this scheme is so well behaved and would seem to be the manner of starting point for making the path integral a well defined mathematical object *[Daubechies and Klauder, 1985]*, tends to indicate that it is a useful portrait of the path integral.

Appendix

Working out the general Gaussian integrals

By differentiating (w.r.t. ν or μ) the Gaussian integral:

$$\int..\int \prod_{j=1,N-1} (du(j)dv(j)/2\pi\hbar)\, \exp[i/\hbar \sum_{k=1,N}\{v(k)u(k) - v^2(k)\Delta t/2\alpha + \nu u(k) + \mu v(k)\}]$$

$$= \exp[-i/\hbar\, \{\, \nu^2\, \Delta t/2\alpha + \nu\mu\, \}]$$

one may develop:

Integral =

$$\int..\int \prod_{j=1,N-1} (du(j)dv(j)/2\pi\hbar)\ \textit{Integrand}\ \exp[i/\hbar \sum_{k=1,N}\{\, v(k)u(k) - v^2(k)\, \Delta t/2\alpha\, \}]$$

Integrand	Integral
1	1
$v^n \quad (n\geq 1)$	0
u	0
vu	$-(\hbar/i)$
$v^n u \quad (n\geq 2)$	0
u^2	$-(\hbar/i)\, \Delta t/\alpha$
vu^2	0
v^2u^2	$2(\hbar/i)^2$
$v^n u^2 \quad (n\geq 3)$	0
u^3	0
vu^3	$3(\hbar/i)^2\, \Delta t/\alpha$
v^2u^3	0
v^3u^3	$-6(\hbar/i)^3$
$v^n u^3 \quad (n\geq 4)$	0

etc.

These expressions continue to be valid to order Δt if α is a function of Q,t; since to this order they may be held constant at the mid-point value. Further, $(\partial/\partial\mu(k))_\nu - (\partial/\partial\mu(k-1))_\nu = \Delta t(\partial^2/\partial t\partial\mu)_\nu$ induces a Δv, and since all currents are held constant (at zero); so the contribution of Δv containing terms is null. It is integrals such as these that tell us that u (ΔQ) contributes with strength order $(\Delta t)^{1/2}$ and v (P) at order $(\Delta t)^{-1/2}$, excepting that for the presence of v's (P's) only (no u's (ΔQ's)) the contribution is zero when the currents are turned off.

From these arguments one concludes that the stochastic terms previously carried are all those that contribute to order Δt.

Chapter Four

Ambiguities in the Dirac Quantization Procedure

Dirac Quantization

(the method of classical analogy)

In this work, which is based on a paper by Chernoff *[1981]*, the Dirac quantization procedure is reviewed and derived from basic postulates, and the resulting ambiguities pointed out. This is relevant to the task of performing a canonical transformation in quantum mechanics; for if a quantization scheme is ambiguous, one cannot use it to induce a quantum canonical transformation from the classical object.

Dirac *[1958]* indicates how a quantum theory might be induced from the classical theory in its Hamiltonian formulation. It is perhaps interesting to note how a formulation so well suited to classical mechanics, namely the Hamiltonian (or modified) action principle with its use of action, Hamiltonian and phase space variables, should also be so suited to the quantum generalization; be it canonical or path integral quantization. Motivated by experimental results, with the need of a superposition principle and probability amplitudes, Dirac *[1958]* was led to representing states by vectors and observables by operators. Having got this far, one has still to determine the evolution (or dynamics) of the quantum system. An analogue with classical mechanics is most easily made when classical mechanics is displayed in terms of the Poisson bracket, which is defined for two classical dynamical variables by:

$$\{u,v\} \equiv (\partial u/\partial q)_p(\partial v/\partial p)_q - (\partial u/\partial p)_q(\partial v/\partial q)_p$$

where this quantity is independent of which canonical coordinates (in this case q and p) are being used *[Goldstein, 1980]*.

Since the Hamilton equations of motion may be written as:

$$\dot{p} = \{p,H\}$$
$$\dot{q} = \{q,H\}$$

so knowledge of the Poisson brackets determines the dynamics of the system.

The Poisson brackets have the following properties:

$$\{u,v\} = -\{v,u\}$$
Antisymmetry

$$\{u,c\} = 0$$

$$\{u_1+u_2,v\} = \{u_1,v\} + \{u_2,v\}$$
$$\{u,v_1+v_2\} = \{u,v_1\} + \{u,v_2\}$$
Linearity

$$\{u_1u_2,v\} = \{u_1,v\}u_2 + u_1\{u_2,v\}$$
$$\{u,v_1v_2\} = \{u,v_1\}v_2 + v_1\{u,v_2\}$$
Leibnitz

$$\{u,\{v,w\}\} + \{v,\{w,u\}\} + \{w,\{u,v\}\} = 0$$
Jacobi Identity

Now Dirac *[1958]* proposed the use of operators for the quantum theory and searched for a quantum analogue to the classical Poisson bracket. By **assuming** that this should satisfy the above properties of the classical Poisson bracket (now taking care of ordering), the quantum Poisson bracket is uniquely determined. This follows from considering:

$$\{u_1u_2,v_1v_2\}$$

and expanding it in two different ways using the 'Leibnitz' property.

$$\{\mathbf{u_1u_2},v_1v_2\}$$
$$= \{u_1,\mathbf{v_1v_2}\}u_2 + u_1\{u_2,\mathbf{v_1v_2}\}$$
$$= \{u_1,v_1\}v_2u_2 + v_1\{u_1,v_2\}u_2 + u_1\{u_2,v_1\}v_2 + u_1v_1\{u_2,v_2\}$$

and

$$\{u_1u_2,\mathbf{v_1v_2}\}$$
$$= \{\mathbf{u_1u_2},v_1\}v_2 + v_1\{\mathbf{u_1u_2},v_2\}$$
$$= \{u_1,v_1\}u_2v_2 + u_1\{u_2,v_1\}v_2 + v_1\{u_1,v_2\}u_2 + v_1u_1\{u_2,v_2\}$$

Equating these leads to:

$$\{u_1,v_1\}(u_2v_2-v_2u_2) = (u_1v_1-v_1u_1)\{u_2,v_2\}$$

Since this condition holds with u_1 and v_1 independent of u_2 and v_2, we have.

$$[u_1,v_1] = i\hbar\{u_1,v_1\}$$
$$[u_2,v_2] = i\hbar\{u_2,v_2\}$$

where $\hbar$ is a constant determined from experiment (the case of $\hbar\neq0$ can only be satisfied by non-commuting variables). In this way we identify the quantum Poisson bracket to be commutation, an operation which also satisfies the other Poisson bracket properties. If it is then further **assumed** *[Dirac, 1958]* that the quantum Poisson brackets obey the same equation as the classical Poisson brackets; the quantum dynamics is specified (see below), and a route to quantization formulated.

To demonstrate that this quantization scheme is in fact ambiguous, define the 'Dirac association' $\mathbb{Q}$ as:

Quantum operator ≡ $\mathbb{Q}$(Classical object)

The postulate motivated above **(P1)** then reads as:

Quantum operator commutator ≡ $i\hbar\,\mathbb{Q}$(Classical Poisson bracket)

i.e. $[\mathbb{Q}(f),\mathbb{Q}(g)] \equiv i\hbar\,\mathbb{Q}(f,g)$

and adding one further assumption **(P2)**

$$\mathbb{Q}(1) \equiv \bar{1}$$

The above postulates specify directly only how to obtain the quantum operator for 1, and one might presume that it is necessary to separately

specify the quantum operators corresponding to polynomials in q and p as Von Neumann did.

It will in fact be shown that the quantum operators for polynomials follow from these postulates alone. They turn out to be generally inconsistent in that not all the quantum operators are uniquely specified. Differing answers deviate by terms in Planck's constant.

To show all this we begin by deriving (from the unmodified Dirac postulates P1, P2) operators for q^2, p^2 and pq in terms of the operators for q and p.

Starting from:

$$\{q,p\} = 1$$

it follows by 'Dirac' *[1958]* (P1 and P2) that:

$$[\bar{q},\bar{p}] = i\hbar\,\bar{1}$$

where

$$\bar{q} \equiv \mathbb{Q}(q),\ \bar{p} \equiv \mathbb{Q}(p)$$

these being left unspecified.

Consider the object of interest (the quantum operator for p^2):

$$\bar{\alpha} \equiv \mathbb{Q}(p^2)$$

Now classically:

$$\{q,p^2\} = 2p \qquad \{p,p^2\} = 0$$

which by 'Dirac' implies:

$$[\bar{q},\bar{\alpha}] = 2i\hbar\bar{p} \qquad [\bar{p},\bar{\alpha}] = \bar{0}$$

it follows that $\bar{\alpha} = \bar{p}^2 + \bar{K}$ where $\bar{K}$ commutes with $\bar{q}$ and $\bar{p}$ (and so anything else) i.e.

$$\mathbb{Q}(p^2) = \bar{p}^2 + \bar{K}$$

similarly

$$\mathbb{Q}(q^2) = \bar{q}^2 + \bar{L}$$

Now to determine $\mathbb{Q}(pq)$ in terms of $\bar{p}$ and $\bar{q}$, look at:

$$(q^2,p^2) = 4pq$$

Let

$$\bar{\zeta} \equiv \mathbb{Q}(pq)$$

then by 'Dirac':

$$[\bar{q}^2 + \bar{L},\bar{p}^2 + \bar{K}] = 4i\hbar\bar{\zeta}$$

since $\bar{K}$ and $\bar{L}$ commute with $\bar{q}$ and $\bar{p}$, they mutually commute. Having assumed that they, like all variables, are a function of $\bar{q}$ and $\bar{p}$ alone. This is seen by Taylor expanding one of (but not both) $\bar{L}$ or $\bar{K}$.

$$[\bar{q}^2,\bar{p}^2] = 4i\hbar\bar{\zeta}$$

$$\bar{q}[\bar{q},\bar{p}]\bar{p} + \bar{q}\bar{p}[\bar{q},\bar{p}] + \bar{p}[\bar{q},\bar{p}]\bar{q} + [\bar{q},\bar{p}]\bar{p}\bar{q} = 4i\hbar\bar{\zeta}$$

$$2(\bar{q}\bar{p} + \bar{p}\bar{q}) = 4\bar{\zeta}$$

having used

$$[\bar{q},\bar{p}] = i\hbar\bar{1}$$

therefore

$$\mathbb{Q}(pq) = (\bar{p}\,\bar{q} + \bar{q}\,\bar{p})/2$$

To further determine $\mathbb{Q}(p^2)$ consider:

$$(pq,p^2) = 2p^2$$

which by 'Dirac' yields:

$$[\,(\bar{p}\bar{q} + \bar{q}\bar{p})/2,\bar{p}^2 + \bar{K}\,] = 2i\hbar(\bar{p}^2 + \bar{K})$$

$$[\bar{p}\bar{q} + \bar{q}\bar{p},\bar{p}^2]/2 = 2i\hbar(\bar{p}^2 + \bar{K})$$

$$(\bar{p}^2[\bar{q},\bar{p}] + \bar{p}[\bar{q},\bar{p}]\bar{p} + \bar{p}[\bar{q},\bar{p}]\bar{p} + [\bar{q},\bar{p}]\bar{p}^2\,)/2 = 2i\hbar(\bar{p}^2 + \bar{K})$$

$$2\bar{p}^2 = 2(\bar{p}^2 + \bar{K})$$

Therefore

$$\bar{K} = 0$$

similarly

$$\bar{L} = 0$$

Hence:

$$\mathbb{Q}(p^2) = \bar{p}^2$$

$$\mathbb{Q}(q^2) = \bar{q}^2$$

$$\mathbb{Q}(qp) = (\bar{q}\bar{p} + \bar{p}\bar{q})/2$$

From this follows the quantum operators for the higher polynomials in q and p. Although it was realized by Groenewold (1946) that starting from $\mathbb{Q}(p^2) \equiv \bar{p}^2$ and $\mathbb{Q}(q^2) \equiv \bar{q}^2$ one could develop quantum operators for other polynomials, these starting operators were given as a supplementary postulate to P1 and P2. Here we have shown that they in fact follow.

To expose the inconsistency we follow the work of Groenewold (1946). Ambiguities arise when determining operators corresponding to higher order polynomials. This line of argument may be continued to determine the operators corresponding to higher order polynomials. For example:

$$\{q^3,q\} = 0 \qquad \{q^3,p\} = 3q^2$$

leads to:

$$\mathbb{Q}(q^3) = \bar{q}^3 + \bar{J}$$

where $\bar{J}$ commutes with $\bar{q}$ and $\bar{p}$, and:

$$\{q^3,pq\}$$

implies that:

$$\mathbb{Q}(q^3) = \bar{q}^3$$

similarly

$$\mathbb{Q}(p^3) = \bar{p}^3$$

$$\mathbb{Q}(pq^2) = 1/2\,(\bar{p}\bar{q}^2 + \bar{q}^2\bar{p}) \qquad \text{from } \{q^3,p^2\} = 6q^2p$$

$$\mathbb{Q}(p^2q) = 1/2\,(\bar{p}^2\bar{q} + \bar{q}\bar{p}^2) \qquad \text{from } \{q^2,p^3\} = 6qp^2$$

with no ambiguities arising up to this point.

Problems arise with terms such as q^2p^2 which have more than one Poisson bracket origin:

$$1/9\,\{q^3,p^3\} = q^2p^2$$

$$1/3\,\{pq^2,p^2q\} = q^2p^2$$

which each lead to a corresponding operator for q^2p^2:

$$\bar{q}^2\bar{p}^2 - 2i\hbar\bar{q}\bar{p} - 2/3\,\bar{i}\hbar^2$$

and

$$\bar{q}^2\bar{p}^2 - 2i\hbar\bar{q}\bar{p} - 1/3\,\bar{i}\hbar^2$$

which differ by $O(\hbar^2)$.

It is in this way that, in general, the Dirac quantization procedure is ambiguous (or inconsistent). It does not uniquely fix the operator ordering.

The difference between this derivation over others is the claim that only P1 and P2 were needed as initial postulates and nothing additional.

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† An hour after writing this acknowledgement it was suggested that Dr. Dowker might be my external examiner. This being the case, I leave it to his imagination as to what I may have written

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