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An occurrence of an effective anharmonic velocity dependent potential

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Abstract. An integrable dynamical problem of a classical neutral particle interacting with an inhomogeneous magnetic field via a magnetic dipole moment is considered; this had previously been studied quantum mechanically. The equation for the centre-of-mass velocity is of second order resembling that of an anharmonic oscillator with velocity replacing position in the equation. The velocity undergoes curious oscillations, where the spin and centre-of-mass degrees of freedom exchange energy, although there is also, in general, a uniform component to the velocity. An application to the motion of a classical 'neutron' in a magnetic domain wall is discussed, and comparison with previous quantum treatments made.

1. Introduction

There are very few dynamics problems which are integrable (in the sense of having a full complement of constants of the motion). In this paper we will discuss an integrable problem classically which previously had been discussed quantum mechanically. It has the dual appeal of having arisen naturally and that the integrability is due to a constant of the motion which is not immediately obvious.

The problem is that of a neutral particle with a magnetic moment interacting with an inhomogeneous magnetic field of a particularly simple form—namely that the field rotates about a fixed direction, say the x axis, as the coordinate x is changed. This problem arose in the context of neutron scattering at a magnetic domain wall (previously treated quantum mechanically by Schärpf (1978)), where the domain wall is a ' $\lambda/2$ ' section of the periodically rotating field, sandwiched between two regions of uniform field, which are antiparallel. One objective of the present calculation was to study whether thinking classically about neutrons in an inhomogeneous magnetic field was as useful as thinking classically about the homogeneous field case. There the utility of classical thought is mathematically due to the equation of motion of the expectation value of the spin only involving the expectation value of the spin itself—thus there is no problem about working out expectation values of a hierarchy of products of operators, which for instance occur in most potential problems apart from the harmonic one. In the inhomogeneous case it is not so obviously useful, and so worth investigating.

In this paper we formulate the equations of motion, and then eliminate the spin degrees of freedom, noting the significance of the extra constant of the motion apart from the energy. We are left with an interesting nonlinear (in terms of \dot{x}) equation for \ddot{x} . It is of the form $\ddot{v} = -\partial V(v)/\partial v$ where v is the velocity and V(v) is a quartic function of v, as in an anharmonic oscillator where the variable is the velocity, not

position. We thus find that in general the centre of mass has an oscillatory velocity with, perhaps, a uniform component as well.

We then study several cases, trying to understand both the centre of mass and spin motion. The results are used to discuss the transmission (or lack of it) of a beam of classical 'neutrons' by a domain wall, and we find under certain circumstances that the particles are transmitted at low and high velocities, but reflected in between.

Finally we compare our results with the quantum case studied by Calvo (1978, 1980) and others (see references in Calvo 1980), and find some interesting similarities.

2. Derivation of equations of motion

We wish to deduce the equations of motion for an uncharged, classical particle with an intrinsic magnetic moment. There is not a unique set of equations for the problem, as posed, as the origin of the magnetic moment determines the form of the equations. We will discuss two possibilities and determine the one we wish by examination of the quantum case.

The first possibility is a magnetic dipole constructed from two magnetic charges of magnitude $\pm M$. Denote the vector describing the separation of the charges by d. We will constrain d to have a fixed magnitude. If the centre-of-mass coordinate is r and both charges have mass m, then the centre-of-mass equation of motion in an inhomogeneous magnetic field, B(r), is (where m is the mass):

$$2m\ddot{r} \simeq M(d \cdot \nabla) B(r). \tag{2.1}$$

Here we have Taylor expanded the magnetic field about the centre of mass. The equation for the relative motion is

$$\frac{1}{2}md^2\hat{d}\times\hat{d} = MB(\mathbf{r})\times d \tag{2.2}$$

where we have equated the torque on the dipole with the moment of inertia times the 'angular' acceleration. $(\hat{d} = d/d)$.

The second possibility is that the magnetic dipole is generated by currents, not magnetic monopoles, for instance a sphere which is neutral overall but, say, the negative charges rotate with respect to the positive charges. If we assume a uniform charge distribution, and just add up to the Lorentz forces, (e/c) $(v \times B)$, on each of the moving charges, we find that:

$$m\ddot{r} = \mu \left(\nabla \cdot \boldsymbol{B}(\boldsymbol{r})\right) - \nabla \left(\mu \cdot \boldsymbol{B}(\boldsymbol{r})\right)$$
(2.3)

and similarly by adding up torques

$$\dot{\boldsymbol{\mu}} = (\boldsymbol{e}/\boldsymbol{m}\boldsymbol{c})(\boldsymbol{\mu} \times \boldsymbol{B}(\boldsymbol{r})) \tag{2.4}$$

where μ is the magnetic dipole moment of the spinning sphere, $\mu = (Ie/mc) \omega$, where ω is the angular velocity and I the moment of inertia of the sphere and m is its mass. If there are no magnetic monopoles then (2.3) becomes

$$m\ddot{\boldsymbol{r}} = -\nabla(\boldsymbol{\mu} \cdot \boldsymbol{B}(\boldsymbol{r})). \tag{2.5}$$

To determine which of the two pairs (2.1) and (2.2) or (2.4) and (2.5) is the natural set of equations of motion corresponding to a neutral quantum particle with spin and a consequent magnetic moment, let us consider the equations of motion for the expectation values of the momentum, p, and the spin, s.

If the quantum Hamiltonian (a classical one is difficult to define, unless we make explicit mention of constituent particles as above, since the spin operators do not have canonical commutation relations as the position and momentum do) is

$$H = p^2/2m + (ge/mc)s \cdot \boldsymbol{B}(\boldsymbol{r})$$
(2.6)

then

$$i\hbar(d/dt)\langle \boldsymbol{p}\rangle = \langle [\boldsymbol{p}, \boldsymbol{H}] \rangle = -i\hbar\langle \nabla((\boldsymbol{g}\boldsymbol{e}/\boldsymbol{m}\boldsymbol{c})\boldsymbol{s} \cdot \boldsymbol{B}(\boldsymbol{r})) \rangle$$
(2.7)

$$i\hbar(d/dt)\langle s \rangle = \langle [s, H] \rangle = i\hbar\langle (ge/mc)s \times B(r) \rangle.$$
(2.8)

If the expectation value is taken with a wavepacket which minimises the positionmomentum uncertainty relationship, and then the limit of Planck's constant going to zero is taken, then the quantities inside the angular brackets are evaluated at the centre of the wavepacket at time t, with small corrections, due to the magnetic field varying over the spatial extent of the wavepacket. This approach was considered in Fradkin and Good (1961) and the subject of classical limits of quantum spinning particles considered in more detail by, for instance, Plahte (1966).

Thus the equations (2.4) and (2.5) correspond to the correct equations of motion. If we wish a physical picture to go with the equations, then that of the differentially rotating positive and negative charge clouds making up a neutral sphere yield such equations of motion, although this picture should not be taken as being the correct *microscopic* classical limit of a particle such as a neutron, of course.

3. Elimination of spin degrees of freedom

In this section we will pick a simple form for an inhomogeneous field, namely a 'helical' field, and show that the spin equations of motion can be integrated, leaving a third-order equation of motion for the position of the particle which will be discussed in detail in § 4. This surprising occurrence of a soluble dynamical problem is due to a hidden constant of the motion, which had been noted for the spin- $\frac{1}{2}$ quantum case by Calvo (1978).

Consider the equation for the magnetic moment (2.4)

$$\dot{\boldsymbol{\mu}} = (\boldsymbol{e}/\boldsymbol{m}\boldsymbol{c})\boldsymbol{\mu} \times \boldsymbol{B}(\boldsymbol{r}(t)). \tag{3.1}$$

It is now natural to use as basis vectors the direction of the local field $\hat{z}(x)$, the direction of motion \hat{x} , and their mutual perpendicular. This set of basis vectors is spatially varying, and corresponds, in the frame of reference of the particle, to a rotating coordinate system, rotating at the apparent angular velocity of the magnetic field.

We now pick the simple case of a magnetic field which rotates uniformly, as a function of position along the x axis, about the x axis, with period a:

$$\boldsymbol{B} = B_0(\hat{\boldsymbol{z}} \cos[(2\pi/a)x] + \hat{\boldsymbol{y}} \sin[(2\pi/a)x])$$
(3.2)

and the problem becomes soluble. This form was motivated by the application, considered in the next section, of a neutron being scattered by a magnetic (Bloch) domain wall, whose field is, to a first approximation, that in (3.2).

The apparent rate of change of μ with respect to the new basis vectors, $\dot{\mu}^*$, can be related to μ , by expansion of μ in terms of the new basis vectors:

$$\dot{\boldsymbol{\mu}}^* = \dot{\boldsymbol{\mu}} + \dot{\boldsymbol{x}}(2\pi/a)\hat{\boldsymbol{x}} \times \boldsymbol{\mu}. \tag{3.3}$$

The second term on the right-hand side describes an apparent torque on the magnetic moment, due to the choice of basis vectors. It is similar to a Coriolis force. Thus the final expression for μ^* is

$$\boldsymbol{\mu}^* = (\boldsymbol{e}/\boldsymbol{m}\boldsymbol{c})(\boldsymbol{\mu} \times \boldsymbol{B}) + \dot{\boldsymbol{x}}(2\pi/\boldsymbol{a})\hat{\boldsymbol{x}} \times \boldsymbol{\mu}. \tag{3.4}$$

We may interpret (3.4) as saying that the magnetic moment moves under the influence of the sum of a constant field and a time varying (as \dot{x} is a function of time) effective field. The difficulty in its solution lies in the time dependence of the second term. By energy conservation, the equation for the velocity is:

$$\dot{x} = [(2/m)(E + \mu \cdot B)]^{1/2}.$$
(3.5)

It is now useful to define some dimensionless variables

$$t' = (eB_0/mc)t \equiv \omega_{\rm L}t, \qquad \dot{x}' = \dot{x}[(2/m)(E + \mu B_0)]^{-1/2}$$

$$b = \mu B_0/E, \qquad \lambda = (2\pi/a)\omega_{\rm L}^{-1}[(2/m)(E + \mu B_0)]^{1/2}.$$
(3.6)

The physical significance of t' and \dot{x}' are: times are measured in units of the inverse Larmor frequency (ω_L) ; the velocity is scaled by its maximum possible value. λ and b are key parameters. λ measures the adiabaticity of the motion, by comparing the lower bound on the time taken by the particle to traverse a period of the oscillation of the field, $[(2/m)(E + \mu B_0)]^{-1/2} a$, with a period of the Larmor precession, $(2\pi)/\omega_L$. For instance if λ is small then the magnetic moment can precess many times around the direction of the local field in the time that the particle takes to traverse an oscillation of the field and thus can adjust adiabatically so that the average magnetic moment points in the direction of the local field; for λ large the converse is true. b compares the maximum 'magnetic' energy, μB_0 , with the total energy. It crudely measures whether the magnetic field is a perturbation to the dynamics or not. In terms of these variables, the equations of motion are (after dividing through by μ)

$$\hat{\boldsymbol{\mu}}^* = \hat{\boldsymbol{\mu}} \times \hat{\boldsymbol{z}} + \lambda \dot{\boldsymbol{x}}' \hat{\boldsymbol{x}} \times \hat{\boldsymbol{\mu}}$$
(3.7)

$$\dot{x}' = (1 + \hat{\mu}_z b)^{1/2} / (1 + b)^{1/2}$$
(3.8)

 $\hat{\mu}$ is the unit vector in the direction of the magnetic moment. The prime on \dot{x}' will be suppressed from now on.

We will now eliminate the spin degrees of freedom from the equations, leaving a nonlinear differential equation for the velocity of the particle, which will be solved in the next section.

Firstly take the z component of (3.7) and represent $\hat{\mu}_z$ by solving (3.8) for it; yielding

$$\hat{\mu}_{y} = [2(1+b)/(\lambda b)]\ddot{x}.$$
(3.9)

This result is not surprising: since we are dealing with a conservative system $\hat{\mu}_z$ can only change by \dot{x} changing, thus we expect a relation between the component of the torque on μ in the z direction (which varies with $\hat{\mu}_y$) and the acceleration. Now the x component of (3.7) is

$$\dot{\boldsymbol{\mu}}_{x}^{*} = \hat{\boldsymbol{\mu}}_{y}. \tag{3.10}$$

Comparing this with (3.9), we see that $\hat{\mu}_x$ and \dot{x} can only differ by a constant:

$$\hat{\mu}_{x} = [2(1+b)/(\lambda b)](\dot{x} - p_{s})$$

$$p_{s} = \dot{x}(t=0) - \lambda b \hat{\mu}_{x}(t=0) / [2(1+b)].$$
(3.11)

This relationship is of great significance; it shows that there is a constant of the motion in addition to the energy, p_s , the screw momentum. This constant was discovered in the quantum case by Calvo (1978). It is due to a hidden symmetry in the problem: a translation of δx followed by a rotation of the spin by $2\pi \delta x/a$ leaves the system unchanged. This 'screw' symmetry gives rise to the conservation of the screw momentum, as the momentum in the x direction and the x component of $\hat{\mu}$ are the generators of corresponding transformations.

There are now expressions for $\hat{\mu}_x$ (3.11), $\hat{\mu}_y$ (3.10) and $\hat{\mu}_z$ (from (3.8)) in terms of \ddot{x} and \dot{x} . If these are substituted into the y component of (3.7) we find

$$\ddot{x} = -2(\dot{x} - p_{\rm s}) - \lambda^2 \dot{x} [(1+b)\dot{x}^2 - 1]/(1+b).$$
(3.12)

If we write $\dot{x} = v$, this can be written in the form:

$$\ddot{v} = -\partial V(v) / \partial v \tag{3.13}$$

where

$$V(v) = \frac{1}{4}\lambda^2 v^4 + (1 - \lambda^2 / [2(1+b)])v^2 - 2p_s v.$$
(3.14)

The form of (3.12) is suggestive of the equation of motion of a particle in a quartic potential, V(x). Thus the motion of the centre of mass of the particle is that of an anharmonic velocity dependent oscillator, where energy is periodically exchanged between the spin and centre-of-mass degrees of freedom.

4. Some solutions to the equations of motion and an application

In this section we will deduce some general features of the motion from the equations derived in § 3. Then we will examine some limiting cases, and see how this behaviour is deduced from the anharmonic oscillator picture which emerged at the end of § 3. Next we will pick a particularly interesting parameter range where the answer is not intuitively obvious and solve the equations of motion there. Finally we will use the model to consider how a classical 'neutron' is reflected from a magnetic domain wall.

As regards general features of the motion, the first point to note is that the velocity, v, must be a periodic function of time, perhaps plus a constant. This just follows from the equation for v being of an oscillator type, which must have periodic solutions as it is one dimensional, and the constant is the analogue of a constant displacement in the 'normal' problem, with x replacing v. By conservation of energy (3.8) $\hat{\mu}_z$ will also be a periodic function of time with the same period; and by equations (3.9) and (3.10) $\hat{\mu}_x$ and $\hat{\mu}_y$ are similarly periodic. With regard to $\hat{\mu}_x$ and $\hat{\mu}_y$, care should be exercised: the fact that they are periodic does not necessarily imply that one Larmor precession occurs during each period of the velocity oscillation—as the azimuthal motion (with respect to the local z axis) of the magnetic moment may be much smaller than 2π —with $\hat{\mu}_x$ and $\hat{\mu}_y$ only undergoing small changes.

Since the equation of motion for v is only cubic in v, it is possible in principle to integrate the equation to yield v(t) in terms of Jacobian elliptic functions (Whittaker and Watson 1973), and moreover since the integrals of elliptic functions are known in closed form x(t) might be obtained. However the method of constructing the solution for a general cubic equation of the form of (3.12) (Whittaker and Watson 1973, pp 513-4) involves solution of cubic algebraic equations and a fair amount of

subsequent manipulation, leading to cumbersome expressions which are hard to interpret. For these reasons we will restrict consideration to three special cases where the equation for v reduces to the harmonic oscillator, although in the last case we will also derive the solution in the fully anharmonic case. These three examples contain three of the physically most interesting cases.

Firstly consider the 'adiabatic' case (λ small). This occurs when there are many periods of the Larmor precession in the time that it takes the particle to traverse one period of the field variation. In that case we expect that the mean direction of the magnetic moment will follow the local field experienced by the particle. In that case we expect the velocity to vary little, as the magnetic energy is conserved.

To see this behaviour emerging from equation (3.13), if we let $\lambda \rightarrow 0$ keeping b fixed (corresponding, say, to letting the length scale of the field variation, a, tend to infinity) then

$$V(v) \simeq v^2 - 2p_{\rm s}v \tag{4.1}$$

so the velocity oscillations are approximately harmonic. The solution to the equation of motion, applying initial conditions $v(t=0) = \dot{x}(0)$ and $\dot{v}(t=0) = 0$ (note by (3.9) this is equivalent to $\mu_y(t=0) = 0$), is

$$v(t) = \dot{x}(t=0) + \hat{\mu}_x(t=0)\lambda b(\cos t - 1)/[2(1+b)].$$
(4.2)

This is first order in λ due to p_s being in part linear in λ . It is interesting to note that (a) the oscillation in the velocity occurs at the Larmor frequency

(b) the mean velocity is not the initial one, but below it. We can now deduce the motion of the magnetic moment

$$\hat{\mu}_{z} \simeq \left[(1+b)\dot{x}(0)^{2} - 1 \right] / b + \lambda \hat{\mu}_{x}(t=0)\dot{x}(t=0)(\cos t - 1).$$
(4.3)

Note that $\hat{\mu}_z$ is smaller on average than its value at t = 0, which is the first term in (4.3). Finally

$$\hat{\mu}_x \simeq \hat{\mu}_x(t=0) \cos t, \qquad \hat{\mu}_y = \hat{\mu}_x(t=0) \sin t.$$
 (4.4)

To the order in λ that we are working, the fluctuations in $\hat{\mu}_z$ do not affect the other components.

Thus a perturbative calculation of the motion in powers of λ yields the expected result, that the velocity is unchanged to lowest order, with the z component of the magnetic moment remaining constant. However the corrections are mildly interesting. Further corrections would yield more Fourier components of the motion, with an amplitude dependent frequency, which would not quite be the Larmor frequency.

Another simple limit is the high velocity limit, where $b \rightarrow 0$. The kinetic energy is dominant and $\lambda \rightarrow \infty$, due to the velocity appearing linearly in λ . This means that the motion will be only weakly perturbed by the existence of the non-uniform field, leading to a small fractional fluctuation in the velocity.

In this limit

$$V(v) \simeq \lambda^2 (v^4/4 - v^2/2). \tag{4.5}$$

This potential has very deep minima at $v = \pm 1$. Since v is measured in units of $[2(E + \mu B_0)/m]^{1/2}$, one of these minima is roughly at the initial velocity of the particle (due to $E/\mu B_0 \gg 1$). The fractional change in v must be small, as the spin degrees of freedom can only absorb a very small amount of the total energy, so we should Taylor

expand V(v) about v = 1. Let $v = 1 + \delta v$, then

$$V(\delta v) \simeq \lambda^2 (\delta v)^2. \tag{4.6}$$

Again the motion is harmonic, with solution

1

$$v = 1 + \delta \cos \lambda t \tag{4.7}$$

(assuming $v(t=0) = 1 + \delta$ and $\dot{v}(t=0) = 0$). Note that in this case (as opposed to the adiabatic case) the frequency is $\lambda \omega_{L}$. This is sensible as λ determines the apparent frequency of field rotation in the frame of the particle, and when this is much larger than the Larmor frequency, as it is here, it will determine the frequency of exchange of energy between the centre-of-mass motion and spin motion.

In the previous two examples, the velocity of the particle varied little as a function of time. The next example goes to the opposite extreme: although the root-mean-square velocity may be near its maximum (1 in dimensionless units), the mean velocity is close to zero. The parameter values for such a situation are as follows: $b \le 0$ implying that the particle has not got a high enough energy to ignore the field in its spin dynamics; $\lambda \to \infty$ which means the particle is not adiabatic—so the spin direction cannot adjust to the local field, and thus let the centre-of-mass motion be unperturbed.

To be more quantitative consider V(v), the potential in the equation for \dot{v} . As $\lambda \rightarrow \infty$ we find (note sign of quadratic term is not positive, remembering sign of b):

$$V(v) \simeq -\frac{1}{2}v^{2}[\lambda^{2}/2(1+b)] + \frac{1}{4}\lambda^{2}v^{4} - 2p_{s}v.$$
(4.8)

The term in p_s is included as there is a term linear in λ in it, namely

$$p_{\rm s} \simeq -[\lambda b/2(1+b)]\hat{\mu}_{\rm x}(t=0). \tag{4.9}$$

As $\lambda \to \infty$, only the quartic and quadratic parts of V(v) are important (unless $v \le 1/\lambda$, an approximate condition for adiabaticity), thus V(v) is symmetric. The importance of the symmetry is that it implies that the average velocity is zero, so the centre-of-mass motion is affected, as predicted above. Note that a symmetric V(v) (and hence zero mean velocity) is even possible for small λ , but requires in that case the initial value of $\hat{\mu}_x$ to be a particular value (such that $p_s = 0$). In the limit of $\lambda \to \infty$ the position is more general: any value of $\hat{\mu}_x$ will lead to zero mean velocity.

We will now consider this case, firstly in the harmonic limit, where $v \ll 1$ (although bigger than $1/\lambda$), and then quote the result for the general anharmonic case.

In the harmonic case we can integrate easily

$$V(t) = \frac{b\hat{\mu}_x(t=0)}{\lambda(1+b)} + \left(v(t=0) - \frac{b\hat{\mu}_x(t=0)}{(1+b)\lambda}\right) \cos\left(\frac{\lambda t}{|1+b|^{1/2}}\right)$$
(4.10)

where v(t=0) = v(0) and $\dot{v}(t=0) = 0$. We see that the average velocity is of order $1/\lambda$, from the first term. The frequency of the velocity oscillations are determined by $\lambda/|1+b|^{1/2}$: the factor of λ can be rationalised as in the last example, the other factor is harder to understand. The behaviour of $\hat{\mu}_z$ can be deduced easily from (4.10) and (3.8)—basically it oscillates in phase with v. To find $\hat{\mu}_{xx}$, we use the fact that p_s is conserved and (4.9) which implies that as $\lambda \to \infty$, p_s conservation is tantamount to $\hat{\mu}_x$ conservation, as the v part of p_s has small weight, hence p_s is insensitive to the fluctuations in v. Thus $\hat{\mu}_x$ is fixed and the change in $\hat{\mu}$ due to $\hat{\mu}_z$ varying, must imply $\hat{\mu}_y$ varies to ensure $\hat{\mu}$ is a unit vector. Thus $\hat{\mu}$ oscillates in the yz plane in phase with the velocity. (4.10) can be integrated to yield x(t)

$$x(t) = x(0) + \frac{b\hat{\mu}_x(0)t}{\lambda(1+b)} + \frac{|1+b|^{1/2}}{\lambda} \left(v(0) - \frac{b\hat{\mu}_x(0)}{\lambda(1+b)}\right) \sin\left(\frac{\lambda t}{|1+b|^{1/2}}\right).$$
(4.11)

Note that in terms of the position, the oscillating component is of the same order as the uniform one, in terms of λ , although of course the uniform part is multiplied by t.

We will now quote the result of a calculation, performed in the appendix, of the motion when v may be of the order of one:

$$v(t) \approx \frac{b\hat{\mu}_x(0)}{\lambda(1+b)} + \left(v(0) - \frac{b\hat{\mu}_x(0)}{\lambda(1+b)}\right) \operatorname{cn}(At, k)$$
(4.12)

where

$$A = \left[2 \left(v(0)^2 - \frac{\lambda^2}{2(1+b)} \right) \right]^{1/2} \lambda, \qquad k = \frac{v(0) - [\lambda b/2(1+b)] \hat{\mu}_x(0)}{\{2(v^2(0) - [\lambda^2/2(1+b)]\}^{1/2}}.$$
 (4.13)

The Jacobian elliptic function cn(At, k) is defined by equation (A8) in the appendix. When v(0) is small $k \approx 0$, and by inspection of (A8) we see that cn reduces to cos with the correct argument. The reason that the reduction described in Whittaker and Watson can be performed in this case $(\lambda \rightarrow \infty)$ is that the quartic is almost symmetric, and the reduction can be performed perturbatively in inverse powers of λ .

The reason that we have considered the three examples above is their relation to the following application of the calculation. An approximation to the magnetic field of a magnetic Bloch domain wall is a section of the helical field, discussed above, of length $\frac{1}{2}a$ with uniform fields, in opposite directions, on either side. Consider the scattering of a classical 'neutron' from this wall (this could be in three dimensions, as if the wall is planar the equations in the other directions separate, momentum in the transverse directions being conserved). This problem was first investigated quantum mechanically by Schärpf (1978). The particle will be transmitted if either

(a) its energy is high enough (i.e. $b \approx 0$) or

(b) if its energy is low enough $(\lambda \simeq 0)$ for the adiabatic approximation to work.

The interesting question is whether it is reflected at an intermediate velocity. The three cases mentioned correspond to the three cases of the helical field discussed in this section.

To decide whether there can be reflection we will use (4.11). The first question to answer is: what is the condition that the particle's velocity reverses before it exits from the wall into uniform field on the opposite side? The particle's velocity changes sign at $t = (\pi/2)\sqrt{|1+b|}/\lambda$ at which time the distance gone is approximately $(\sqrt{|1+b|}/\lambda)v(0)$. We wish this to be less than $\frac{1}{2}a$ (in dimensional units). This requirement in dimensional units is (after a little manipulation):

$$\frac{1}{2}a > \frac{1}{2}(a/\pi)(\frac{1}{2}m\dot{x}(0)^2/|E|)^{1/2}.$$
(4.14)

Thus for sufficiently small incident velocities, the particle turns about before the end of the wall. Note however that $\dot{x}(0)$ must be large enough to avoid adiabatic transmission, implying that

$$\dot{x}(0) > a(\omega_{\rm L}/2\pi).$$
 (4.15)

With its initial velocity between these limits the particle will be reflected, as the velocity will be negative for a period $\pi\sqrt{|1+b|}/\lambda$ which more than cancels the positive distance initially travelled, plus the small (of order λ^{-2}) contribution from the uniform velocity. It is also possible for the motion to be confined to the domain wall.

5. Discussion and conclusions

In this section we will compare the results of the last section with previous work on the quantum problem by Calvo (1978, 1980) and others (see references in Calvo 1980). Then conclusions will be drawn. Firstly some of Calvo's results will be stated. The Hamiltonian for the system may be written as:

$$H = p^2/2m + (ge/mc)s \cdot \boldsymbol{B}(x).$$
(5.1)

If B(x) is of helical form (3.2) then it is easy to check that $p_s(=p-(2\pi/a)s_x)$ commutes with *H*. This can then be transformed to a spinor basis aligned along the local field (analogous to the basis vectors employed in the classical case)

$$H = [p + (2\pi/a)s_x]^2 / 2m + (ge/mc)B_0s_z$$
(5.2)

which now commutes with p, an operator with the significance (in the new basis) of the screw momentum. The first term is the kinetic energy (the term in s_x subtracts off the effect of the rotating spinors) and the second is the magnetic energy.

A particularly simple case where comparisons can be made is the weak field case, where $(e/mc)gB_0s \ll (\hbar^2/2m)(2\pi/a)^2$. In that case the allowed energies (as functions of p) are a set of parabolae specified by $[p + (2\pi/a)n\hbar)]^2/m$ where n runs from -sto +s through the integers on half-integers. Now if the second term is finite it couples these states, and the effect is particularly important when states on two parabolae are degenerate. An example would be when (for an integer spin system) p = 0 and $n = \pm 1$. The parabolae hybridise and split, like bands in a solid. The splitting can be calculated by the same techniques as nearly free electron theory in solids (e.g. Ziman 1972). In fact at p = 0 any unperturbed state will be degenerate with another—as there is always an -n corresponding to the n labelling the parabola that the state is on. Thus all states will be at band edges for p = 0, which will be commented on later. It is also interesting to note that Calvo's work can be extended to yield evanescent states in the gaps, and for spin- $\frac{1}{2}$ (which only has one gap, as there are only two parabolae) the state in the middle of the gap is actually an eigenstate of s_y , which seems to have no physical interpretation.

The first point of comparison between the classical and quantum results is to remember that for $p_s = 0$ classically, the mean velocity was zero. This agrees with the quantum result that all states at p = 0 are at band edges, and so have zero group velocity. The more complicated comparison is the behaviour away from $p_s = 0$. Classically we find that the group velocity is small in the sense that the average value of the velocity is small compared to the root-mean-square velocity, until a certain value of momentum, p. This can be gauged by considering the conserved screw momentum:

$$p_{s} = \dot{x} - [b\lambda/2(1+b)]\hat{\mu}_{x}.$$
(5.3)

Now in dimensionless units \dot{x} is bounded from above by one (as it is measured in units of the maximum possible velocity). Thus if we find the momenta for which the constant in front of $\hat{\mu}_x$ is less than one, they will estimate the region where \dot{x} is approximately conserved, and hence the mean velocity is the root-mean-square velocity. Using the expressions for b and λ (3.6) we find that p_s is

$$p_{\rm s} = \dot{x} - \left(\frac{\mu}{e/mc}\right) \frac{2\pi}{a} \frac{2}{p} \hat{\mu}_{x}.$$
(5.4)

Thus we wish $[\mu/(e/mc)](2\pi/a)(2/p)$ to be small. Note that $\mu/(e/mc)$ has units of action (as has \hbar or angular momentum). The equivalent statement quantum mechanically is that $s(\pi/a)/p \ll 1$.

We thus have a correspondence between s and $\mu/(e/mc)$, as expected. For sufficiently large p, defined by the satisfying of the above inequalities, ordinary momentum is conserved. For smaller p, classically the mean velocity tends to zero, which corresponds to the quantum dispersion relation looking like a set of solid state bands (for $p \le s(\pi/a)$), with small *average* group velocity (averaging over the region of p_s between 0 and $s(\pi/a)$).

It would be appealing to quantise the classical model by an analogous technique to WKB. The difficulty is that the Hamiltonian has a matrix nature due to the spinor part of the states, thus leaving us with a problem of the form:

$$(\mathbf{d}^2/\mathbf{d}x^2)\boldsymbol{\psi}(x) = (\mathbf{M}(x) - E\mathbf{1}) \cdot \boldsymbol{\psi}(x).$$
(5.5)

If $\mathbf{M}(x)$ were spatially constant then we could have a solution in terms of an exponential, however it is not. Thus we need something like a time ordered product (cf integrating the Schrödinger equation with a time dependent potential). One possibility for doing this, at large s (hence in the semiclassical spin limit), is to use the fact that the spin operators almost commute at large s. One technique for this is the Magnus expansion (Magnus 1954) which exploits the almost commutativity of matrices involved in a matrix differential equation.

To conclude, we have looked at a new classical integrable dynamical system, the integrability being due to the screw symmetry of the magnetic field. It shows peculiar behaviour, such as anharmonic velocity oscillations, although it is not spatially confined, associated with a periodic exchange of energy between the spin and centre-of-mass degrees of freedom. Finally we have related some of the classical results to previous quantum work.

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Appendix

We wish to integrate the equation

$$\lambda^{-2}\dot{v}^{2} + \frac{1}{4}(v^{4} - v^{4}(0)) - \frac{1}{2}A(v^{2} - v^{2}(0)) - B(v - v(0)) = 0$$
(A1)

where B is a small quantity of order λ^{-1} . This equation can be solved in terms of elliptic functions (e.g. Whittaker and Watson 1973, pp 513-4). This requires the solution of the quartic equation in v (disregarding the term in \dot{v}). In general this is a difficult procedure, with lengthy algebraic expressions which are nearly impossible to interpret. Thus we will only attempt a perturbative solution of (A1), where the term multiplied by B is the perturbation. We will write the integral of (A1) in the form of the integral representation of the Jacobian elliptic function cn(x, k).

$$v_1^{(0)} = v(0) \qquad v_2^{(0)} = -v(0)$$

$$v_{\pm}^{(0)} = \pm i(v(0)^2 - 2A)^{1/2} \equiv \pm iM.$$
(A2)

To first order in B

$$v_1 = v(0) \qquad v_2 = -v_0 + \varepsilon \qquad \varepsilon = -2B/(v(0)^2 - A)$$

$$v_{\pm} = \pm iM + \varepsilon_{\pm} \qquad \varepsilon_{\pm} = -B(M \pm iv(0))/[M(v(0)^2 - A)].$$
(A3)

The next part of the prescription for solution (Whittaker and Watson 1973) is to take the roots of the quartic in the pairs $(v - v_1)(v - v_2)$ and $(v - v_+)(v - v_-)$ and complete the squares in the respective quadratics to yield:

$$(v - v_1)(v - v_2) = (v + \alpha)^2 - (v(0) + \alpha)^2$$

(v - v_+)(v - v_-) = (v + \alpha)^2 - (v(0) + \alpha)^2 + 2(v(0)^2 - A) (A4)

where

$$\alpha = B/(v(0)^2 - A). \tag{A5}$$

Then we can integrate (A1) formally as

$$\lambda t = -\int_{v(0)}^{v} \left\{ \left[(v(0) + \alpha)^2 - (v' + \alpha)^2 \right] \times \left[(v' + \alpha)^2 + 2(v(0)^2 - A) - (v(0) + \alpha)^2 \right] \right\}^{-1/2} dv'.$$
(A6)

Now change variable to $w = (v' + \alpha)/(v(0) + \alpha)$:

$$\lambda t = \frac{1}{v(0) + \alpha} \int_{v + \alpha/v(0) + \alpha}^{1} \left\{ \left[1 - w^2 \right] \left[w^2 + 2(v(0)^2 - A)/(v(0) + \alpha)^2 - 1 \right] \right\}^{-1/2} dw$$
(A7)

and use the definition of cn(x, k):

$$x = \int_{\operatorname{cn}(x,k)}^{1} (1-t^2)^{-1/2} [(1-k^2) + k^2 t^2]^{-1/2} \,\mathrm{d}t \tag{A8}$$

we see that the solution of (A1) is

$$v(t) = -\alpha + (\nu(0) + \alpha) \operatorname{cn}([2(\nu(0)^2 - A)]^{1/2} \lambda t, (\nu(0) + \alpha) / [2(\nu(0)^2 - A)]^{1/2}).$$
(A9)

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