International Journal of Theoretical Physics, Vol. 39, No. 1, 2000

Quantum Mechanics on Path Space and Point Interactions on a Circle

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Received August 31, 1999

In this paper we analyze quantum mechanics formulated in terms of wave functions defined on what may be called the *path space*, rather than the traditional physical space. An explicit theory of quantum mechanics on a circle is given which can be readily applied to describe a superconducting current flowing around a superconducting ring with a Josephson junction. The path space approach provides an elegant and natural interpretation of the current flow across the Josephson junction. A striking feature of the theory is the emergence of a superselection rule inherent in the fundamental structure of the theory, without needing additional ad hoc assumptions. Other point interactions are discussed, including a δ-potential on a circle and the standard Kronig–Penny model of a crystal lattice on the real line.

1. INTRODUCTION

In 1931 Dirac [1] pointed out a striking ambiguity in the wave function $\phi(x)$, namely that the position probability density function $|\phi(x)|^2$ only determines the wave function up to an arbitrary phase factor. Writing the wave function in the form

$$\phi(x) = R(x)e^{\lambda S(x)}, \qquad \lambda = i/\hbar \tag{1}$$

where $R(x)$ and $S(x)$ are real-valued functions of x, it is clear that adding a constant to the phase function S produces no physically observable consequences. In other words, it is the phase difference which is physically significant, not the actual value of the phase. The situation resembles the potential function in classical mechanics, i.e., it is only the potential difference which is significant. This realization opens the way to generalize quantum mechanics

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0020-7748/00/0100-0127$18.00/0

to embody multivalued wave functions. A formal approach is through the introduction of a path space and functions defined on the path space. There have been quite a number of general formulations along such lines. In this paper we shall endeavor to keep the mathematics to a bare minimum by avoiding general and abstract discussions. Instead we shall confine ourselves to concrete examples which have direct physical applications, making full use of some of the existing general formulations [2–4].

2. PATH SPACE

Let $\mathbb{M}$ be a Riemannian manifold and m a point in $\mathbb{M}$. In the standard formulation of quantum mechanics, with $\mathbb{M}$ as the physical space, we would first introduce complex-valued functions $\phi(m)$ on $\mathbb{M}$ which are square-integrable with respect to a given volume element $d\mu(m)$ on $\mathbb{M}$, i.e.,

$$\int_{\mathbb{M}} \phi^*(m)\phi(m)\, d\mu(m) \leq \infty \tag{2}$$

With the usual definition of scalar product

$$\langle\phi|\psi\rangle = \int_{\mathbb{M}} \phi^*(m)\psi(m)\, d\mu(m) \tag{3}$$

these functions form a scalar product space which can be completed to form a Hilbert space, which will be denoted by $\mathcal{H}(\mathbb{M})$. A function ϕ in $\mathcal{H}(\mathbb{M})$ is normalized if

$$\int_{\mathbb{M}} \phi^*(m)\phi(m)\, d\mu(m) = 1 \tag{4}$$

All functions we refer to from $\mathcal{H}(\mathbb{M})$ are assumed to be normalized from now on. Functions ϕ in $\mathcal{H}(\mathbb{M})$ give rise to probability density functions $|\phi(m)|^2$, and any two functions ϕ_1, ϕ_2 in $\mathcal{H}(\mathbb{M})$ differing by an arbitrary local phase[2] $\alpha_{1,2}(m)$,i.e.,

$$\phi_1(m) = e^{i\alpha_{1,2}(m)}\phi_2(m) \tag{5}$$

give rise to the same probability density function since $|\phi_1(m)|^2 = |\phi_2(m)|^2$. For a quantum particle moving in $\mathbb{M}$, the standard approach is to associate the Hilbert space $\mathcal{H}(\mathbb{M})$ with the particle and ϕ in $\mathcal{H}(\mathbb{M})$ as possible wave functions, with $|\phi(m)|^2$ interpreted as the position probability density function of the particle on $\mathbb{M}$. We can see that there is no observational distinction

[2] The phase is local in that its value is dependent on $m \in \mathbb{M}$. If it has a constant value for all $m \in \mathbb{M}$ it is called global.

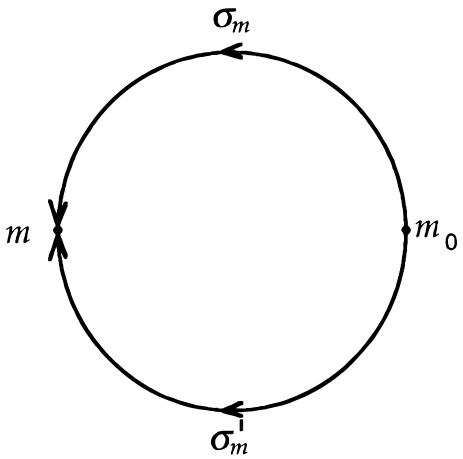

Fig. 1. Two paths in $\mathbb{M}$ joining m_0 to m.

between wave functions differing by an arbitrary global phase factor since it does not affect any expectation values.[3] As a consequence of this, the states of the system are identified one-to-one with one-dimensional subspaces of $\mathcal{H}(\mathbb{M})$ [6, 7].

The phase indeterminacy can be given a systematic and geometric formulation which can take into account specific topological properties of $\mathbb{M}$. Dirac already realized this possibility and proposed a kind of path space formulation of quantum mechanics which we now discuss [1].

Given a manifold $\mathbb{M}$, choose some point $m_0 \in \mathbb{M}$, which may be called the origin and is to be held fixed from now on. We assume that $\mathbb{M}$ is connected so that any point m in $\mathbb{M}$ may be joined to m_0 by a path.[4] Let σ_m be any path from m_0 to m. There is an infinite set Π_m of paths

$$\Pi_m = \{\sigma_m, \sigma'_m, \sigma''_m, \ldots\} \tag{6}$$

linking m_0 to m, of which σ_m and σ'_m are but two (see Fig. 1).

We shall denote by

$$\Pi(\mathbb{M}) = \{\Pi_m : m \in \mathbb{M}\} \tag{7}$$

the set of all paths from the origin m_0 to all points $m \in \mathbb{M}$, and refer to $\Pi(\mathbb{M})$ as the *path space* on the manifold $\mathbb{M}$ centered at the origin m_0.

Two paths may be different in a variety of ways. There is a sophisticated scheme to classify paths, i.e., homotopy theory. We shall not digress into

[3] A local phase will generally affect the expectation value, albeit not the position probability density function.

[4] A path in a manifold means a differentiable curve in the manifold.

this branch of mathematics. Instead we shall confine ourselves to manifolds $\mathbb{M}$ of one and two dimensions where we can classify paths in an intuitive and pictorial manner. Moreover, many mesoscopic and macroscopic quantum systems are confined to one- or two-dimensional physical spaces. Two paths σ_m and σ'_m on $\mathbb{M}$ are said to be homotopic or homotopically equivalent if they can be continuously deformed into one another. Whether two paths are homotopic depends on the topological nature of $\mathbb{M}$. If $\mathbb{M}$ is the plane $\mathbb{R}^2$, then any two paths, as depicted in Fig. 1, are homotopic. However, if $\mathbb{M}$ is a plane with a hole, i.e., with a region removed, then not all the paths are homotopic. Figure 2 serves to illustrate this situation. Here, not all paths are homotopic; the missing hole spoils the topology of the plane, so that not all paths are continuously deformable into one another. We have to examine how the paths enclose the hole.

The paths σ'_m and σ''_m in Fig. 2a are homotopic, but neither is homotopic to the path σ_m because of the missing hole. The path σ_m is not homotopic to the path $\sigma_{m,1}$ in Fig. 2b, which is formed by a loop (closed curve) $\mathscr{L}_1$ around the hole in an anticlockwise direction once followed by σ_m, since the loop encloses the hole, it cannot be contracted to the point m_0.

Path σ_m in Fig. 2a is not homotopic to the path $\sigma_{m,-1}$ in Fig. 3, since $\sigma_{m,-1}$ is made of a loop $\mathscr{L}_{-1}$ around the hole in the clockwise direction once followed by σ_m.

It is generally the case that two paths are homotopic if they go around the origin in the same way. Before we classify paths we introduce a classification of the loops starting and ending at m_0 in $\Pi(\mathbb{M})$:

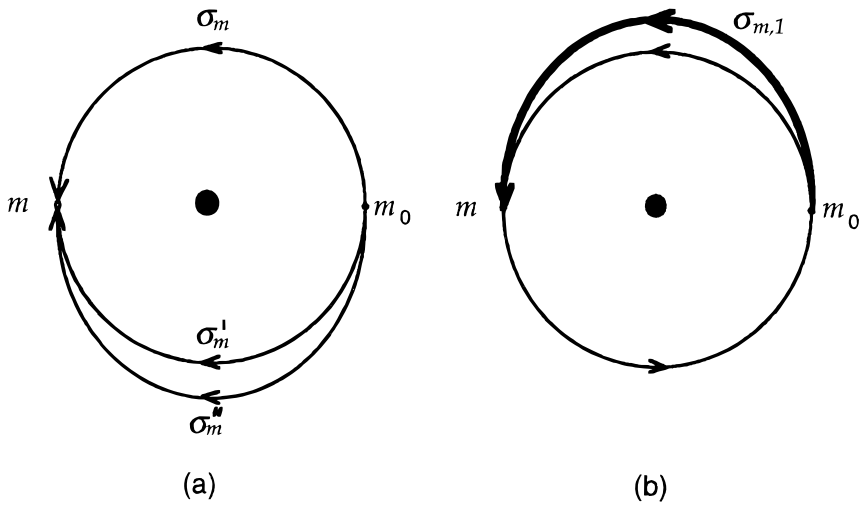

Fig. 2. Paths in $\mathbb{M}$.

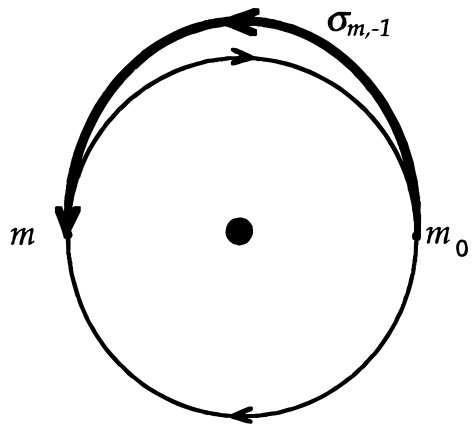

Fig. 3. The path $\sigma_{m,-1}$.

Class 0: $[\mathscr{L}_0] = \{$all loops not enclosing the hole$\}$

Class 1: $[\mathscr{L}_1] = \{$all loops circling the hole once in an anticlockwise direction$\}$

Class -1: $[\mathscr{L}_{-1}] = \{$all loops circling the hole once in a clockwise direction$\}$

$\vdots$

Class l: $[\mathscr{L}_l] = \{$all loops circling the hole l times in an anticlockwise direction, $\ell > 0\}$

Class $-l$: $[\mathscr{L}_{-l}] = \{$all loops circling the origin l times in a clockwise direction, $l > 0\}$

$\vdots$

These are called homotopic classes of loops, and the integer l of the class $[\mathscr{L}_l]$ is known as the winding number of the class. A member of $[\mathscr{L}_l]$ will be denoted by $\mathscr{L}_l$. We shall use this classification of loops to classify paths.

Let $[\sigma_{m,0}]$ denote the set of all paths from m_0 to m curving around the hole in an anticlockwise direction, but not enclosing the hole. The path σ_m of Fig. 1a is an element of this set. A general path in Π_m will either be in the set $[\sigma_{m,0}]$ or will circle the hole a number of times before ending up at the point m. For example, in Fig. 2b the path $\sigma_{m,1}$ is a sequence of two curves $\mathscr{L}_1 \in [\mathscr{L}_1]$ followed by $\sigma_m \in [\sigma_{m,0}]$. We shall denote this symbolically by

$$\sigma_{m,1} = \sigma_m * \mathscr{L}_1 \tag{8}$$

Similarly, for the path $\sigma_{m,-1}$ in Fig. 3 we have

$$\sigma_{m,-1} = \sigma_m * \mathscr{L}_{-1} \tag{9}$$

It follows that any path in Π_m which is homotopic to $\sigma_{m,1}$ is of the form of

a sequence of two curves, one from $[\mathscr{L}_1]$ followed by one from $[\sigma_{m,0}]$. We can collect all paths in Π_m homotopic to $\sigma_{m,1}$ shown in Fig. 2 to form a class to be denoted by

$$[\sigma_{m,1}] = [\sigma_{m,0}] * [\mathscr{L}_1] \tag{10}$$

Generally, we can divide all the paths in Π_m into such classes according to whether they are homotopic to a sequence of two curves, one from $[\mathscr{L}_l]$ followed by one from $[\sigma_{m,0}]$. Such classes are to be denoted by

$$[\sigma_{m,l}] = [\sigma_{m,0}] * [\mathscr{L}_l], \qquad l = 0, \pm 1, \pm 2, \ldots \tag{11}$$

with a member of the class denoted by $\sigma_{m,l}$.

Clearly the homotopic nature of the path space is independent of the choice of the origin.

3. FUNCTIONS ON PATH SPACE

Consider a mapping f of the set of paths on $\mathbb{M}$ to the set of complex numbers $\mathbb{C}$:

$$f: \quad \Pi(\mathbb{M}) \to \mathbb{C} \quad \text{by} \quad \sigma_{m,\,l} \to f(\sigma_{m,l}) \in \mathbb{C} \tag{12}$$

Such a mapping may be regarded as a complex-valued function on the path space $\Pi(\mathbb{M})$. The value of the function $f(\sigma_{m,l})$ depends on the endpoint m as well as the path $\sigma_{m,l}$. In other words, $f(\sigma_{m,l})$ may be viewed as a multivalued function on $\mathbb{M}$.

We do not want arbitrary functions on $\Pi(\mathbb{M})$. Instead we want a smaller set of functions on $\Pi(\mathbb{M})$ satisfying the following five physically motivated conditions [2–4]:

1. *Single-valueness up to a phase as functions on* $\mathbb{M}$. A function f on $\Pi(\mathbb{M})$ is said to be single-valued up to a phase as a function on $\mathbb{M}$ if its modulus $|f(\sigma_{m,l})|$ depends only on the endpoint m, not on the path linking the origin to m. This condition ensures that $f(\sigma_{m,l})$ can give rise to a well-defined probability density function $|f(\sigma_{m,l})|^2$ on $\mathbb{M}$ whenever $|f(\sigma_{m,l})|^2$ is integrable and normalized with respect to a chosen volume element for integration on $\mathbb{M}$.

This requirement means that the path dependence of the function will be present only in the phase, i.e., given two paths $\sigma'_{m,l'}$ and $\sigma_{m,l}$, there exists a real-valued function $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ such that

$$f(\sigma'_{m,l'}) = \{\exp[i\vartheta(\sigma'_{m,l'}, \sigma_{m,l})]\}\, f(\sigma_{m,l}) \tag{13}$$

We call $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ a *path difference function* between paths $\sigma'_{m,l'}$ and $\sigma_{m,l}$. Generally $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ may be different for different f.

2. *Universal path difference function*. Two functions f and g on $\Pi(\mathbb{M})$ are said to share a path difference function $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ if

$$f(\sigma'_{m,l'}) = \{\exp[i\vartheta(\sigma'_{m,l'}, \sigma_{m,l})]\}f(\sigma_{m,l}) \tag{14}$$

$$g(\sigma'_{m,l'}) = \{\exp[i\vartheta\ (\sigma'_{m,l'}, \sigma_{m,l})]\}g(\sigma_{m,l}) \tag{15}$$

The path difference function in Eq. (13) is said to be *universal* to a set of functions on $\Pi(\mathbb{M})$ if this path difference function is shared by all the functions in the set.

A set of functions on $\Pi(\mathbb{M})$ which are single-valued up to a phase as functions on $\mathbb{M}$ and which share a path difference function $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ form a vector space. To appreciate this, let f and g be two functions on $\Pi(\mathbb{M})$. Let us try to define their sum $f + g$ as a function on $\Pi(\mathbb{M})$ by

$$(f + g)(\sigma_{m,l}) = f(\sigma_{m,l}) + g(\sigma_{m,l}) \tag{16}$$

Then we must have

$$(f + g)\,(\sigma'_{m,l'}) = f(\sigma'_{m,l'}) + g(\sigma'_{m,l'}) \tag{17}$$

If they share a path difference function, then their sum, as defined by Eq. (16), will share the same path difference function, i.e.,

$$\begin{aligned}(f + g)(\sigma'_{m,l'}) &= f(\sigma'_{m,l'}) + g(\sigma'_{m,l'}) \\ &= \{\exp[i\vartheta(\sigma'_{m,l'}, \sigma_{m,l})]\}\ f(\sigma_{m,l}) \qquad (18) \\ &\quad + \{\exp[i\vartheta(\sigma'_{m,l'}, \sigma_{m,l})]\}g(\sigma_{m,l}) \\ &= \{\exp[i\vartheta(\sigma'_{m,l'}), \sigma_{m,l})]\}(f(\sigma_{m,l}) + g(\sigma_{m,l})) \qquad (19) \\ &= \{\exp[i\vartheta(\sigma'_{m,l'}, \sigma_{m,l})]\}(f + g)(\sigma_{m,l})\end{aligned}$$

The desire to form a vector space is motivated by the need for a superposition principle in quantum mechanics. In other words, the state space of an orthodox quantum system must be a vector space so that we can form a superposition of two different states. It follows that if we are to use functions on path space to represent the states of a given quantum system, we must choose one definite universal path difference function $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ to be shared by all its states. A new universal path difference function would then correspond to a new physical system and vice versa. This will have important consequences on the properties of quantum theory formulated on path space functions.

The path difference function $\vartheta(\sigma'_{m,l'}, \sigma_{m,l})$ may be regarded as a measure of the difference between the paths $\sigma'_{m,l'}$, and $\sigma_{m,l}$. We expect $\vartheta(\sigma'_{m,l'},$

$\sigma_{m,l}) = 0$ if $\sigma'_{m,l'}$ and $\sigma_{m,l}$ are identical. A natural generalization of this to homotopic paths is given below.

3. *Homotopic functions*. A function f on $\Pi(\mathbb{M})$ is called a *homotopic function* if at every point $m \in \mathbb{M}$ the path difference function for any two homotopic paths $\sigma'_{m,l}$, and $\sigma_{m,l}$ satisfies

$$\vartheta(\sigma'_{m,l}, \sigma_{m,l}) = 0 \tag{20}$$

so that

$$f(\sigma'_{m,l}) = \{\exp[i\vartheta(\sigma'_{m,l}, \sigma_{m,l})]\}f(\sigma_{m,l}) = f(\sigma_{m,l}) \tag{21}$$

for homotopic paths.

We are now in a position to relate functions on the path space $\Pi(\mathbb{M})$ to functions on $\mathbb{M}$ in the following manner:

(a) For each $m \in \mathbb{M}$ choose a direct path from m_0 to m, $\sigma_{m,0} \in [\sigma_{m,0}]$. Then define a function ϕ on these direct paths for all $m \in \mathbb{M}$. Since the paths are chosen and fixed from the start, this function ϕ becomes a function on $\mathbb{M}$, i.e., it is a single-valued function on $\mathbb{M}$ with a unique value $\phi(m)$ at each point $\mathbb{M}$.

(b) Choose a path difference function $\vartheta(\sigma_{m,l}, \sigma_{m,0})$ and define a function f on $\Pi(\mathbb{M})$ in terms of ϕ by

$$f(\sigma_{m,l}) = \{\exp[i\vartheta(\sigma_{m,l}, \sigma_{m,0})]\}\phi(m) \tag{22}$$

In general f is multivalued on $\mathbb{M}$, i.e., the value of f at $\mathbb{M}$ changes with the winding number l. If the manifold $\mathbb{M}$ is the plane $\mathbb{R}^2$ without any holes, the situation simplifies considerably, since all paths from m_0 to m are homotopic to $\sigma_{m,0}$. It follows that a homotopic function f on the path space $\Pi(\mathbb{M})$ coincides with a single-valued function ϕ on $\mathbb{M}$. There is then no point in generalizing functions on $\mathbb{M}$ to $\Pi(\mathbb{M})$. Quantum mechanics formulated in terms of homotopic wave functions on the path space $\Pi(\mathbb{M})$ will be identical to the usual theory in terms of wave functions on the physical space $\mathbb{M}$.

When $\mathbb{M}$ does not have the topology of $\mathbb{R}$ or $\mathbb{R}^2$ a theory based on the path space will have new features. Before we can do this we need to introduce further conditions on the path space functions.

In standard quantum theory on $\mathbb{M}$, any wave function can be given a phase factor without affecting the state described by the wave function, as long as the phase is a global one. To reflect this property we shall introduce the following item.

4. *Globally homotopic functions*. A homotopic function f on $\Pi(\mathbb{M})$ is said to be a *global* one if the path difference function amounts to the addition of a phase which is dependent on the winding numbers l and l' and independent

of $m \in \mathbb{M}$. This means that the path difference function $\vartheta(\sigma'_{m,\ell'}, \sigma_{m,\ell})$ for any pair of curves $\sigma_{m,\ell}$ and $\sigma'_{m,\ell'}$ is of the form

$$\vartheta(\sigma'_{m,\ell'}, \sigma_{m,\ell}) = \vartheta(\sigma'_{m',\ell'}, \sigma_{m',\ell}) = \vartheta(\ell', \ell) \tag{23}$$

We can rewrite Eq. (22) as

$$f(\sigma_{m,\ell}) = e^{i\vartheta(\ell,0)}\phi(m) \tag{24}$$

To arrive at the value $f(\sigma_{m,\ell})$, we can imagine taking the value of $\phi(m)$ around a loop of the hole l times, with each loop around resulting in an additional phase. We desire the path difference function to vary in a well-behaved manner as we increase the winding number. This is made clear in the next item.

5. *Additivity of the path difference function.* A path difference function is said to be *additive* if it increases by the same amount as we increase the winding number by 1, i.e., $\vartheta(\ell, 0)$ is of the form

$$\vartheta(l, 0) = l\hbar\lambda \qquad \text{for some real parameter} \quad \lambda \in [0, 2\pi) \tag{25}$$

So, each time we loop the hole, we simply pick up a phase λ; this phase is to be referred to as a *universal path difference constant*.

Let $\mathcal{F}_\lambda(\Pi(S^1))$ denote the set of functions on $\Pi(S^1)$ satisfying the five properties listed above with a chosen universal path difference constant λ. Since every function f in $\mathcal{F}_\lambda(\Pi(S^1))$ takes the same value for homotopic paths, we can reduce the set $\mathcal{F}_\lambda(\Pi(S^1))$ of functions on the space of paths to a corresponding set of functions on the space $\{[\sigma_{m,l}]\}$ of homotopic classes of paths. However, for notational convenience we shall retain the set $\mathcal{F}_\lambda(\Pi(S^1))$ and talk about functions on the space of paths rather than on the space of homotopic classes of paths.

4. QUANTIZATION IN THE PATH SPACE $\Pi(S^1)$

Let us consider setting up a quantum theory on the circle $\mathbb{M} = S^1$ of radius r. The circle S^1 is topologically similar to the plane $\mathbb{R}^2$ with a hole, so our previous constructs apply with little alteration. We take as our coordinate on S^1 the angle variable $\theta \in [0, 2\pi)$, which measures the angular distance from some fixed point m_0 on S^1 coordinated by $\theta = 0$ to any other point m coordinated by θ.

4.1. The Hilbert Space

We now construct a Hilbert space out of functions defined on the path space $\Pi(S^1)$. We start with the set $\mathcal{F}_\lambda(\Pi(S^1))$ of functions on $\Pi(S^1)$ satisfying

the five properties listed in the preceding section with a chosen universal path difference constant λ. A function $f_\lambda \in \mathscr{F}_\lambda(\Pi(S^1))$ will then be of the form

$$f_\lambda(\sigma_{m,l}) = e^{il\hbar\lambda}\phi(m), \qquad m \in S^1 \tag{26}$$

where ϕ is a single-valued function on S^1. We can conveniently rewrite functions in $\mathscr{F}_\lambda(\Pi(S^1))$ as multivalued functions of the coordinate θ, i.e., as a multivalued function $F_\lambda(\theta, l)$ of angle θ and winding number l of the path $\sigma_{m,l}$:

$$f_\lambda(\sigma_{m,l}) = F_\lambda(\theta, l) = e^{il\hbar\lambda}\phi(\theta), \qquad \theta \in [0, 2\pi) \tag{27}$$

Sharing the same universal path difference constant λ, these functions can be added to form a vector space. An l-independent scalar product can also be defined as

$$\langle f_\lambda | f'_\lambda \rangle_\lambda = \langle F_\lambda | F'_\lambda \rangle_\lambda = \int_0^{2\pi} F^*_\lambda(\theta, l)\, F'_\lambda(\theta, l)\, d\mu(\theta) \tag{28}$$

The volume element is taken as $d\mu(\theta) = d\theta$. This scalar product space can be completed in the usual way to form a Hilbert space $\mathscr{H}_\lambda(\Pi(S^1))$. We have in effect a set of Hilbert spaces $\mathscr{H}_\lambda = \mathscr{H}_\lambda(\Pi(S^1))$ parameterized by the universal path difference constant λ. Each $\mathscr{H}_\lambda$ contains functions which change phase by the same amount λ when taken around a single loop anticlockwise. It should be stressed that we cannot superpose functions from different $\mathscr{H}_\lambda$'s. Let

$$F_\lambda(\theta, l) = e^{il\hbar\lambda}\phi(\theta) \in \mathscr{H}_\lambda, \qquad F'_{\lambda'}(\theta, l) = e^{il\hbar\lambda'}\phi'(\theta) \in \mathscr{H}_{\lambda'} \tag{29}$$

If we carry out a formal sum, we get

$$F_\lambda(\theta, l) + F'_{\lambda'}(\theta, l) = e^{il\hbar\lambda}\,\phi(\theta) + e^{il\hbar\lambda'}\,\phi'(\theta) \tag{30}$$

which belongs to neither $\mathscr{H}_\lambda(\Pi(S^1))$ nor $\mathscr{H}_{\lambda'}(\Pi(S^1))$.

Let us examine the description of the functions in $\mathscr{H}_\lambda(\Pi(S^1))$ in more detail before we introduce operators. The first thing to note is that looping around the circle can be described by introducing an extended coordinate variable θ_{ex} which varies from $-\infty$ to ∞. The first loop around anticlockwise corresponds to θ_{ex} taking values in the range $[2\pi, 4\pi)$, and the first loop around clockwise corresponds to values in the range $[-2\pi, 0)$ and so on. So, we can imagine functions in $\mathscr{H}_\lambda$ to be functions defined for $\theta_{ex} \in \mathbb{R} = (-\infty, \infty)$.

We conclude that functions in $\mathscr{H}_\lambda(\Pi(S^1))$ can be treated explicitly in one of the following forms:

1. As single-valued functions $f_\lambda(\sigma_{m,l})$ on the path space $\Pi(S^1)$
2. As multivalued functions $F_\lambda(\theta, l)$ on the circle S^1

3. As single-valued functions $\Psi_\lambda(\theta_{ex})$ on $\mathbb{R}$ related to $F_\lambda(l, \theta)$, and hence to $f_\lambda(\sigma_{m,l})$ by

$$\Psi_\lambda(\theta_{ex}) = F_\lambda(\theta, l) = f_\lambda(\sigma_{m,l}) = e^{i\ell\hbar\lambda}\,\phi(\theta), \qquad \text{where} \quad \theta_{ex} = \theta + 2l\pi \tag{31}$$

In the rest of the paper we shall always adhere to the notation $\theta_{ex} \in (-\infty, \infty)$, $\theta \in [0, 2\pi)$, and the relation $\theta_{ex} = \theta + 2l\pi$, whenever these variables are mentioned. The reasons for introducing $\Psi_\lambda(\theta_{ex})$ are twofold: first, we are more familiar in dealing with single-valued functions on $\mathbb{R}$ than multivalued functions on S^1 or functions on path space, and, more importantly, the variable θ_{ex} embodies a notion of continuity of flow as we go around and around the circle, a notion very useful in appreciating some important mathematical models of physical situations, such as a current flowing around a conducting ring.

To help us appreciate the whole situation, we can compare the Hilbert spaces $\mathcal{H}_\lambda(\Pi(S^1))$ with the familiar space L^2 $(0, 2\pi)$ of square-integrable functions $\psi(\theta)$ on the open interval $(0, 2\pi)$ with respect to the volume element $d\theta$. First, introduce a formal translation operator $\hat{T}_\alpha$ acting on $\Psi_\lambda(\theta_{ex})$ by

$$\hat{T}_\alpha \Psi_\lambda(\theta_{ex}) = \Psi_\lambda(\theta_{ex} - \alpha) \tag{32}$$

The effect is literally to translate the function $\Psi_\lambda(\theta_{ex})$ by the amount α. Translating the function by a loop around S^1 can be effected by

$$\hat{T}_{2\pi} \Psi_\lambda(\theta_{ex}) = \Psi(\theta_{ex} - 2\pi) = F_\lambda(\theta, l + 1) \tag{33}$$

We shall consider $\mathcal{H}_{\lambda=0}$ and $\mathcal{H}_{\lambda\neq 0}$ separately as follows:

1. $\mathcal{H}_{\lambda=0}$: We can establish a natural mapping between $\mathcal{H}_{\lambda=0}$ and $L^2(0, 2\pi)$. First, each continuous function $\psi(\theta) \in L^2(0, 2\pi)$ can be related to a $\Psi_{\lambda=0}(\theta_{ex}) \in \mathcal{H}_{\lambda=0}$ by

$$\Psi_{\lambda=0}(\theta_{ex}) = \psi(\theta), \qquad \theta_{ex} \neq 2l\pi \tag{34}$$

$$\Psi_{\lambda=0}(0) = \psi(0_+) = \lim_{\theta\to 0} \psi(\theta) \tag{35}$$

$$\Psi_{\lambda=0}(2l\pi) = \Psi_{\lambda=0}(0) \tag{36}$$

When translated by 2π, $\Psi_{\lambda=0}(\theta_{ex})$ just repeat themselves:

$$\hat{T}_{2\pi} \Psi_{\lambda=0}(\theta_{ex}) = \Psi_{\lambda=0}(\theta_{ex}) \tag{37}$$

These functions are called *periodic* in θ_{ex} on account of Eqs. (36) and (37). A typical example is

$$\Psi_{\lambda=0}(\theta_{ex}) = e^{i\ell\hbar n\theta} \qquad \text{for some integer} \quad n \tag{38}$$

However, not every function is periodic in a continuous manner in θ_{ex}, i.e., being periodic and continuous in θ_{ex}. Consider the following continuous function in $L^2(0, 2\pi)$:

$$\overline{\psi}(\theta) = e^{i\ell\hbar\beta\theta/2\pi}, \qquad \text{where } \beta \text{ is a real number, but not an integer multiple of } \pi \tag{39}$$

The corresponding function $\overline{\Psi}_{\lambda=0}(\theta_{ex})$ is given by

$$\overline{\Psi}_{\lambda=0}(\theta_{ex}) = e^{i\hbar\beta\theta/2\pi}, \qquad \theta_{ex} \neq 2l\pi \tag{40}$$

$$\overline{\Psi}_{\lambda=0}(2l\pi) = \overline{\Psi}_{\lambda=0}(0) = \overline{\psi}(0_+) = 1 \tag{41}$$

There is a discontinuity at $\theta_{ex} = 2l\pi$ since

$$\overline{\Psi}_{\lambda=0}(2\pi_-) = \lim_{\theta_{ex}\to 2\pi_-} \overline{\Psi}_{\lambda=0}(\theta_{ex}) = e^{i\hbar\beta} \neq \overline{\Psi}_{\lambda=0}(2\pi) = 1 \tag{42}$$

Having to be periodic, the function $\overline{\Psi}_{\lambda=0}$ is discontinuous at $\theta_{ex} = 2l\pi$. We can conveniently symbolize the relations defined by (34) and (36) between $L^2(0, 2\pi)$ and $\mathcal{H}_{\lambda=0}$ by writing[5]

$$\Psi_{\lambda=0} = \hat{U}_{\lambda=0}\psi \tag{43}$$

Clearly $\hat{U}_{\lambda=0}$ may be regarded as a unitary operator relating $L^2(0, 2\pi)$ to $\mathcal{H}_{\lambda=0}$.

2. $\mathcal{H}_{\lambda\neq 0}$: Again this can be mapped to $L^2(0, 2\pi)$, but in a different manner. Each continuous function $\psi(\theta) \in L^2(0, 2\pi)$ can be mapped to $\Psi_{\lambda\neq 0}(\theta_{ex}) \in \mathcal{H}_{\lambda\neq 0}$ by

$$\Psi_{\lambda\neq 0}(\theta_{ex}) = e^{i\hbar l\lambda}\psi(\theta), \qquad \theta_{ex} \neq 2l\pi \tag{44}$$

$$\Psi_{\lambda\neq 0}(0) = \psi(0_+) \tag{45}$$

$$\Psi_{\lambda\neq 0}(2l\pi) = e^{i\hbar l\lambda}\,\Psi_{\lambda\neq 0}(0) \tag{46}$$

These functions are called *quasiperiodic*. A typical example is

$$\Psi_{\lambda\neq 0}(\theta_{ex}) = e^{i\hbar(n+\lambda/2\pi)\theta} \qquad \text{for some integer } n \tag{47}$$

Again there are discontinuities generally. For example, in (39) we have

$$\overline{\Psi}_{\lambda\neq 0}(\theta_{ex}) = e^{il\hbar\lambda}\overline{\psi}(\theta) = e^{il\hbar\lambda}\,e^{i\ell\hbar\beta\theta/2\pi}, \qquad \theta_{ex} \neq 2l\pi \tag{48}$$

$$\overline{\Psi}_{\lambda\neq 0}(2l\pi) = e^{il\hbar\lambda}\overline{\Psi}(0_+) = e^{il\hbar\lambda} \tag{49}$$

[5] Since continuous functions ψ in $L^2(0, 2\pi)$ form a dense set, relations (34) and (36) can be continuously extended to give a definition of a unique bounded operator $\hat{U}_{\lambda=0}$ on the entire Hilbert space $L^2(0, 2\pi)$.

Clearly there are discontinuities at $\theta_{ex} = 2l\pi$. For example, we have

$$\overline{\Psi}_{\lambda\neq 0}(2\pi_-) = e^{i\hbar\lambda}e^{i\beta} \neq \overline{\Psi}_{\lambda\neq 0}(2\pi) = e^{i\hbar\lambda} \tag{50}$$

We can similarly symbolize the relations defined by (44)–(46) between $L^2(0, 2\pi)$ and $\mathcal{H}_{\lambda\neq 0}$ by writing

$$\Psi_{\lambda\neq 0} = \hat{U}_{\lambda\neq 0}\psi \tag{51}$$

Again $\hat{U}_{\lambda\neq 0}$ may be regarded as a unitary operator relating $L^2(0, 2\pi)$ to $\mathcal{H}_{\lambda\neq 0}$.

To define self-adjoint differential operators in $L^2(0, 2\pi)$, we usually introduce a differential expression to act on the dense subset $C_0^\infty(0, 2\pi)$ of infinitely differentiable functions of compact support in $(0, 2\pi)$, i.e., for each $\varphi(\theta) \in C_0^\infty(0, 2\pi)$ there is an interval $[\theta_1, \theta_2] \subset (0, 2\pi)$ such that $\varphi(\theta) = 0$ for θ lying outside $[\theta_1, \theta_2]$. This would produce symmetric operators, and we can then go on to unearth their selfadjoint extensions. In our present situation we shall proceed similarly in $\mathcal{H}_\lambda(\Pi(S^1))$. First we shall single out a similar set of smooth functions in $\mathcal{H}_\lambda(\Pi(S^1))$. Let $C_{0;\lambda}^\infty(\Pi(S^1))$ be the set of functions $\Phi_\lambda(\theta_{ex})$ in $\mathcal{H}_\lambda(\Pi(S^1))$ defined in terms of $\varphi(\theta) \in C_0^\infty(0, 2\pi)$ according to Eq. (44)–(46). These functions possess the following properties:

1. $\Phi_\lambda(\theta_{ex})$ is infinitely differentiable with respect to θ_{ex}.
2. For every $\Phi_\lambda(\theta_{ex})$ there exists a closed interval $[\theta_1, \theta_2] \subset (0, 2\pi)$ such that $\Phi_\lambda(\theta_{ex})$ vanishes for every value of θ_{ex} corresponding to θ lying outside the interval $[\theta_1, \theta_2]$.

Clearly $C_{0;\lambda}^\infty(\Pi(S^1))$ is a dense subset of $\mathcal{H}_\lambda(\Pi(S^1))$, being the unitary equivalence of the subset $C_0^\infty(0, 2\pi)$, which is known to be dense in $L^2(0, 2\pi)$.

Intuitively we can see that functions defined on the path space $\Pi(S^1)$ can be perceived to be defined on a helix (Fig. 4). The extended angle variable θ_{ex} can be visualized as varying along the helix, and a differentiation with respect to θ_{ex} as a differentiation along the helix. The values of such functions at corresponding points on successive loops differ by a phase factor.

Note that although functions $\Phi_\lambda(\theta_{ex})$ are formally defined for the entire range of values of $\theta_{ex} \in (-\infty, \infty)$, the scalar product involves an integral only over the range $(0, 2\pi)$:

$$\langle\Phi_\lambda(\theta_{ex})|\Phi_\lambda(\theta_{ex})\rangle_\lambda = \int_0^{2\pi} \Phi_\lambda^*(\theta_{ex})\Phi_\lambda(\theta_{ex})\, d\theta_{ex} \tag{52}$$

4.2. The Position and Momentum Operators in $\mathcal{H}_\lambda(\Pi(S^1))$

We can define the angular position operator on the Hilbert space $\mathcal{H}_\lambda(\Pi(S^1))$ as either $\hat{\theta}_\lambda$,

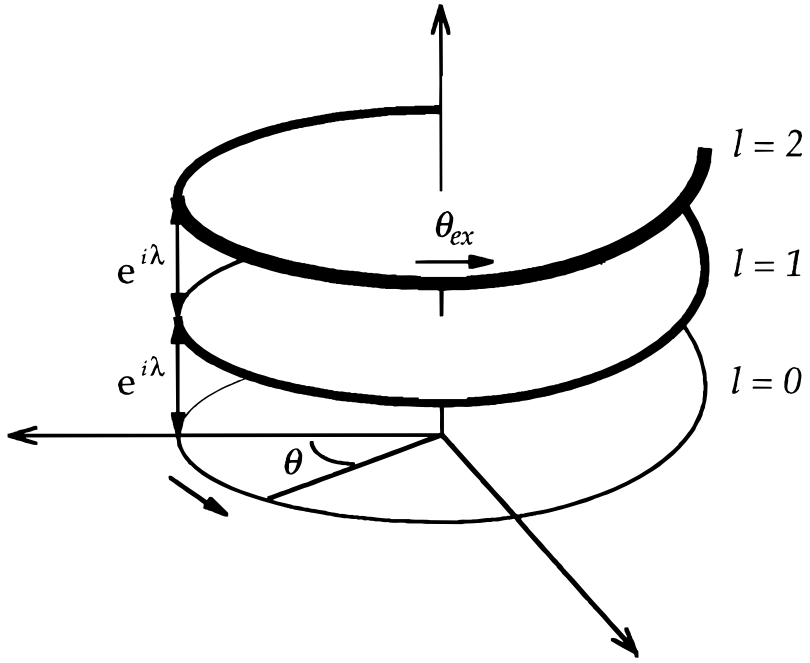

Fig. 4. The path space forms a helix.

$$\hat{\theta}_\lambda F_\lambda(\theta, l) = \theta F_\lambda(\theta, l) \tag{53}$$

or $\hat{\theta}_{ex,\lambda}$,

$$\hat{\theta}_{ex,\lambda}\Psi_\lambda(\theta_{ex}) = \theta_{ex}\Psi_\lambda(\theta_{ex}) \tag{54}$$

with expectation values similarly given either by

$$\langle F_\lambda(\theta, l)|\hat{\theta}_\lambda F_\lambda(\theta, l)\rangle_\lambda = \int_0^{2\pi} F_\lambda^*(\theta, l)\theta\, F_\lambda(\theta, l)\, d\theta \tag{55}$$

or by

$$\langle \Psi_\lambda(\theta_{ex})|\hat{\theta}_{ex,\lambda}\Psi_\lambda(\theta_{ex})\rangle_\lambda = \int_0^{2\pi} \Psi_\lambda^*(\theta_{ex})\theta_{ex}\Psi_\lambda(\theta_{ex})\, d\theta_{ex} \tag{56}$$

This angular position operator is a bounded self-adjoint operator which acts in the same way in all $\mathscr{H}_\lambda(\Pi(S^1))$, independent of λ. One can say that there is a unique angular position operator on the circle S^1, denoted simply by $\hat{\theta}$ or $\hat{\theta}_{ex}$. Note that although θ_{ex} as a variable has a formal range of $(-\infty, \infty)$ of values, the operator expression $\hat{\theta}_{ex}$ has only finite expectation values.

It is more involved when we come to define a self-adjoint (linear) momentum operator; momentum operators are unbounded, a fact requiring careful specification of their domains of operation. Let us first recall the operator $\hat{p}_0 = (-i\hbar/r)d/d\theta$ acting on the dense domain $C_0^\infty(0, 2\pi)$ in the Hilbert space $L^2(0, 2\pi)$. It is well known that this operator is only symmetric, but it admits a one-parameter family of self-adjoint extensions $\hat{p}_\lambda = (-i\hbar/r)d/d\theta$ characterized by their domains $\mathcal{D}_\lambda(0, 2\pi) \subset L^2(0, 2\pi)$ which consist of absolutely continuous functions $\varphi_\lambda(\theta)$ on the interval $(0, 2\pi)$ satisfying the following quasiperiodic boundary condition [8]:

$$\varphi(2\pi_-) = e^{i\lambda}\varphi(0_+), \qquad \lambda \in [0, 2\pi) \tag{57}$$

In $\mathcal{H}_\lambda(\Pi(S^1))$ we can similarly introduce an operator $\hat{\wp}_{0;\lambda}$ acting on $C^\infty_{0;\lambda}(\Pi(S^1)) \subset \mathcal{H}_\lambda(\Pi(S^1)$ by

$$\hat{\wp}_{0;\lambda}\Phi_\lambda(\theta_{ex}) = -\frac{i\hbar}{r}\frac{\partial\Phi_\lambda(\theta_{ex})}{\partial\theta_{ex}}, \qquad \Phi_\lambda(\theta_{ex}) \in C^\infty_{0;\lambda}(\Pi(S^1)) \tag{58}$$

This operator is symmetric, and not self-adjoint in $\mathcal{H}_\lambda(\Pi(S^1))$. We now need to investigate possible self-adjoint extensions to $\hat{\wp}_{0;\lambda}$ in $\mathcal{H}_\lambda(\Pi(S^1))$. Let us now consider the following two cases:

1. In the Hilbert space $\mathcal{H}_{\lambda=0}(\Pi(S^1))$. Since functions in $\mathcal{H}_{\lambda=0}(\Pi(S^1))$ satisfy the periodic boundary condition, the natural self-adjoint extension is the one corresponding to $\hat{p}_\lambda$ in $L^2(0, 2\pi)$ with $\lambda = 0$. In other words, we have a self-adjoint extension to $\hat{\wp}_{0\lambda=0}$, denoted by $\hat{\wp}_{\lambda=0}$, defined on the domain consisting of functions in $\mathcal{H}_{\lambda=0}(\Pi(S^1))$ which are absolutely continuous[6] in $\theta_{ex} \in \mathbb{R}$. Note that the continuity requirement implies that functions in the domain of operation of $\hat{\wp}_{\lambda=0}$ are periodic in a continuous manner in θ_{ex}.
2. In Hilbert space $\mathcal{H}_{\lambda\neq0}(\Pi(S^1))$. Since functions in $\mathcal{H}_{\lambda\neq0}(\Pi(S^1))$ satisfy the quasiperiodic boundary condition, the natural self-adjoint extension is the one corresponding to $\hat{p}_\lambda$ in $L^2(0, 2\pi)$ with $\lambda \neq 0$. In other words we have a self-adjoint extension to $\hat{\wp}_{0;\lambda\neq0}$, denoted by $\hat{\wp}_{\lambda\neq0}$, defined on the domain consisting of functions in $\mathcal{H}_{\lambda\neq0}(\Pi(S^1))$ which are absolutely continuous in θ_{ex}. These functions satisfy quasiperiodic boundary conditions (46) in a continuous manner in θ_{ex}.

Note that $\hat{\wp}_\lambda$ possesses a purely discrete spectrum $p_{\lambda,n}$ with normalized eigenfunctions $\varphi_{p_{\lambda,n}}$ given by

$$\varphi_{p_{\lambda,n}}(\theta_{ex}) = (1/\sqrt{2\pi})\exp[i\hbar(n + \lambda/2\pi)\theta_{ex}] \tag{59}$$

with $p_{\lambda,n} = (1/r)\hbar(n + \lambda/2\pi)$ for some integer n.

[6] Absolutely continuous functions are once differentiable almost everywhere [8].

The striking feature here is that it is possible to single out a *preferred* extension $\hat{\wp}_{\lambda\neq 0}$ acting on absolutely continuous functions in each Hilbert space $\mathcal{H}_{\lambda\neq 0}(\Pi(S^1))$, a situation not available in $L^2(0, 2\pi)$.

4.3. Kinetic Energy Operators in $\mathcal{H}_\lambda(\Pi(S^1))$

The system we have in mind is a quantum circuit system where an electron or a current in a superconductor is confined to flow around a circular conducting ring. There are two scenarios: (1) the ring is cut so that a very narrow insulating gap appears to interrupt the otherwise continuous ring, and (2) we have a continuous ring without any cut. Clearly the first case is more complex and more interesting. An electron or a superconducting current is capable of tunneling through the insulating gap, known as a tunneling junction or a Josephson junction, respectively, to maintain a steady current flow. Physically an insulating gap in the ring represents a perturbation or a local interaction to the free flow of the electron or a superconducting current at the cut. Such an interaction is referred to as a *point interaction*. A systematic and rigorous mathematical analysis of point interactions is available [12]. Traditional treatments consist in introducing a Hamiltonian with a kind of δ-function potential [13, 14] or some ad hoc theory [15] put in by hand. Now, a ring with a cut at $\theta = 0$, denoted by S^1_c, may be visualized as a circle with the point $\theta = 0$ removed. We can establish a theory on the Hilbert space $L^2(S^1_c)$, since we can identify $L^2(S^1_c)$ naturally with $L^2(0, 2\pi)$. To obtain a kinetic energy operator in $L^2(0, 2\pi)$ we start with the differential operator $\hat{K}_0$ on $C_0^\infty(0, 2\pi)$:

$$\hat{K}_0 = -\frac{\hbar^2}{2mr^2}\frac{\partial^2\psi(\theta)}{\partial\theta^2}, \qquad \psi(\theta) \in C_0^\infty(0, 2\pi) \tag{60}$$

This operator is symmetric. An obvious self-adjoint extension is simply

$$\hat{K}_\lambda = \frac{1}{2m}\hat{p}_\lambda^2 \tag{61}$$

However, $\hat{K}_0$ possesses a large number of other self-adjoint extensions, some of which will be discussed in what follows [11].

Clearly we can transfer all the technical results from $L^2(0, 2\pi)$ to the Hilbert space $\mathcal{H}_\lambda(\Pi(S^1))$ in a unitary manner using the unitary operator $\hat{U}_\lambda$ introduced earlier. We shall illustrate this by constructing an explicit theory to model the Josephson effect in a superconducting ring interrupted by a narrow cut. This result would demonstrate that a path space approach is a natural way to proceed.

4.4. A Model Theory of Josephson Effect in $\mathscr{H}_\lambda(\Pi(S^1))$

Within $L^2(0, 2\pi)$ there is a class of self-adjoint extensions $\hat{K}_{a,b}$ to $\hat{K}_0$ which are characterized by two real parameters a, b in the sense that the extension operator $\hat{K}_{a,b}$ acts on a domain $\mathscr{D}_{a,b} \in L^2(0, 2\pi)$ consisting of twice-differentiable functions $\psi(\theta)$ in $L^2(0, 2\pi)$ satisfying the following boundary conditions [11]:

$$\psi'(2\pi_-) = a\psi(2\pi_-) + b\psi(0_+) \tag{62}$$

$$\psi'(0_+) = -a\psi(0_+) - b\psi(2\pi_-) \tag{63}$$

where the prime represents differentiation, i.e., $\psi'(\theta) = d\psi(\theta)/d\theta$. To transfer these results in $L^2(0, 2\pi)$ to $\mathscr{H}_\lambda(\Pi(S^1))$, we can write down the corresponding operators in $\mathscr{H}_\lambda(\Pi(S^1))$ by

$$\hat{\mathscr{H}}_{a,b;\lambda} = \hat{U}_\lambda \hat{K}_{a,b} \hat{U}_\lambda^\dagger \tag{64}$$

and through $\hat{U}_\lambda$ we can write down the corresponding boundary conditions at $\theta_{ex} = 2\pi$ for the functions in the domain of $\hat{\mathscr{H}}_{a,b;\lambda}$:

$$\Psi'_\lambda(2\pi_-) = a\,\Psi_\lambda(2\pi_-) + be^{-i\lambda}\Psi_\lambda(2\pi_+) \tag{65}$$

$$e^{-i\lambda}\Psi'_\lambda(2\pi_+) = -ae^{-i\lambda}\Psi_\lambda(2\pi_+) - b\Psi_\lambda(2\pi_-) \tag{66}$$

The resulting self-adjoint operator in $\mathscr{H}_\lambda(\Pi(S^1))$ will be denoted by $\hat{\mathscr{H}}_{a,b;\lambda}$.

In a superconductor the electrons form pairs known as Cooper pairs which go around the superconductor to form a measurable electrical current known as a supercurrent. The totality of these Cooper pairs constitutes what is known as the *condensate*, which can tunnel through the Josephson junction to form a stable direct current. We can model such a physical system in the Hilbert space $\mathscr{H}_\lambda(\Pi(S^1))$. An electrical current is caused by the condensate going around and around the circle. In the standard macroscopic wave function approach [15] the condensate as a whole can be represented by a single quasiparticle. To describe this quasiparticle in the Hilbert space $\mathscr{H}_\lambda(\Pi(S^1))$ we would identify (1) the quasiparticle's position with the extended angular position operator $\hat{\theta}_{ex}$ which has a formal range of values $(-\infty, \infty)$, (2) the quasiparticle's (linear) momentum with the operator $\hat{\wp}_\lambda$ in $\mathscr{H}_\lambda(\Pi(S^1))$, and (3) the quasiparticle's state with a normalized function $\Psi_\lambda(\theta_{ex}) \in \mathscr{H}_\lambda(\Pi(S^1))$.

To have a current flow we require the state to be an eigenfunction of the momentum operator $\hat{\wp}_\lambda$ in $\mathscr{H}_\lambda(\Pi(S^1))$, i.e., $\varphi_{p_{\lambda,n}}(\theta_{ex})$ given by Eq. (59), since an electrical current is proportional to the momentum [10]. To maintain a stable and time-independent current the state must be a stationary state, i.e., it must be an eigenfunction of the Hamiltonian of the system. In the traditional treatment an ad hoc arrangement has to be devised to set up a Hamiltonian for this superconducting system [15]. In our present theory, all

we need is to take the self-adjoint operator $\hat{\mathcal{H}}_{a,b;\lambda}$ in $\mathscr{H}_\lambda(\Pi(S^1))$ specified by boundary conditions (65), (66) as the Hamiltonian. The requirement that $\varphi_{p_{\lambda,n}}$ be an eigenfunction of $\hat{\mathcal{H}}_{a,b;\lambda}$ acting as the Hamiltonian means that $\varphi_{p_{\lambda,n}}$ must satisfy the self-adjointness boundary conditions (65), (66). Substituting $\varphi_{p_{\lambda,n}}$ into (65, 66) gives

$$0 = a + b\cos\lambda \tag{67}$$

$$p_{\lambda,n} = (\hbar b/r)\sin\lambda \tag{68}$$

The parameter a is seen to be dependent on λ and the other parameter b, i.e., $a = -b\cos\lambda$. Equation (68) then leads to

$$p_{\lambda,n} = p_0 \sin\lambda, \qquad p_0 = \hbar b/r \tag{69}$$

This in effect is the famous Josephson equation, when we take the supercurrent to be proportional to $p_{\lambda,n}$ [10, 11]. The physical interpretation is transparent now. The wave function $\varphi_{p_{\lambda,n}}(\theta_{ex})$ describing the system can be regarded as a continuous single-valued function of the extended position variable θ_{ex}. When the quasiparticle passes the junction in completing a loop, i.e., θ_{ex} increases by 2π, the phase of the wave function increases smoothly by λ. This phase is the all-important quantity here since it determines the magnitude of the supercurrent through $p_{\lambda,n}$. The traditional description in terms of functions of θ will have to consider multivalued functions on S^1 where the wave function changes abruptly at the junction.

4.5. Superselection Rules

In the case of a superconducting current going around in a circle discussed above, the current is of a macroscopic magnitude and there is no evidence of any state being a superposition of states corresponding to different supercurrent, e.g., there is no superposition of $\varphi_{p_{\lambda,n}}(\theta_{ex})$ and $\varphi_{p_{\lambda',n}}(\theta_{ex})$ corresponding to currents with different phase constants λ and λ'. This can be explained by the existence of a superselection rule forbidding such a superposition [10, 11]. There has been a lot of controversy about superselection rules ever since they were introduced to tackle the quantum measurement problem [5], on account of the difficulty in establishing a superselection rule within orthodox quantum mechanics. There have been many attempts to derive superselection rules based on various physical arguments. Here we have a derivation not based on an ad hoc argument, but directly on the fundamental structure of the theory. Quantum mechanics on path space automatically generates a whole family of Hilbert spaces $\mathscr{H}_\lambda(\Pi(S^1))$ in such a way that functions from different spaces $\mathscr{H}_\lambda(\Pi(S^1))$ and $\mathscr{H}_{\lambda'}(\Pi(S^1))$ cannot be added together, as shown in the argument following Eq. (30). In other words, the

theory has a built-in superselection rule forbidding any superposition of functions from different spaces of the family. This would then explain why, physically, there is no superposition of $\varphi_{P_{\lambda,n}}(\theta_{ex})$ and $\varphi_{P_{\lambda',n}}(\theta_{ex})$ corresponding to currents with different phase constants λ and λ'. One can include superselection rules explicitly in the theory by forming a direct integral Hilbert space

$$\mathscr{H}^{\oplus} = \int^{\oplus} \mathscr{H}_{\lambda}(\Pi(S^1))\, d\mu(\lambda) \tag{70}$$

A systematic formulation of superselection rules in terms of direct integral Hilbert spaces and a justification of the superselection rule in superconductivity in terms of standard microscopic BCS theory have recently been presented by Wan *et al.* [18].

4.6. Circular Motion in a δ-Potential

Within $L^2(0, 2\pi)$ there is a class of self-adjoint extensions $\hat{K}_\delta$ to $\hat{K}_0$ given by the following boundary conditions (Appendix):

$$-\frac{2mV_0}{\hbar^2}\,\psi(2\pi_-) = \psi'(2\pi_-) - e^{i\lambda}\,\psi'(0_+), \qquad V_0 > 0 \tag{71}$$

$$-\frac{2mV_0}{\hbar^2}\,e^{i\lambda}\,\psi(0_+) = \psi'(2\pi_-) - e^{i\lambda}\,\psi'(0_+) \tag{72}$$

When these are transferred to $\mathscr{H}_\lambda(\Pi(S^1))$, using $\hat{U}_\lambda$, we get

$$-\frac{2mV_0}{\hbar^2}\,\Psi(2l\pi_-) = \Psi'(2l\pi_-) - \Psi'(2l\pi_+) \tag{73}$$

$$-\frac{2mV_0}{\hbar^2}\,\Psi(2l\pi_+) = \Psi'(2l\pi_-) - \Psi'(2l\pi_+) \tag{74}$$

These are the standard boundary conditions for a repulsive δ-potential centered at $\theta_{ex} = 2l\pi$ [12–14, 18]. It follows that we can visualize $\hat{K}_\delta$ acting as a Hamiltonian with a simple point interaction in the form of a repulsive δ-potential of strength V_0 centered[7] at the cut in S^1_c. The corresponding

[7] Intuitively, such a Hamiltonian may be written as

$$-\frac{\hbar^2}{2mr^2}\frac{d^2}{d\theta^2} + V_0\,\delta(\theta)$$

operator $\hat{\mathcal{H}}_{\delta;\lambda} = \hat{U}_\lambda \hat{K}_\delta \hat{U}_\lambda^\dagger$ in $\mathcal{H}_\lambda(\Pi(S^1))$ admits the following eigenfunctions:

$$\Psi(\theta_{ex}) = Ae^{i\hbar l\lambda}\left(e^{ik\theta} + \left(\frac{e^{i\lambda} - e^{2ik\pi}}{e^{-2ik\pi} - e^{i\lambda}}\right)e^{-ik\theta}\right), \qquad \theta_{ex} \neq 2l\pi \tag{75}$$

where A is a normalization constant, and k is a real constant related to λ and V_0 by

$$k = -\frac{mV_0}{\hbar^2}\left(\frac{\sin 2k\pi}{\cos 2k\pi - \cos\lambda}\right) \tag{77}$$

The corresponding eigenvalues are $E = (\hbar k)^2/2m$. An attractive δ-potential can be similarly constructed.

Surprising as it may seem, a self-adjoint extension of a symmetric kinetic energy operator can behave like a Hamiltonian with an effective potential. We have recently demonstrated that a large class of point interactions for one-dimensional systems on the real line $\mathbb{R}$ can be identified with various self-adjoint extensions to the kinetic energy operator on the real line with a cut because they are both characterized by boundary conditions [16]. The characterization of point interactions by boundary conditions at the cut spans a comprehensive range of physical effects. Another example of these is seen in the following section.

All these just reinforce a fundamental assumption of quantum mechanics that observables should be represented by self-adjoint operators, if at all possible [17].

4.7. Circular Motion in a δ'-Potential

Another simple point interaction involves a so-called δ'-potential. Consider a self-adjoint extension $\hat{K}_{\delta'}$ to $\hat{K}_0$ determined by the following boundary conditions (Appendix):

$$-\frac{2mV_0}{\hbar^2}(\psi(2\pi_-) - e^{i\lambda}\psi(0_+)) = e^{i\lambda}\psi'(0_+), \qquad V_0 > 0 \tag{78}$$

$$-\frac{2mV_0}{\hbar^2}(\psi(2\pi_-) - e^{i\lambda}\psi(0_+)) = \psi'(2\pi_-) \tag{79}$$

When transferred to $\mathcal{H}_\lambda(\Pi(S^1))$ the above conditions become

$$-\frac{2mV_0}{\hbar^2}(\Psi(2l\pi_-) - \Psi(2l\pi_+)) = \Psi'(2l\pi_+) \tag{80}$$

$$-\frac{2mV_0}{\hbar^2}(\Psi(2l\pi_-) - \Psi(2l\pi_+)) = \Psi'(2l\pi_-) \tag{81}$$

These are the standard boundary conditions for a repulsive δ'-potential centered at $\theta_{ex} = 2l\pi$ [12, 18]. The corresponding operator $\hat{\mathcal{H}}_{\delta';\lambda} = \hat{U}_\lambda \hat{K}_{\delta'} \hat{U}_\lambda^\dagger$ in $\mathcal{H}_\lambda(\Pi(S^1))$ admits the following eigenfunctions:

$$\Psi(\theta_{ex}) = Ae^{i\hbar l\lambda}\left(e^{ik\theta} + \left(\frac{e^{2ik\pi} - e^{i\lambda}}{e^{-2ik\pi} - e^{i\lambda}}\right)e^{-ik\theta}\right), \qquad \theta_{ex} \neq 2l\pi \tag{82}$$

where A is a normalization constant, and k is a real constant related to λ and V_0 by

$$k = \frac{4mV_0}{\hbar^2}\left(\frac{\cos 2k\pi - \cos\lambda}{\sin 2k\pi}\right) \tag{83}$$

The corresponding eigenvalues are $E = (\hbar k)^2/2m$.

4.8. The Kronig–Penny Model and the Path Space of S^1

Functions in the Hilbert space $\mathcal{H}_\lambda(\Pi(S^1))$ resemble Bloch functions in solid-state physics. Take the idealized example of a Kronig–Penny model of a one-dimensional periodic crystal lattice, which pictures the effect of the one-dimensional crystal as an infinite array of δ-potentials, of strength V_0, evenly spaced on the point set $Z = \{x_l = la,\ l = 0, \pm 1, \pm 2, \ldots\}$ on the real line $\mathbb{R}$ [13, 14]. The Hamiltonian for an electron in such a crystal is traditionally written as

$$\hat{H}_{\mathrm{KP}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_l V_0\,\delta(x - la) \tag{84}$$

An alternative and mathematically rigorous definition of this Hamiltonian is to introduce the kinetic energy operator by the differential expression $-(\hbar^2/2m)\,d^2/dx^2$ acting on $C_0^\infty(\mathbb{R} - Z)$. The resulting operator is symmetric, but it possesses infinitely many self-adjoint extensions. One of the self-adjoint extensions, denoted by $\hat{K}_{\mathrm{KP}}$, is specified by a domain consisting of continuous functions in $L^2(\mathbb{R})$ which are twice-differentiable on $\mathbb{R} - Z$ and satisfying the following δ-potential boundary condition at every point in Z [12]:

$$\psi'(x_{l+}) - \psi'(x_{l-}) = \left(\frac{2m}{\hbar^2}V_0\right)\psi(x_l), \qquad x_l \in Z \tag{85}$$

For example, one can easily check that the generalized eigenfunctions of $\hat{H}_{\mathrm{KP}}$ satisfy this boundary condition [14]. We can therefore identify $\hat{H}_{\mathrm{KP}}$ with $\hat{K}_{\mathrm{KP}}$.

Generally for a perfectly periodic potential with periodicity a the generalized eigenfunctions of the Hamiltonian are known to be of the form [14]

$$\eta_k(x) = e^{ikx}u_k(x) \tag{86}$$

where k is a real number and $u_k(x)$ is a periodic function of x, i.e.,

$u_k(x - a) = u_k(x)$. These are Bloch functions in solid-state physics. Using the translation operator $\hat{T}_\alpha$ again, we have, for any integer l,

$$\hat{T}_{la}\eta_k(x) = \eta_k(x - la) = e^{-ikla}\,\eta_k(x) \tag{87}$$

Since the derivative $u_k'(x)$ is periodic on account of the periodicity of $u_k(x)$, the derivative $\eta_k'(x)$ also satisfies (87), i.e.,

$$\eta_k'(x) = ik\eta_k(x) + e^{ikx}\,u_k'(x) \Rightarrow \hat{T}_{la}\eta_k'(x) = e^{-ikla}\,\eta_k'(x) \tag{88}$$

For the specific case of periodic δ-potentials, $\eta_k(x)$ must also satisfy the following additional boundary conditions [12] at $x = la$, where the δ-potentials are centered:

$$\eta_k'(la_+) - \eta_k'(la_-) = \left(\frac{2m}{\hbar^2}V_0\right)\eta_k(la) \qquad \text{and} \qquad \eta_k(la_+) - \eta_k(la_-) = 0 \tag{89}$$

It appears at first sight that Bloch functions arise naturally as functions in our path space theory on S^1, since every $\mathscr{H}_\lambda(\Pi(S^1))$ consists of quasiperiodic functions Ψ_λ in θ_{ex}. A quantum particle going around and around in S^1 with a single δ-potential also appears to resemble a particle in the Kronig–Penny model moving in the straight line $\mathbb{R}$ encountering a δ-potential periodically, especially when we set the periodicity $a = 2\pi$. However, a simple identification of Bloch functions with functions in $\mathscr{H}_\lambda(\Pi(S^1))$ fails since Bloch functions possess a range of phase constants k, while once a $\mathscr{H}_\lambda(\Pi(S^1))$ is chosen, the phase constant λ is fixed. So we have to form an appropriate direct integral space over $\mathscr{H}_\lambda(\Pi(S^1))$ with different λ. This can be achieved technically by first constructing a Hamiltonian with a δ-potential in $L^2(0, 2\pi)$ defined on a domain satisfying the following additional boundary conditions:

$$\begin{aligned} &\psi_k(2\pi_-) = e^{i\lambda}\,\psi_k(0_+), \qquad \psi_k'(2\pi_-) = e^{i\lambda}\psi_k'(0_+) \\ &\psi_k(\pi_-) = \psi_k(\pi_+), \qquad \psi_k'(\pi_+) - \psi_k'(\pi_-) = V_0\psi_k(\pi) \end{aligned} \tag{90}$$

In other words, we are taking a Hamiltonian in $L^2(0, 2\pi)$ of the form

$$\hat{K}_\lambda + \frac{2m}{\hbar^2}V_0\,\delta(\theta - \pi) \tag{91}$$

These conditions resemble conditions (89) for Bloch functions $\eta_k(x)$ for some specific k. One then has to perform a direct integral of these Hamitonians, corresponding to different λ, to obtain a final Hamiltonian in order to be able to compare with $\hat{H}_{KP}$ [12]. Finally, one can transfer the results on $L^2(0, 2\pi)$ to a corresponding direct integral of $\mathscr{H}_\lambda(\Pi(S^1))$.

It is clear that the origin of the quasiperiodic nature of the wave function in the path space theory on the circle S^1, and in a periodic potential in traditional solid-state physics with $\mathbb{R}$ as the physical space is, fundamentally different.

5. CONCLUDING REMARKS

We have seen that the path space offers a formulation of quantum mechanics which can naturally lead to new physical insights under certain circumstances. The application of the path space formulation to closed circuit configurations is particularly interesting in view of its easy accommodation of physical quantities like the momentum operator $\hat{\wp}_\lambda$ together with its eigenfunctions (59), which are single-valued and continuous functions of the extended angle variable θ_{ex}. This constrasts sharply with the need for discontinuous and possibly multivalued functions in the traditional formulation in the Hilbert space $L^2(S_c^1)$. When the path space formalism is employed to describe the condensate in a circuit with a Josephson junction, the superselection rules emerge in a natural manner.

APPENDIX

Let $AC(S_c^1)$ be the set of absolutely continuous functions ϕ on S_c^1 such that

$$\frac{d\phi}{d\theta} \in AC(S_c^1), \qquad \frac{d^2\phi}{d\theta^2} \in L^2(S_c^1) = L^2(0, 2\pi)$$

Let $\underline{\alpha} = \{\alpha'_-, \alpha_-, \alpha'_+, \alpha_+\}$ and $\underline{\beta} = \{\beta'_-, \beta_-, \beta'_+, \beta_+\}$ be two sets of complex numbers subject to the following two conditions:

(C1) The first set is not a multiple of the second set, i.e., there is no number δ such that $\alpha'_- = \delta\beta'_-$, $\alpha_- = \delta\beta_-$, $\alpha'_+ = \delta\beta'_+$, and $\alpha_+ = \delta\beta_+$.

(C2) These complex numbers are related by

$$\alpha'^*_-\alpha_- - \alpha^*_-\alpha'_- = \alpha'^*_+\alpha_+ - \alpha^*_+\alpha'_+, \qquad \beta'^*_-\beta_- - \beta^*_-\beta'_- = \beta'^*_+\beta_+ - \beta^*_+\beta'_+$$

$$\alpha'^*_-\beta_- - \alpha^*_-\beta'_- = \alpha'^*_+\beta_+ - \alpha^*_+\beta'_+, \qquad \beta'^*_-\alpha_- - \beta^*_-\alpha'_- = \beta'^*_+\alpha_+ - \beta^*_+\alpha'_+$$

Finally, let $\mathcal{D}_{\underline{\alpha},\underline{\beta}}$ be a subset of $AC(S_c^1)$ consisting of functions ϕ satisfying the following boundary conditions:

$$\alpha'_-\,\phi'_- - \alpha_-\phi_- = \alpha'_+\phi'_+ - \alpha_+\phi_+ \tag{92}$$

$$\beta'_-\,\phi'_- - \beta_-\phi_- = \beta'_+\phi'_+ - \beta_+\phi_+ \tag{93}$$

where ϕ'_- and ϕ'_+ are the derivatives of ϕ with respect to θ evaluated at $\theta = 0$ and $\theta = 2\pi$, respectively. All self-adjoint extensions of $\hat{K}_0$ are given by the following theorem [9]:

Theorem. The operator $\hat{K}_{\underline{\alpha},\underline{\beta}}$ defined on the domain $\mathcal{D}_{\underline{\alpha},\underline{\beta}}$ by

$$\hat{K}_{\underline{\alpha},\underline{\beta}}\phi = -\frac{\hbar^2}{2mr^2}\frac{d^2\phi}{d\theta^2}, \qquad \forall\phi \in \mathcal{D}_{\underline{\alpha},\underline{\beta}}$$

is self-adjoint in $L^2(0, 2\pi)$ and conversely every self-adjoint extension of $\hat{K}_0$ is of this form.

We have the following two cases:

1. *Case* 1. δ-potential: Boundary conditions (71), (72) amount to choosing

$$\begin{aligned} \alpha'_- &= e^{i\lambda}, \quad \alpha_- = 0, \\ \alpha'_+ &= 1, \quad \alpha_+ = -(2mV_0/\hbar^2) \\ \beta'_- &= e^{i\lambda}, \quad \beta_- = (2mV_0/\hbar^2)e^{i\lambda}, \\ \beta'_+ &= 1, \quad \beta_+ = 0 \end{aligned} \tag{94}$$

Conditions (C1) and (C2) are satisfied. It follows that (71), (72) do lead to a self-adjoint extension of $\hat{K}_0$ in $L^2(0, 2\pi)$.

2. *Case* 2. δ'-potential: Boundary conditions (78), (79) amount to choosing

$$\begin{aligned} \alpha'_- &= -e^{i\lambda}, \quad \alpha_- = -(2mV_0/\hbar^2)e^{i\lambda}, \\ \alpha'_+ &= 0, \quad \alpha_+ = -(2mV_0/\hbar^2) \\ \beta'_- &= 0, \quad \beta_- = -(2mV_0/\hbar^2)e^{i\lambda}, \\ \beta'_+ &= 1, \quad \beta_+ = -(2mV_0/\hbar^2) \end{aligned} \tag{95}$$

Conditions (C1) and (C2) are satisfied. It follows that (78), (79) do lead to a self-adjoint extension of $\hat{K}_0$ in $L^2(0, 2\pi)$.

ACKNOWLEDGMENT

C.T. gratefully acknowledges financial support from EPSRC.

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