

On the Hindered Circulation of Charged Particles around Rings Enclosing a Varying Magnetic Flux

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The dynamics of charged particles moving on a circular ring of negligible thickness is investigated. The ring has a time-dependent magnetic flux passing through it and contains a scalar potential consisting of one or more attractive wells which can bind the particle in negative energy states. For a scalar potential containing a double well structure formed from delta function potentials, the eigenfunctions, in the presence of a static flux, are determined exactly. Only the lowest two eigenstates have negative energies and these are weakly split by tunnelling. For variations of the flux that cause negligible mixing of these states with positive energy states we truncate the system to only the negative energy states. These two states constitute a novel kind of two-level system whose time evolution we have determined for fluxes that change suddenly or at a constant rate. In the latter case we find a coherent oscillation between the instantaneous eigenfunctions of the Hamiltonian. © 1994 Academic Press, Inc.

1. INTRODUCTION

When a particle moves on a ring of negligible thickness, it is natural to use the angular coordinate φ to describe its position. In classical mechanics, such an angular variable hardly merits a second glance as to its status as a descriptive coordinate. Apart from a possible restriction of its range (e.g., to the interval $-\pi$ to π), an angular coordinate appears on the same footing as cartesian coordinates such as x , y , or z . In quantum mechanics the situation is not quite so simple. A particle on a ring has a wavefunction $\psi(\varphi)$ with the periodicity

$$\psi(\varphi + 2\pi) = \psi(\varphi). \quad (1.1)$$

The product $\varphi\psi(\varphi)$ lies outside the space of functions obeying Eq.(1.1), indicating that φ is inadmissible as an operator on the space of wavefunctions. A necessary requirement for a function of φ to be allowed as an operator is that the function have a 2π periodicity.

There has been much previous work on the kinematic/geometric aspects of phase angles: it can be traced, for instance, from Refs. [1].

Here we aim at exposing some of the less obvious quantum dynamical properties of a system having an angular degree of freedom, namely a charged particle moving on a ring which encloses a magnetic flux. We are aware that such systems have come under investigation since microfabrication techniques have allowed the construction of small metallic rings with mesoscopic properties [2]. However, we have not seen any detailed discussion of the less elementary dynamical properties of such motion, and the present work aims to initiate such a discussion.

We consider a particle moving on a circle in the presence of both scalar and vector potentials. Each is chosen to respect the identification of the points φ and $\varphi + 2\pi$, and between them they allow us to prove some nontrivial properties of the system.

This paper is arranged as follows. In Sections 2 and 3 we determine general expressions for the quantization condition and eigenfunctions of a particle on a circle with a general symmetric potential and a *static* flux. In Section 4 we apply these results to potentials containing one and two attractive delta function wells. In Section 5 the problem with a double well potential is truncated to the lowest two eigenstates of the Hamiltonian, and the time evolution equation is determined when the magnetic flux varies with time. Section 6 treats the time evolution when the magnetic flux changes suddenly. In Section 7 the time evolution operator is found, in approximate form, for a magnetic flux that changes at a constant rate, and two applications of this approximation are made in Section 8. Section 9 is a brief summary and there are four appendices, three of which discuss different aspects of motion on a circle. We use a prime, ', to denote the differentiation of a function with respect to its argument and an overdot, $\dot{}$, to denote differentiation with respect to time.

2. PRELIMINARIES FOR THE TIME INDEPENDENT SCHRÖDINGER EQUATION

We consider a particle of mass m , charge e , moving on a circle of radius R with the angle φ describing its position. In what follows we ignore the spin (if any) of the particle and treat only its spatial degree of freedom.

The particle experiences a scalar potential $V(\varphi)$ that is periodic:

$$V(\varphi + 2\pi) = V(\varphi) \quad (2.1)$$

and a vector potential, \mathbf{A} , with a component, A , only in the φ direction, independent of φ and, until further notice, independent of time.

The line integral of \mathbf{A} around the circle specifies the net magnetic flux through the circle. Any dependence of \mathbf{A} on the radial coordinate is irrelevant since we require \mathbf{A} only on the circle.

In units of the flux quantum,

$$\Phi_0 = h/e, \quad (2.2)$$

the magnetic flux is

$$\mu = \oint \mathbf{A} \cdot d\mathbf{l} / \Phi_0 = eAR/\hbar. \quad (2.3)$$

The time independent Schrödinger equation of the system is

$$\left[\frac{1}{2m} \left(-\frac{i\hbar}{R} \frac{d}{d\varphi} - eA \right)^2 + V(\varphi) \right] \psi(\varphi) = E\psi(\varphi), \quad (2.4)$$

where ψ obeys the periodic boundary condition given in Eq. (1.1).

With the introduction of the dimensionless quantities

$$u(\varphi) = (2mR^2/\hbar^2) V(\varphi), \quad (2.5)$$

$$\varepsilon = (2mR^2/\hbar^2) E \quad (2.6)$$

we can write the time independent Schrödinger equation in a dimensionless form. With $\partial \equiv \partial/\partial\varphi$, we have

$$[-(\partial - i\mu)^2 + u(\varphi)]\psi = \varepsilon\psi. \quad (2.7)$$

Henceforth we shall refer to this as the time independent Schrödinger equation and to ε as the energy.

We define an auxiliary function

$$f(\varphi) = \exp(-i\mu\varphi) \psi(\varphi) \quad (2.8)$$

which satisfies

$$[-\partial^2 + u(\varphi)]f(\varphi) = \varepsilon f(\varphi). \quad (2.9)$$

The physical identity of the positions φ and $\varphi + 2\pi$ is embodied in the boundary condition of Eq. (1.1), and it follows that $f(\varphi)$ obeys the boundary condition

$$f(\varphi + 2\pi) = \exp(-2\pi i\mu) f(\varphi). \quad (2.10)$$

Equation (2.10) shows that the function $f(\varphi)$ acquires a phase change each time φ is incremented by 2π . The same happens when the coordinate of an energy eigenfunction in a one-dimensional crystal is increased by one period of the lattice. (This analogy underlies the version of the quantization condition outlined in Appendix A.) The difference between the two problems is that for a particle on a circle only a single phase factor, $\exp(-2\pi i\mu)$, is picked out by the external magnetic field, whereas in a crystal all phase factors are permitted and these label the states in a band of the crystal. Consequently, an eigenstate on the circle, for a fixed magnetic field, corresponds to only a single state of a band in the crystal.

3. GENERAL FORM OF THE QUANTIZATION CONDITION AND WAVEFUNCTIONS FOR SYMMETRIC POTENTIALS

We assume throughout that the potential $u(\varphi)$ appearing in Eq. (2.9) is symmetric about a reference point which we take to be $\varphi=0$. We restrict φ to the interval $(-\pi, \pi)$ and impose the boundary conditions

$$\begin{aligned} f(\pi) &= \exp(-2\pi i\mu) f(-\pi) \\ f'(\pi) &= \exp(-2\pi i\mu) f'(-\pi) \end{aligned} \quad (3.1)$$

which are equivalent to Eq. (2.10).

To proceed, we consider Eq. (2.9) for general values of ε . It has two linearly independent solutions, which may be arranged to have definite parity. Let us take them as $f_o(\varphi)$ and $f_e(\varphi)$, where the functions are odd and even, respectively:

$$f_o(-\varphi) = -f_o(\varphi), \quad f_e(-\varphi) = f_e(\varphi). \quad (3.2)$$

We impose the boundary conditions of Eq. (3.1) on

$$f(\varphi) = f_e(\varphi) + cf_o(\varphi), \quad (3.3)$$

which, up to an overall normalization, is the general solution to Eq. (2.9). Using the definite parities from Eq. (3.2) we obtain

$$f_e(\pi) + cf_o(\pi) = \exp(-2\pi i\mu)[f_e(\pi) - cf_o(\pi)] \quad (3.4a)$$

$$f'_e(\pi) + cf'_o(\pi) = \exp(-2\pi i\mu)[-f'_e(\pi) + cf'_o(\pi)]. \quad (3.4b)$$

Eliminating the amplitude ratio, c , from these equations yields the quantization condition on the energy ε ,

$$[f_o(\pi) f'_e(\pi) + f_e(\pi) f'_o(\pi)] + \cos(2\pi\mu)[f_o(\pi) f'_e(\pi) - f_e(\pi) f'_o(\pi)] = 0. \quad (3.5)$$

A shorter form of Eq. (3.5) emerges on noting two points: (i) The first term in square brackets is a total derivative. (ii) The coefficient of $\cos(2\pi\mu)$ is the Wronskian of the two solutions f_o and f_e and is independent of where it is evaluated. A particularly simple form is obtained at $\varphi=0$; it leads to the compact form for the quantization condition,

$$\frac{d}{d\varphi} [f_o(\varphi) f_e(\varphi)]|_{\varphi=\pi} - f_e(0) f'_o(0) \cos(2\pi\mu) = 0. \quad (3.6)$$

To find the amplitude ratio, c , of Eq. (3.3), we solve Eqs. (3.4a) and (3.4b) separately for c . A simple form for c is obtained if we add the results from

Eqs. (3.4a) and (3.4b). With similar considerations to those leading to the quantization condition, this leads to

$$c = \frac{i \cos(2\pi\mu)(d/d\varphi)[f_o(\varphi) f_e(\varphi)]|_{\varphi=\pi} - f_e(0) f'_o(0)}{2 \sin(2\pi\mu) f_o(\pi) f'_o(\pi)}. \quad (3.7)$$

Using the quantization condition, Eq. (3.6), to eliminate the coefficient of $\cos(2\pi\mu)$, we obtain the compact form

$$c = -\frac{i}{2} \sin(2\pi\mu) \frac{f_e(0) f'_o(0)}{f_o(\pi) f'_o(\pi)}. \quad (3.8)$$

Equation (3.6) for the quantization condition and Eq. (3.8) for the wavefunction amplitude ratio apply for general symmetric potentials, whose particular form determines f_o and f_e up to a multiplicative factor.

4. EXAMPLES OF EIGENFUNCTIONS AND EIGENVALUES FOR PARTICULAR POTENTIALS

To see some of the content of the general results of the previous section we shall consider two different potentials. To avoid the need for distracting discussions about approximation schemes for the functions f_o and f_e we choose potentials involving only Dirac delta functions, which admit results in closed form. In terms of the potential $u(\varphi)$ of Eq. (2.5) we choose

$$u_1(\varphi) = -2\lambda\delta(\varphi) \quad (4.1)$$

$$u_2(\varphi) = -2\lambda\delta(\varphi - \pi/2) - 2\lambda\delta(\varphi + \pi/2), \quad (4.2)$$

where for definiteness we restrict the parameter λ to be positive. We shall find it natural to express the functions $f_e(\varphi)$ and $f_o(\varphi)$ in terms of the variable

$$k = \sqrt{-\varepsilon}. \quad (4.3)$$

Appendix A sketches an alternative approach, applicable to any number of evenly spaced delta functions, but probably less ready to supply all the information we shall need about wavefunctions.

(i) *Single Delta Function Potential*

For the potential $u_1(\varphi)$ of Eq. (4.1) we find that

$$f_o(\varphi; k) = \sinh(k\varphi) \quad (4.4a)$$

$$f_e(\varphi; k) = \cosh(k\varphi) - (\lambda/k) \sinh(k|\varphi|). \quad (4.4b)$$

The quantization condition, Eq. (3.6), yields the relation

$$k = \frac{\lambda \sinh(2\pi k)}{\cosh(2\pi k) - \cos(2\pi\mu)}. \quad (4.5)$$

We shall consider solutions of this equation only for the case of negative energies and furthermore assume that

$$\Gamma_1 \equiv 2 \exp(-2\pi\lambda) \ll 1. \quad (4.6)$$

Then the expression on the right of Eq. (4.5) can be developed as a series in Γ_1 . Only a single negative energy state exists having

$$k = \lambda [1 + \Gamma_1 \cos(2\pi\mu) + O(\Gamma_1^2)] \quad (4.7)$$

and

$$\varepsilon = -\lambda^2 [1 + 2\Gamma_1 \cos(2\pi\mu) + O(\Gamma_1^2)]. \quad (4.8)$$

The factor Γ_1 is associated with a particle of energy $\varepsilon = -\lambda^2$ tunnelling an angular distance of 2π through the potential. Thus the cosine modulation of the energy results from the particle tunnelling around the circle and simultaneously being affected by the line integral of \mathbf{A} —that is, the magnetic flux through the circle. In classical mechanics, apart from there being no tunnelling, there would also be no effect of the magnetic field on the motion or energy of the particle, since the Lorentz force is everywhere normal to the circle.

It is interesting to note from Eq. (4.8) that for $\mu = 0$, tunnelling around the circle shifts the energy downward. We devote Appendix B to a discussion of this topic.

Let us now consider the implications of Eq. (3.8) for the amplitude ratio. We find that

$$c = -i \sin(2\pi\mu) \Gamma_1 + O(\Gamma_1^2). \quad (4.9)$$

By virtue of Eqs. (2.8), (4.4a), and (4.4b) the eigenfunction then reads

$$\psi(\varphi) \approx N \exp(i\mu\varphi) [f_e(\varphi; k) - i \sin(2\pi\mu) \Gamma_1 f_o(\varphi; k)]. \quad (4.10)$$

N is a real normalization constant such that $\langle \psi | \psi \rangle \equiv \int_{-\pi}^{\pi} d\varphi |\psi|^2 = 1$. Note that the value of k used in the functions f_e and f_o has to be taken from Eq. (4.7).

(ii) Double Delta Function Potential

For the potential $u_2(\varphi)$ of Eq. (4.2) we find, in the range $\pi > \varphi > 0$,

$$\begin{aligned} f_0(\varphi; k) &= \cosh(k\pi/2) \sinh(k\varphi), & \pi/2 > \varphi > 0 \\ &= \cosh(k\pi/2) \sinh(k\varphi) - (\lambda/k) \sinh(k\pi) \sinh[k(\varphi - \pi/2)], & \pi > \varphi > \pi/2 \end{aligned} \quad (4.11a)$$

$$\begin{aligned}
f_e(\varphi; k) &= \sinh(k\pi/2) \cosh(k\varphi), & \pi/2 > \varphi > 0 \\
&= \sinh(k\pi/2) \cosh(k\varphi) - (\lambda/k) \sinh(k\pi) \sinh[k(\varphi - \pi/2)], & \pi > \varphi > \pi/2.
\end{aligned} \tag{4.11b}$$

For positive φ , $f_o(\varphi; k)$ and $f_e(\varphi; k)$ achieve their maximum values at $\varphi = \pi/2$. The particular normalizations of f_o and f_e have been chosen by hindsight so as to yield the simplest form for the amplitude ratios.

After some rearrangement, the quantization condition following from Eq. (3.6) can be written in the form

$$\left(k - \frac{\lambda \sinh(\pi k)}{\cosh(\pi k) - \cos(\pi\mu)} \right) \left(k - \frac{\lambda \sinh(\pi k)}{\cosh(\pi k) + \cos(\pi\mu)} \right) = 0. \tag{4.12}$$

Alternatively, Eq. (4.12) emerges as a special case of Eq. (A.10) in Appendix A.

We again consider only solutions with negative energies and assume that

$$\Gamma_2 = 2 \exp(-\pi\lambda) \ll 1. \tag{4.13}$$

Equation (4.12) yields a pair of negative energy states with

$$k_{\pm} = \lambda [1 \pm \Gamma_2 \cos(\pi\mu)] + O(\Gamma_2^2) \tag{4.14}$$

and energies

$$\varepsilon_{\pm} = -\lambda^2 [1 \pm 2\Gamma_2 \cos(\pi\mu)] + O(\Gamma_2^2). \tag{4.15}$$

In other words, the ‘‘tunnel splitting’’ between the ground and the first excited states is modified by the magnetic flux.

The amplitude ratios c_{\pm} are given, with no approximation, by

$$c_+ = -i \tan(\pi\mu/2)$$

$$c_- = -i \cot(\pi\mu/2)$$

and lead to the normalized eigenfunctions¹

$$\psi_+(\varphi) \approx N_+ \exp(i\mu\varphi) [\cos(\pi\mu/2) f_e(\varphi; k_+) - i \sin(\pi\mu/2) f_o(\varphi; k_+)] \tag{4.16a}$$

$$\psi_-(\varphi) \approx N_- \exp(i\mu\varphi) [-i \sin(\pi\mu/2) f_e(\varphi; k_-) + \cos(\pi\mu/2) f_o(\varphi; k_-)], \tag{4.16b}$$

with N_{\pm} taken to be real.

For most values of μ , Eqs. (4.10) and (4.16) yield essentially complex energy eigenfunctions, reflecting the fact that stationary states on a circle threaded by a magnetic field carry a nonzero current $j = -(ie/2)(\psi^* \psi' - \psi'^* \psi)$. The same

¹ The main purpose of our notation $f_{e,o}(\varphi; k)$ is, precisely, to emphasize that the k -vectors used in $\psi_+(\varphi)$ and $\psi_-(\varphi)$ are generally different.

conclusion follows directly from the spectrum (i.e., from Eq. (4.8) or Eq. (4.15)), in view of the relation

$$j = -d\epsilon/d\mu. \quad (4.17)$$

The origin of Eq. (4.17) is best appreciated by considering an adiabatic (arbitrarily slow) increment $d\mu$ over a time interval dt . Then Faraday's law entails an e.m.f. $-d\mu/dt$, leading to an energy change $d\epsilon = dt(-d\mu/dt)j = -jd\mu$ which is equivalent to Eq. (4.17).

Finally, we recall that Byers and Yang [3] have formulated theorems about the energy spectrum of a particle on a circle in a magnetic field. In Appendix C we discuss these theorems in the light of the explicit results of Eqs. (4.8) and (4.15).

5. EQUATION OF MOTION IN THE DOUBLE DELTA FUNCTION POTENTIAL WHEN μ VARIES WITH TIME

We now consider the dynamical behaviour of the system by allowing μ to vary with time. It is assumed that the variations with μ are slow on the scale of λ^{-2} so that any mixing of the negative energy states with those of positive energy is negligible. Working in this approximation it is consistent to deal with our system truncated to only the negative energy states.

A single delta function potential, with its single negative energy level, leads to a trivial dynamical problem that is determined by the adiabatic theorem: energy and wavefunctions are given by Eq. (4.8) and by $\exp[-i \int^t ds \epsilon(\mu(s))] \psi(\varphi)$ with $\psi(\varphi)$, from Eq. (4.10), governed by the instantaneous value $\mu(t)$ of the flux. Accordingly, the interesting dynamical problem to study is the behaviour of the two negative energy levels of the double delta function potential, $u_2(\varphi)$ of Eq. (4.2).

To investigate the dynamics induced by a variation of μ with time, we omit arguments φ , and set

$$\begin{aligned} \psi(t) = & a(t) \exp \left[-i \int_0^t ds \epsilon_+(\mu(s)) \right] \psi_+(\mu(t)) \\ & + b(t) \exp \left[-i \int_0^t ds \epsilon_-(\mu(s)) \right] \psi_-(\mu(t)). \end{aligned} \quad (5.1)$$

The parametric dependence of ψ_{\pm} on $\mu(t)$ is displayed explicitly. Next we substitute ψ into the time dependent Schrödinger equation

$$[-(\partial - i\mu(t))^2 + u(\varphi)] \psi = i \partial_t \psi. \quad (5.2)$$

² We use a time variable, t , that is rescaled relative to the time, t_{original} that occurs in the original, unscaled, Schrödinger equation. The relation between the times is $t = (2mR^2/\hbar) t_{\text{original}}$.

Projecting the resulting equation onto ψ_+ and ψ_- , respectively and using η , defined in terms of the energy levels of Eq. (4.15) by

$$\begin{aligned}\eta(t) &= -\int_0^t ds [\varepsilon_+(\mu(s)) - \varepsilon_-(\mu(s))] \\ &\approx 4\lambda^2 \Gamma_2 \int_0^t ds \cos(\pi\mu(s)),\end{aligned}\quad (5.3)$$

it follows that

$$\dot{a} + \langle \psi_+ | \dot{\psi}_+ \rangle a + e^{-i\eta} \langle \psi_+ | \dot{\psi}_- \rangle b = 0 \quad (5.4a)$$

$$\dot{b} + \langle \psi_- | \dot{\psi}_- \rangle b + e^{i\eta} \langle \psi_- | \dot{\psi}_+ \rangle a = 0. \quad (5.4b)$$

The time derivatives such as $\langle \psi_+ | \dot{\psi}_+ \rangle$ appearing in the above equations are more naturally expressed as derivatives with respect to μ , since it is the variation of this parameter that induces the time dependence of the ψ_{\pm} . We thus write $\langle \psi_+ | \dot{\psi}_+ \rangle = \dot{\mu} \langle \psi_+ | \partial\psi_+ / \partial\mu \rangle$ etc. In Appendix D we show that

$$\begin{aligned}\langle \psi_+ | \partial\psi_+ / \partial\mu \rangle &= 0, & \langle \psi_- | \partial\psi_- / \partial\mu \rangle &= 0 \\ \langle \psi_- | \partial\psi_+ / \partial\mu \rangle &= \langle \psi_+ | \partial\psi_- / \partial\mu \rangle = -i\frac{\pi}{2}\Gamma_2 + O(\Gamma_2^2).\end{aligned}\quad (5.5)$$

Thus the amplitudes a and b follow from the equation of motion

$$\frac{d}{dt} \begin{pmatrix} a \\ b \end{pmatrix} = i\frac{\pi}{2}\Gamma_2 \dot{\mu}(t) M(t) \begin{pmatrix} a \\ b \end{pmatrix}, \quad (5.6)$$

where $M(t)$ is the matrix

$$M(t) = \begin{pmatrix} 0 & e^{-i\eta(t)} \\ e^{i\eta(t)} & 0 \end{pmatrix} \equiv \sigma_1 \cos \eta(t) + \sigma_2 \sin(\eta(t)) \quad (5.7)$$

and σ_i , $i = 1, 2, 3$, are the usual Pauli matrices.

We should note that in Eq. (5.6), the coefficient of $\dot{\mu}(t)$, namely $i(\pi/2)\Gamma_2$ has only been calculated to leading order in Γ_2 and, as a consequence, the equation is not an exact description of the time evolution.

6. SUDDEN CHANGES OF μ

As an application of Eq. (5.6), let us consider a change of $\mu(t)$ that is fast on the timescale Γ_2^{-1} but still slow on the scale of λ^{-2} , so as to stay in the two level truncation.

Then we can adopt a Heaviside step form for μ ,

$$\mu(t) = \mu_0 \Theta(t) \quad (6.1)$$

leading to

$$\frac{d}{dt} \begin{pmatrix} a \\ b \end{pmatrix} = i \frac{\pi}{2} \Gamma_2 \mu_0 \delta(t) M(t) \begin{pmatrix} a \\ b \end{pmatrix}. \quad (6.2)$$

In this equation the known matrix $M(t)$ is continuous at $t=0$ and equal to the Pauli matrix σ_1 . By contrast, the unknown functions (a, b) remain to be determined and may not be assumed to be continuous.

To solve for (a, b) we diagonalize σ_1 and obtain

$$\frac{d}{dt} \ln(a \pm b) = \pm i \frac{\pi}{2} \Gamma_2 \mu_0 \delta(t). \quad (6.3)$$

These differential equations for $(a \pm b)$ may be integrated and with

$$\begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} a(t < 0) \\ b(t < 0) \end{pmatrix} \quad (6.4)$$

we obtain

$$\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \exp \left(i \frac{\pi}{2} \Gamma_2 \mu_0 \Theta(t) \sigma_1 \right) \begin{pmatrix} a_i \\ b_i \end{pmatrix}. \quad (6.5)$$

The manifestation of the sudden approximation that appears above is very simple and should be contrasted with the standard treatment where the overlaps such as $\langle \psi_+(\mu_0) | \psi_+(0) \rangle$ are required.

7. EVOLUTION UNDER μ INCREASING LINEARLY WITH TIME

We continue to work with the lowest two levels of the double delta potential and consider, for simplicity, the case where μ , over some time interval, changes linearly with time. Thus we set

$$\mu = \beta t \quad (7.1)$$

with β independent of t .³

Let us consider $K(t)$ the 2×2 matrix that evolves $\begin{pmatrix} a(0) \\ b(0) \end{pmatrix}$ from time zero to time t :

$$\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = K(t) \begin{pmatrix} a(0) \\ b(0) \end{pmatrix}. \quad (7.2)$$

³ For small but not necessarily constant β , it is fairly straightforward to design a stationary-phase approximation to the transition amplitudes between ψ_{\pm} ; it accommodates the leading-order contributions, which arise from the level-crossings that occur at half-integer values of μ . The drawback of the method is that, after many level crossings, it accumulates errors far faster than the procedure described below.

Then $K(t)$ obeys⁴

$$\frac{d}{dt} K(t) = i \frac{\pi}{2} \Gamma_2 \dot{\mu} M(t) K(t), \quad K(0) = 1. \quad (7.3)$$

Here it proves convenient to use $\mu = \beta t$ rather than t as the independent variable. Instead of writing $K(t(\mu))$, $\eta(t(\mu))$, and $M(t(\mu))$ we write $K(\mu)$ etc. We find from Eqs. (5.3) and (5.7) that

$$M(\mu) = \sigma_1 \cos \eta(\mu) + \sigma_2 \sin \eta(\mu), \quad (7.4)$$

$$\eta(\mu) = \alpha \sin(\pi\mu), \quad \alpha = \frac{4\lambda^2}{\pi\beta} \Gamma_2 \quad (7.5)$$

and the $K(\mu)$ obeys⁵

$$\frac{d}{d\mu} K(\mu) = i \frac{\pi}{2} \Gamma_2 M(\mu) K(\mu). \quad (7.6)$$

The formal solution to this equation is

$$K(\mu) = T \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^\mu dv M(v) \right], \quad (7.7)$$

where T is the time ordering operator.

We shall argue below that

$$K(\mu) = \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^\mu dv M(v) + O(\mu\Gamma_2^2) \right] \quad (7.8)$$

supplies an accurate approximation for values of μ such that $\mu\Gamma_2^2 \ll 1$ but with no restriction on $\mu\Gamma_2$.

The approximation to $K(\mu)$ stems from three facts.

- (i) The matrix $M(\mu)$ is periodic over an interval of $O(1)$:

$$M(\mu + 2) = M(\mu). \quad (7.9)$$

⁴ The matrix M depends on t and hence the problem is not translationally invariant in time. It would be more explicit (and cumbersome), to write $K(t; 0)$ rather than $K(t)$ since K evolves the amplitudes from time zero to time t . We shall use the notation $K(t)$ with the warning that $K(t_1)K(t_2)$ does not, generally, equal $K(t_1 + t_2)$.

⁵ Although Γ_2 is small by assumption, we stress that solutions are required for values of α that may be large as well as small.

Because of this, $K(\mu + 2)$ obeys the same equation as $K(\mu)$ and from $\lim_{\mu \rightarrow 0} K(\mu + 2) = K(2)$ it follows that we can write

$$K(\mu + 2) = K(\mu) K(2), \quad (7.10)$$

a result equivalent to Floquet's theorem on periodic functions.

(ii) The elements of $M(\mu)$ are of $O(1)$.

(iii) $\Gamma_2 \ll 1$.

To derive Eq. (7.8) we consider two cases:

(1) $\mu < 2$. Here, since $M(\mu)$ is $O(1)$, $(\pi/2) \Gamma_2 \int_0^\mu dv M(v)$ is $O(\Gamma_2)$ and K obeys

$$K(\mu) = 1 + i \frac{\pi}{2} \Gamma_2 \int_0^\mu dv M(v) + O(\Gamma_2^2) \quad (7.11a)$$

$$= \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^\mu dv M(v) + O(\Gamma_2^2) \right]. \quad (7.11b)$$

Since μ is $O(1)$ we can, equivalently, write the correction to the integral in the exponent as $O(\mu \Gamma_2^2)$, making Eq. (7.11b) identical to Eq. (7.8).

(2) $\mu = \mu_1 + 2n$; $\mu_1 < 2$, n is an integer. Here we repeatedly use the property of Eq. (7.10):

$$K(\mu_1 + 2n) = K(\mu_1) K(2n) = K(\mu_1) [K(2)]^n \quad (7.12)$$

with $K(\mu_1)$ and $K(2)$ given by Eq. (7.11a) for $\mu = \mu_1$ and 2, respectively. We then have

$$\begin{aligned} [K(2)]^n &= \left(1 + i \frac{\pi}{2} \Gamma_2 \int_0^2 dv M(v) + O(\Gamma_2^2) \right)^n \\ &= \exp \left[n \log \left(1 + i \frac{\pi}{2} \Gamma_2 \int_0^2 dv M(v) + O(\Gamma_2^2) \right) \right] \\ &= \exp \left[i \frac{\pi}{2} \Gamma_2 n \int_0^2 dv M(v) + O(n \Gamma_2^2) \right] \\ &= \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^{2n} dv M(v) + O(n \Gamma_2^2) \right], \end{aligned} \quad (7.13)$$

the last step using the periodicity of $M(\mu)$. Last, we write

$$\begin{aligned} K(\mu_1) [K(2)]^n &= \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^{\mu_1} dv M(v) + O(\Gamma_2^2) \right] \\ &\quad \times \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^{2n} dv M(v) + O(n \Gamma_2^2) \right]. \end{aligned} \quad (7.14)$$

Since the integrals in the two exponents are of order Γ_2 and $n\Gamma_2$, respectively, we can add them, to form a single integral, with the generation of additional, $O(n\Gamma_2^2)$ corrections. Since n is $O(\mu)$, the resulting form is equivalent to Eq. (7.8), the result we sought to establish.

We note, finally, that there is another source for the $O(\mu\Gamma_2^2)$ corrections to the integral in Eq. (7.8). These come from the $O(\Gamma_2^2)$ correction in Eq. (5.5), which combine with the $O(\mu)$ contribution of the integral of $M(v)$ to give a correction to the stated order. It follows that to calculate beyond the order we have already established requires significantly more effort.

8. TWO APPLICATIONS OF THE APPROXIMATE EVOLUTION OPERATOR

In this section we apply the approximation to the evolution operator

$$K(\mu) \approx \exp \left[i \frac{\pi}{2} \Gamma_2 \int_0^\mu dv M(v) \right] \quad (8.1)$$

to two different situations.

(i) Sudden variations in μ . Let us return to the case of sudden variations of μ , treated in Section 6. We assume μ has the form

$$\begin{aligned} \mu(t) &= 0 & t < 0 \\ &= \mu_0 t/T, & T > t > 0 \\ &= \mu_0 & t > T. \end{aligned} \quad (8.2)$$

Equation (8.1) applies for μ in the range $\mu_0 > \mu > 0$; outside this range, $K(\mu)$ is constant. In the limit $T \rightarrow 0$, we would then expect to reproduce the results of Section 6. We have, from Eqs. (7.5) and (8.2),

$$\alpha = \frac{4\lambda^2}{\pi\mu_0} T\Gamma_2. \quad (8.3)$$

Thus, in the limit $T \rightarrow 0$, the parameter α vanishes. It follows from Eqs. (7.4) and (7.5) that

$$\lim_{T \rightarrow 0} M(\mu) = \sigma_1. \quad (8.4)$$

Substitution into Eq. (8.1) for $\mu = \mu_0$ (corresponding to times $t > T$) then yields

$$K(\mu_0) = \exp \left[i \frac{\pi}{2} \Gamma_2 \mu_0 \sigma_1 \right] \quad (8.5)$$

which is equivalent to Eq. (6.5). More generally we could keep T finite and trace the evolution of the amplitudes through the region of changing μ .

(ii) Variations at arbitrary speed over times $\sim(\beta\Gamma_2)^{-1}$. Equation (8.1) is a good approximation to $K(\mu)$, provided the inequality $\mu\Gamma_2^2 \ll 1$ is satisfied. Since Γ_2 is small we may consider values of $\mu \equiv \beta t$ which are of order Γ_2^{-1} , i.e., large but still satisfying the inequality. In order to evaluate $K(\mu)$, we require an integral over $M(v)$ which from Eqs. (7.4) and (7.5) involves

$$C(\mu; \alpha) \equiv \int_0^\mu dv \cos(\alpha \sin(\pi v)) \quad (8.6)$$

and

$$S(v; \alpha) \equiv \int_0^\mu dv \sin(\alpha \sin(\pi v)). \quad (8.7)$$

With δ the fractional part of $\mu/2$,

$$\delta = \mu/2 - [\mu/2], \quad 1 > \delta \geq 0, \quad (8.8)$$

we can write

$$\begin{aligned} C(\mu; \alpha) &= \mu \int_0^1 dv \cos(\alpha \sin(\pi v)) \\ &\quad + \left[\int_0^{2\delta} dv \cos(\alpha \sin(\pi v)) - 2\delta \int_0^1 dv \cos(\alpha \sin(\pi v)) \right] \\ &= \mu J_0(\alpha) + O(1) \end{aligned} \quad (8.9)$$

$$S(\mu; \alpha) = \int_0^{2\delta} dv \sin(\alpha \sin(\pi v)) = O(1), \quad (8.10)$$

where J_0 is a Bessel function of the first kind with order zero [4].

Since $C(\mu; \alpha)$ and $S(\mu; \alpha)$ enter the exponent in $K(\mu)$ only premultiplied by Γ_2 , we can make a further approximation by keeping only the systematically increasing part of $M(\mu)$, i.e., omitting the $O(1)$ corrections to $C(\mu; \alpha)$ and *all* of $S(\mu; \alpha)$ which is $O(1)$. The result has a simple form,

$$\begin{aligned} K(\mu) &= e^{i(\pi/2) \Gamma_2 J_0(\alpha) \mu \sigma_1 (1 + O(\Gamma_2))} \\ &= \left\{ \cos \left(\frac{\pi}{2} \Gamma_2 J_0(\alpha) \mu \right) + i \sigma_1 \sin \left(\frac{\pi}{2} \Gamma_2 J_0(\alpha) \mu \right) \right\} (1 + O(\Gamma_2)), \end{aligned} \quad (8.11)$$

which is useful when $(\pi/2) \Gamma_2 J_0(\alpha) \mu$ is not small compared with unity.

Recall, from Eqs. (5.1) and (7.2) that $K(\mu)$ acts on $\binom{a(0)}{b(0)}$ to yield $\binom{a(t)}{b(t)}$ which are the amplitudes of the eigenstates $\psi_\pm(\mu(t))$ of the instantaneous Hamiltonian

corresponding to flux $\mu(t)$.⁶ Thus the implication of Eq. (8.11) is that for a flux increasing linearly with real time, the system oscillates coherently between the adiabatic basis states $\psi_+(\mu(t))$ and $\psi_-(\mu(t))$, so that if it started from $\psi_+(\mu(t))$ at time $t=0$, then it would be in $\psi_-(\mu(t))$ when $\mu=1/(\Gamma_2 J_0(\alpha))$, i.e., at time $1/(\beta\Gamma_2 J_0(\alpha))$. Thus with

$$\gamma = \beta\Gamma_2 J_0(\alpha), \quad (8.12)$$

we have in general that

$$\begin{aligned} \psi(t) \approx & \left[\cos\left(\frac{\pi}{2}\gamma t\right) a(0) + i \sin\left(\frac{\pi}{2}\gamma t\right) b(0) \right] \exp\left[-i \int_0^t ds \varepsilon_+(\mu(s))\right] \psi_+(\mu(t)) \\ & + \left[i \sin\left(\frac{\pi}{2}\gamma t\right) a(0) + \cos\left(\frac{\pi}{2}\gamma t\right) b(0) \right] \exp\left[-i \int_0^t ds \varepsilon_-(\mu(s))\right] \psi_-(\mu(t)). \end{aligned} \quad (8.13)$$

Note that there is an exception to the coherent oscillations between the adiabatic basis states if $J_0(\alpha)=0$, i.e., if the parameter α is a zero of the Bessel function.

9. SUMMARY

In this work we have investigated the dynamical behaviour of a charged particle on a ring subject to both a scalar potential and a time dependent magnetic flux through the ring. For the case of a scalar potential with a double well structure, the lowest two eigenstates form a novel kind of two level system whose time evolution we have determined for fluxes that change either suddenly or at constant but otherwise arbitrary speed.

APPENDIX A:

N UNIFORMLY SPACED DELTA POTENTIALS ON A RING ENCLOSING FLUX

We reformulate the eigenvalue problem along the lines familiar from energy bands in a one-dimensional crystal. The analogy is instructive and furnishes a convenient expression for determining the eigenvalues for arbitrary N . Consider the equation

$$-\partial^2 f(x) - 2\lambda \sum_n \delta(x-na) f(x) = q^2 f(x). \quad (A.1)$$

⁶ ψ_+ and ψ_- change with time only due to their parametric dependence on $\mu=\mu(t)$. As μ increases by unity, they transform, apart from a phase factor, into each other. Furthermore, at $\mu=n+\frac{1}{2}$, n =integer, the eigenvalues, Eq. (4.15), cross each other. Eq. (8.11) therefore describes the consequences of many level crossings.

The range of the summation (i.e., the number of lattice sites), the lattice spacing a , and the boundary conditions are left open until further notice. We can switch from positive to negative energy by the replacement $q \rightarrow ik$.

The general solution of Eq. (A.1) can be written

$$f(x) = r_n \cos[q(x - na)] + s_n \sin[q(x - na)], \quad na \leq x \leq (n+1)a. \quad (\text{A.2})$$

Then the continuity of f and the jump condition on $\partial\phi$ across $x = na$ may be manipulated to yield

$$\begin{pmatrix} r \\ s \end{pmatrix}_{n+1} = Z(q; a) \begin{pmatrix} r \\ s \end{pmatrix}_n \quad (\text{A.3})$$

$$Z(q; a) = \begin{bmatrix} \cos(qa), & \sin(qa) \\ (-\sin(qa) - (2\lambda/q) \cos(qa)), & (\cos(qa) - (2\lambda/q) \sin(qa)) \end{bmatrix}. \quad (\text{A.4})$$

By induction $(r, s)_{n+N} = Z^N(r, s)_n$. The eigenvalues of Z read

$$z_{\pm} = \cos(qa) - (\lambda/q) \sin(qa) \pm [(\cos(qa) - (\lambda/q) \sin(qa))^2 - 1]^{1/2}. \quad (\text{A.5})$$

On an unbounded lattice, propagation is possible only in the allowed bands, where the radicand is negative and the z_{\pm} thereby complex, of modulus unity and complex conjugates of each other. Accordingly, bands are allowed subject to

$$-1 \leq \cos(qa) - (\lambda/q) \sin(qa) \leq 1. \quad (\text{A.6})$$

On a ring with N sites we have $a = 2\pi/N$ and identify f in Eq. (A.1) with the auxiliary function f from Eqs. (2.8)–(2.10). In particular, the boundary condition Eq. (2.10) now requires that $(r, s)_N = (r, s)_0 \exp(-2\pi i\mu)$; thus Z^N has an eigenvalue

$$z_{\pm}^N = \exp(-2\pi i\mu), \quad (\text{A.7})$$

whence

$$z_{\pm} = \exp[-2\pi i(\mu + p)/N], \quad p = 0, 1, \dots, (N-1), \quad (\text{A.8})$$

which in the light of Eq. (A.5) entails

$$\cos(2\pi q/N) - (\lambda/q) \sin(2\pi q/N) = \cos[2\pi(\mu + p)/N], \quad p = 0, 1, \dots, (N-1). \quad (\text{A.9})$$

For negative energies ($q \rightarrow ik$) this reads,

$$\cosh(2\pi k/N) - (\lambda/q) \sinh(2\pi k/N) = \cos[2\pi(\mu + p)/N], \quad p = 0, 1, \dots, (N-1). \quad (\text{A.10})$$

Setting $N=1$, $p=0$, we recover Eq. (4.5); setting $N=2$ and $p=0, 1$ we recover, respectively, the first and second factors on the left of Eq. (4.12).

APPENDIX B: TUNNEL LOWERING ON A CIRCLE

We consider a single symmetric attractive potential on a circle without magnetic flux and estimate by how much the ground-state energy is lower than for the same potential on the unbounded x -axis. For simplicity, we shall (eventually) restrict ourselves to a tightly bound state in a narrow well, where the ranges of the potential and wavefunction are both much smaller than the circumference of the circle. This covers the situation considered in the body of the paper. The method is an adaptation of a more general procedure developed elsewhere [5].

The real, nodeless, even-parity ground states on the line and circle obey⁷

$$-\psi_0''(x) + u(x)\psi_0(x) = \varepsilon_0\psi_0(x), \quad \psi_0(\pm\infty) = 0 \quad (\text{B.1})$$

$$-\psi''(x) + u(x)\psi(x) = (\varepsilon_0 + \Delta)\psi(x), \quad \psi'(-L) = 0 = \psi'(L). \quad (\text{B.2})$$

We introduce an (even) function $g(x)$ defined by

$$\psi(x) = g(x)\psi_0(x); \quad (\text{B.3})$$

then the boundary condition $\psi'(L) = 0$ entails the effective quantization condition

$$g'\psi_0|_{x=L} = -g\psi_0'|_{x=L}. \quad (\text{B.4})$$

We shall obtain an approximation to the energy shift Δ through suitable approximations to g and ψ_0 .

Subject to the simplifying assumptions stated above, we may, over most of the circle (including the "outer regions" $x \sim \pm L$) write

$$\psi_0(x) \approx M \exp(-q|x|), \quad q \equiv -\sqrt{\varepsilon_0}, \quad (\text{B.5})$$

where M is a constant. By hindsight, we choose to norm g through

$$g(0) = 1 \quad (\text{B.6})$$

and expect appreciable departures of $g(x)$ from unity only where ψ_0 is very small.

Substituting Eq. (B.3) into Eq. (B.2) and then multiplying by ψ_0 , one eventually obtains

$$\frac{d}{dx}(g'\psi_0^2) = -\Delta g\psi_0^2(x). \quad (\text{B.7})$$

⁷ It is worth noting that, for even-parity states on a circle, the first periodicity condition (namely $\psi(-L) = \psi(L)$) is satisfied automatically, leaving only the Neumann boundary conditions indicated in Eq. (B.2). Conversely, for odd-parity states, the second periodicity condition $\psi'(-L) = \psi'(L)$ is satisfied automatically, leaving only the Dirichlet conditions $\psi(L) = 0 = \psi(-L)$, which are those considered in [5].

Since g is even and $g'(0)$ therefore vanishes, this integrates to

$$g'(x) \psi_0^2(x) = -\Delta \int_0^x dx' g(x') \psi_0^2(x'). \quad (\text{B.8})$$

Division by ψ_0^2 and further integration, plus Eq. (B.6), then lead to

$$g(L) = 1 - \Delta \int_0^L dx \psi_0^{-2}(x) \int_0^x dx' g(x') \psi_0^2(x'). \quad (\text{B.9})$$

Finally we substitute into Eq. (B.4) from Eq. (B.9), and the expression for $g'(L)$ obtained from Eq. (B.8). Some rearrangement then yields

$$\begin{aligned} \Delta \left\{ \int_0^L dx g(x) \psi_0^2(x) + \psi_0(L) \psi_0'(L) \int_0^L dx \psi_0^{-2}(x) \right. \\ \left. \times \int_0^x dx' g(x') \psi_0^2(x') \right\} = \psi_0(L) \psi_0'(L). \end{aligned} \quad (\text{B.10})$$

Equation (B.10), still exact and exploited systematically in [5], governs Δ . Under our present assumptions, i.e., to leading order in $\exp(-qL)$, it is readily approximated as follows: (i) The first term within the curly brackets reduces to half the normalization integral for ψ_0 , i.e. to $\frac{1}{2}$. (ii) In the second term, the outer integral is dominated by the region $x \sim L$, where ψ_0 nearly vanishes, according to Eq. (B.5). Hence the inner integral can (here as in the first term) be replaced by $\frac{1}{2}$. (iii) In the outer integral, ψ_0^2 is approximated by Eq. (B.5); and (iv) so is $\psi_0(L) \psi_0'(L) \approx -qM^2 \exp(-2qL)$ on both sides of Eq. (B.10). We find

$$\Delta \approx -4qM^2 \exp(-2qL). \quad (\text{B.11})$$

This confirms the fact, already plausible from Eq. (B.10), that Δ is negative.⁸

To make the connection with the ground-state energy of Eq. (4.8) for $\mu=0$, we consider the potential $-2\lambda \delta(x)$ and choose $L=\pi$. This yields

$$q = \lambda, \quad M = \sqrt{\lambda}, \quad \Delta \approx -4\lambda^2 \exp(-2\pi\lambda) \equiv -2\lambda^2 \Gamma_1 \quad (\text{B.12})$$

in complete accordance with Eq. (4.8).

APPENDIX C: DIFFERENT REALISATIONS OF THE BYERS-YANG THEOREMS

In this appendix we examine how different scalar potentials, $u(\varphi)$, can result in quite different realisations of the theorems originally formulated by Byers and Yang [3] for the problem of fluxoid quantization in superconducting rings.

⁸To put this conclusion into mathematical perspective, we note that it follows from replacing the boundary conditions at infinity in Eq.(B.1) by Neumann conditions at $\pm L$. By contrast, Dirichlet conditions at $\pm L$ raise the energy (i.e., they yield a positive Δ), as discussed in [5].

For our purposes, the theorems simply assert that the set of energy levels is even and periodic in μ , with period unity; where, as in Eq. (2.3), μ is the magnetic flux through the circle, measured in units of $\Phi_0 \equiv h/e$.

For orientation we first consider the case of vanishing potential. Solving Eq. (2.7) for this case with periodic boundary conditions, one finds eigenfunctions $(2\pi)^{-1/2} \exp(in\varphi)$ and eigenvalues

$$E_n = (n + \mu)^2, \quad n = 0, \pm 1, \pm 2, \pm 3, \dots \quad (\text{C.1})$$

Thus under the change $\mu \rightarrow \mu + 1$ individual levels move to the position of one of neighbouring levels before the change. But the set of energy levels $\{E_n : n = 0, \pm 1, \pm 2, \dots\}$ maps back into itself:

$$\{E_n\} \xrightarrow{\mu \rightarrow \mu + 1} \{E_n\}. \quad (\text{C.2})$$

It is therefore periodic with period unity. Furthermore, since both the labels n and $-n$ are included, the set is even in μ .

Quite different behaviour, but equally compatible with the theorems, is exhibited by Eqs. (4.8) and (4.15), which, although only a subset of the complete spectrum, do constitute closed sets under the change $\mu \rightarrow \mu + 1$.

Equation (4.8) gives the ground state energy for a single delta function potential on a circle. In this case the level does not move to a neighbouring level as μ changes by unity. Instead it simply oscillates with μ , with period 1.

Equation (4.15) gives, for a pair of closely spaced states in a double well potential on a circle, another type of behaviour. Here the change $\mu \rightarrow \mu + 1$ results in the two levels interchanging their position.

APPENDIX D: DETERMINING COEFFICIENTS IN THE EQUATION OF MOTION FOR THE DOUBLE DELTA FUNCTION POTENTIAL

In this appendix we calculate the matrix elements $\langle \psi_+ | \partial \psi_+ / \partial \mu \rangle$, $\langle \psi_- | \partial \psi_- / \partial \mu \rangle$, $\langle \psi_- | \partial \psi_+ / \partial \mu \rangle$, and $\langle \psi_+ | \partial \psi_- / \partial \mu \rangle$ for the double delta function potential on a circle. The Dirac notation corresponds to $\langle a | b \rangle = \int_{-\pi}^{\pi} d\varphi a^*(\varphi) b(\varphi)$; * denotes complex conjugate.

It will be useful to rewrite Eqs. (4.16a), (4.16b) by introducing the real functions

$$F_{e\pm}(\varphi) = N_{\pm} f_e(\varphi; k_{\pm}) \quad (\text{D.1})$$

$$F_{o\pm}(\varphi) = N_{\pm} f_o(\varphi; k_{\pm}). \quad (\text{D.2})$$

With the abbreviations

$$s = \sin(\pi\mu/2), \quad c = \cos(\pi\mu/2) \quad (\text{D.3})$$

and the omission of φ arguments we can write⁹

$$\psi_+ = \exp(i\mu\varphi)[cF_{e+} - isF_{o+}] \quad (\text{D.4a})$$

$$\psi_- = \exp(i\mu\varphi)[-isF_{e-} + cF_{o-}]. \quad (\text{D.4b})$$

(1) *Calculation of $\langle \psi_+ | \partial\psi_+ / \partial\mu \rangle$ and $\langle \psi_- | \partial\psi_- / \partial\mu \rangle$*

Both of these matrix elements vanish identically. To see this we calculate, e.g., $\langle \psi_+ | \partial\psi_+ / \partial\mu \rangle$. We have

$$\begin{aligned} \partial\psi_+ / \partial\mu &= i\varphi\psi_+ + \exp(i\mu\varphi)(\pi/2)[-sF_{e+} - icF_{o+}] \\ &\quad + \exp(i\mu\varphi)[c \partial F_{e+} / \partial\mu - is \partial F_{o+} / \partial\mu] \end{aligned} \quad (\text{D.5})$$

the last line following since F_{e+} and F_{o+} depend on k_+ which itself depends on μ . Then, since F and $\partial F / \partial\mu$ have the same parity,

$$\begin{aligned} \langle \psi_+ | \partial\psi_+ / \partial\mu \rangle &= i\langle \psi_+ | \varphi | \psi_+ \rangle - (\pi/2)sc\{F_{e+} | F_{e+} \rangle - \langle F_{o+} | F_{o+} \rangle\} \\ &\quad + \{c^2 \langle F_{e+} | \partial F_{e+} / \partial\mu \rangle + s^2 \langle F_{o+} | \partial F_{o+} / \partial\mu \rangle\}. \end{aligned} \quad (\text{D.6})$$

A comparison of this expression with the explicit form of $\partial\langle \psi_+ | \psi_+ \rangle / \partial\mu$ indicates that we can write

$$\langle \psi_+ | \partial\psi_+ / \partial\mu \rangle = i\langle \psi_+ | \varphi | \psi_+ \rangle + \frac{1}{2} \partial\langle \psi_+ | \psi_+ \rangle / \partial\mu. \quad (\text{D.7})$$

Use of Eq. (D.4a) and the definite parities of the $F_{o,e}$ causes the first term on the right to vanish. The second term is identically zero since $\langle \psi_+ | \psi_+ \rangle = 1$ for all μ .

(2) *Calculation of $\langle \psi_- | \partial\psi_+ / \partial\mu \rangle$ and $\langle \psi_+ | \partial\psi_- / \partial\mu \rangle$*

Explicit calculation, following from Eq. (D.5), indicates that $\langle \psi_- | \partial\psi_+ / \partial\mu \rangle$ is purely imaginary, and so is $\langle \psi_+ | \partial\psi_- / \partial\mu \rangle$. Combining this information with orthogonality of ψ_- and ψ_+ quickly yields the identity $\langle \psi_- | \partial\psi_+ / \partial\mu \rangle \equiv \langle \psi_+ | \partial\psi_- / \partial\mu \rangle$.

The calculation of $\langle \psi_- | \partial\psi_+ / \partial\mu \rangle$ may be simplified if we determine $1/2(\langle \psi_- | \partial\psi_+ / \partial\mu \rangle + \langle \psi_+ | \partial\psi_- / \partial\mu \rangle)$. We find, with similar considerations to those used in the calculation of $\langle \psi_+ | \partial\psi_+ / \partial\mu \rangle$, that

$$\begin{aligned} \langle \psi_- | \partial\psi_+ / \partial\mu \rangle &\equiv \langle \psi_+ | \partial\psi_- / \partial\mu \rangle = i/2\{(\langle F_{e-} | \varphi | F_{o+} \rangle + \langle F_{o-} | \varphi | F_{e-} \rangle) \\ &\quad - \pi/2(\langle F_{e-} | F_{e+} \rangle + \langle F_{o-} | F_{o+} \rangle)\} \\ &\quad + (1/2) \frac{\partial}{\partial\mu} \langle \psi_- | \psi_+ \rangle \end{aligned} \quad (\text{D.8})$$

and the μ derivative vanishes since $\langle \psi_- | \psi_+ \rangle = 0$ for all μ .

⁹ It is tempting, but not obviously correct, to assume that $F_{e\pm}(\varphi)$ and $F_{o\pm}(\varphi)$ are normalised to unity. We can only be certain that ψ_{\pm} are an orthonormal set.

The above equation is written in the form

$$\begin{aligned} \langle \psi_- | \partial \psi_+ / \partial \mu \rangle \equiv \langle \psi_+ | \partial \psi_- / \partial \mu \rangle = i \left\{ -(\pi/2) \int_0^\pi d\varphi (F_{e-} - F_{o-})(F_{e+} - F_{o+}) \right. \\ \left. + \int_0^\pi d\varphi (\varphi - \pi/2)(F_{e-} F_{o+} + F_{o-} F_{e+}) \right\}. \end{aligned} \quad (\text{D.9})$$

The first integral is straightforward since, on account of Eqs. (D.1), (D.2), and (4.11),

$$F_e - F_o = N \sinh[k(\pi/2 - \varphi)] \quad (\text{D.10})$$

and leads to

$$\int_0^\pi d\varphi (F_{e-} - F_{o-})(F_{e+} - F_{o+}) = N_+ N_- \left(\frac{e^{(k_+ + k_-)\pi/2}}{2(k_+ + k_-)} + O(1) \right). \quad (\text{D.11})$$

To obtain the leading behaviour it is sufficient to evaluate N_+ and N_- with k taken to zeroth order in Γ_2 . From Eq. (4.14) this is $k = \lambda$ and a straightforward calculation gives

$$N_+ N_- \approx 8\lambda e^{-2\lambda\pi}. \quad (\text{D.12})$$

Using this and the values of k_\pm taken from Eq. (4.14) gives

$$\int_0^\pi d\varphi (F_{e-} - F_{o-})(F_{e+} - F_{o+}) \approx 2e^{-\pi\lambda} \equiv \Gamma_2. \quad (\text{D.13})$$

The second integral in Eq. (C.9) can be shown to be of order Γ_2^2 and hence may be neglected to leading order in Γ_2 . We thus have

$$\langle \psi_- | \partial \psi_+ / \partial \mu \rangle \equiv \langle \psi_+ | \partial \psi_- / \partial \mu \rangle = -i(\pi/2)\Gamma_2 + O(\Gamma_2^2). \quad (\text{D.12})$$

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Note added in proof. The first-order homogeneous differential equation (6.2) with its delta-function coefficient becomes unambiguous only when the delta-function is defined explicitly as the limit either of a local or of a separable representation, since the solutions of the equation continue to depend on the type of representation, even in the limit. Equation (6.3) is appropriate to local representations, dictated by the physics of our system. Such ambiguities are discussed more generally elsewhere (G. Barton and D. Waxman, "Wave equations with point-support potentials having dimensionless strength parameters," Sussex preprint, 1993).

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