Quantum Mechanics of a Particle with Two Magnetic Impurities

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Abstract

A two-dimensional quantum mechanical system consisting of a particle coupled to two magnetic impurities of different strengths, in a harmonic potential, is considered. Topological boundary conditions at impurity locations imply that the wave functions are linear combinations of two-dimensional harmonics. A number of low-lying states are computed numerically, and the qualitative features of the spectrum are analyzed.

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1 Introduction

A distinctive feature of the topology of two-dimensional space is that a pointlike object renders it multiply connected. A closed path taking a particle around the object is characterized by a winding number, showing how many times the object has been encircled; and in the path-integral formalism, paths with different winding numbers may carry different overall phase factors.

A simple physical incarnation of this general principle is a system of charged particles in the presence of "magnetic impurities", i.e. magnetic flux points (two-dimensional projections of flux tubes) at given points in space. There is no classical interaction force, since the magnetic field outside an impurity vanishes; however, the electromagnetic vector potential being topologically nontrivial, the dynamics of the particle is influenced (the Aharonov-Bohm effect [1]). Identifying impurities with particles themselves leads to the concept of anyon statistics [2], whereby the wave function acquires a nontrivial phase factor when the positions of two particles are continuously interchanged. The anyon model is not exactly solvable for more than two particles, because the usual representation of the multiparticle wave function (which is now a multivalued function of its complex arguments) in terms of products of single-particle functions is not possible.

Obviously, the two-dimensional model with magnetic impurities may be viewed as a projection of a three-dimensional system in which the impurities are infinite solenoids, and the longitudinal motion is free.

Topological models of this kind are interesting because of their relevance to the fractional quantum Hall effect [3], which is a two-dimensional phenomenon and where the elementary excitations are believed to be anyonic. For a particle coupled to a random Poissonian distribution of magnetic impurities, calculations of the density of states averaged over the positions of the impurities have been performed [4], with some interesting qualitative conclusions. The model is no less fascinating, however, as an example of quite a generic quantum-mechanical system in multiply connected space.

Last but not least, there is a direct connection with the problem of winding number distribution of random paths [5]. In fact, the partition function of one particle in the presence of N impurities is essentially a Fourier transform of the sequence $P_{m_1 m_2 \ldots m_N}$ of probabilities that a random closed path winds m_k times around point k for all $k = 1, \ldots, N$. Since it is known from past experience [6] that the partition function of such systems can be computed with precision better by several orders of magnitude (with comparable computational time expense) by means of finding the spectrum directly rather than by Monte Carlo simulating the winding number distribution, one tends to believe that finding the levels is the right way to go in pursuit of a good numerical, and possibly analytic, estimate of the probability distribution in question.

The system of one particle coupled to one impurity is trivial (standard A-B). The kinetic angular momentum with respect to the impurity acquires a fractional part equal to the magnetic flux modulo the flux quantum, and the energy levels, which depend on the momentum, shift accordingly. In this paper we consider the problem of one particle coupled to two impurities [7]. A harmonic potential is used as the most convenient long-

distance regulator. There appears a new dimensionless parameter, the ratio of the distance between the two impurities to the harmonic length. (In the thermodynamic limit, when the harmonic frequency vanishes, it is the ratio of that distance to the thermal wavelength that becomes relevant.) Searching for the wave function as a linear combination of two-dimensional harmonics and imposing boundary conditions at the positions of the impurities boils down to the standard procedure: there arises a system of linear equations for the coefficients, and the levels are those values of energy at which the determinant vanishes.

We find numerically the ground state and the first two excited states and observe how their energies depend on the strengths of the impurities (i.e. the values of the fluxes they carry) and the distance between them. At certain conditions there is a nonperturbative behavior at vanishing distance, whose nature is the same as in the case of the A-B ground state [8]: a nonsingular wave function turns into a singular one. The present calculation is a starting step in the evaluation of the partition function, with the subsequent inference of the two-point winding number distribution.

2 Two-dimensional harmonics and boundary conditions

The single-particle two-dimensional harmonic oscillator Hamiltonian is ($\hbar = 1$)

$$H = -\frac{1}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\,\frac{\partial}{\partial r} + \frac{1}{r^2}\,\frac{\partial^2}{\partial \varphi^2}\right) + \frac{m\omega^2}{2}\,r^2 \ . \tag{1}$$

Upon introducing the dimensionless length $\rho = \sqrt{m\omega}r$ and energy $\mathcal{E} = E/\omega$ and separating the wave function as $\psi(\rho,\varphi) = f(\rho)\,\mathrm{e}^{\mathrm{i}l\varphi}$, the energy eigenvalue equation $H\psi = E\psi$ reduces to the radial equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{1}{\rho}\,\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{l^2}{\rho^2} - \rho^2 + 2\mathcal{E}\right) f(\rho) = 0 \ . \tag{2}$$

Its two linearly independent solutions can be expressed in terms of the confluent hypergeometric functions [9]:

$$f_{l,\mathcal{E}}(\rho) = \rho^{|l|}\,\mathrm{e}^{-\frac{\rho^2}{2}}\,M(a,b,\rho^2) \ , \tag{3}$$

$$g_{l,\mathcal{E}}(\rho) = \rho^{|l|}\,\mathrm{e}^{-\frac{\rho^2}{2}}\,U(a,b,\rho^2) \ , \tag{4}$$

where

$$a = \frac{|l|+1-\mathcal{E}}{2} \ , \qquad b = |l|+1 \ . \tag{5}$$

$M(a,b,\rho^2)$ is regular at $\rho = 0$ but in general grows exponentially at $\rho \to \infty$; on the contrary, $U(a,b,\rho^2)$ falls off at infinity but is singular at the origin. It is only in the special case of $a = -n$, where $n = 0, 1, 2, \ldots$, that the two solutions actually coincide and

represent a wave function that is regular both at zero and infinite ρ; hence, the familiar two-dimensional harmonic spectrum

$$\mathcal{E} = 2n + |l| + 1 \ , \tag{6}$$

with the integer angular momentum $l = 0, \pm 1, \pm 2, \ldots$ (the wave function being single-valued).

When the particle encircles an impurity with flux Φ at the origin, one can always work in the singular gauge where the flux has been erased but the wave function acquires an extra factor of $\exp(\mathrm{i}\alpha\varphi)$, where the "impurity strength" is, by definition, $\alpha = \Phi/\Phi_0$, with the flux quantum $\Phi_0 = 2\pi/e$. Thus, moving the particle around the origin brings up a phase factor of $\exp(2\mathrm{i}\alpha\pi)$; for fractional α, the wave function becomes multivalued. This is achieved by a shift $l \mapsto l + \alpha$; accordingly, the spectrum becomes

$$\mathcal{E} = 2n + |l + \alpha| + 1 \ , \tag{7}$$

Note that the phase factor—and the spectrum—is periodic in α with period 1; i.e., it is only the fraction of the flux quantum that matters.

Let us now place two impurities on the plane: one of strength α_1 at the point with polar coordinates $(\rho_0, 0)$ and another one of strength α_2 at (ρ_0, π). The most general particle wave function inside the circle $\rho = \rho_0$ is

$$\psi_-(\rho, \varphi) = \sum_{l=-\infty}^{\infty} c_l \, f_{l,\mathcal{E}}(\rho) \, \mathrm{e}^{\mathrm{i}l\varphi} \ . \tag{8}$$

Outside the same circle, adding 2π to φ amounts to encircling both impurities 1 and 2, which should yield a phase factor of $\exp[2\mathrm{i}(\alpha_1 + \alpha_2)\pi]$. The wave function, therefore, must be

$$\psi_+(\rho, \varphi) = \sum_{l=-\infty}^{\infty} d_l \, g_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho) \, \mathrm{e}^{\mathrm{i}(l+\alpha_1+\alpha_2)\varphi} \ . \tag{9}$$

On the circle $\rho = \rho_0$ we must require continuity of the function $\psi(\rho, \varphi)$ and its normal, i.e. radial derivative. There remain, however, the boundary conditions associated with encircling the individual impurities; those cannot be satisfied with one global relation between $\psi_-(\rho_0, \varphi)$ and $\psi_+(\rho_0, \varphi)$. Rather, one has to introduce branch cuts such that encircling zero, one, or both impurities would involve crossing different combinations of the cuts, and impose phase differences between the opposite sides of each cut. Indeed, if the two cuts are made as shown on Fig. 1, the boundary conditions are satisfied. E.g., encircling impurity 1 counterclockwise yields a phase factor of $\exp[-2\mathrm{i}\alpha_2\pi] \times \exp[2\mathrm{i}(\alpha_1 + \alpha_2)\pi] = \exp[2\mathrm{i}\alpha_1\pi]$. Thus, the boundary conditions are

$$\psi_-(\rho_0, \varphi) = \psi_+(\rho_0, \varphi) \qquad (0 \le \varphi < \pi) \ ; \tag{10}$$

$$\psi_-(\rho_0, \varphi) = \mathrm{e}^{-2\mathrm{i}\alpha_2\pi}\psi_+(\rho_0, \varphi) \qquad (\pi \le \varphi < 2\pi) \ , \tag{11}$$

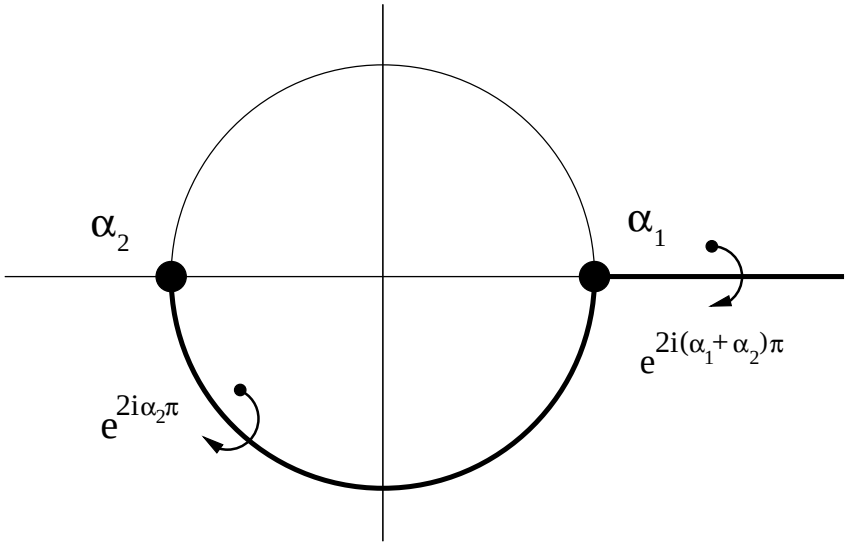


Figure 1: The two branch cuts and associated phase differences.

or, substituting the explicit expressions (8)–(9),

$$\sum_{l=-\infty}^{\infty} c_l\, f_{l,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}l\varphi} = \sum_{l=-\infty}^{\infty} d_l\, g_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}(l+\alpha_1+\alpha_2)\varphi} \qquad (0 \le \varphi < \pi)\ ; \quad (12)$$

$$\sum_{l=-\infty}^{\infty} c_l\, f_{l,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}l\varphi} = \mathrm{e}^{-2\mathrm{i}\alpha_2\pi} \sum_{l=-\infty}^{\infty} d_l\, g_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}(l+\alpha_1+\alpha_2)\varphi} \qquad (\pi \le \varphi < 2\pi)\ . \quad (13)$$

Exactly the same conditions have to hold for the normal derivatives $\partial\psi_{\pm}(\rho,\varphi)/\partial\rho$, implying

$$\sum_{l=-\infty}^{\infty} c_l\, f'_{l,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}l\varphi} = \sum_{l=-\infty}^{\infty} d_l\, g'_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}(l+\alpha_1+\alpha_2)\varphi} \qquad (0 \le \varphi < \pi)\ ; \quad (14)$$

$$\sum_{l=-\infty}^{\infty} c_l\, f'_{l,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}l\varphi} = \mathrm{e}^{-2\mathrm{i}\alpha_2\pi} \sum_{l=-\infty}^{\infty} d_l\, g'_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0)\, \mathrm{e}^{\mathrm{i}(l+\alpha_1+\alpha_2)\varphi} \qquad (\pi \le \varphi < 2\pi) \quad (15)$$

$[f'_{l,\mathcal{E}}(\rho) \equiv \partial f_{l,\mathcal{E}}(\rho)/\partial\rho]$. These equations depend on energy as a parameter, and energy levels are those values of $\mathcal{E}$ for which all four can be satisfied simultaneously.

3 Numerical procedure

In order to project out single Fourier components, one should multiply Eqs. (12)–(15) by $\mathrm{e}^{-\mathrm{i}k\varphi}$, for integer k, and integrate over φ from 0 to 2π. In practice, however, the l summation will be truncated to a finite number of terms, say $2N$. It is impossible to satisfy the boundary conditions at all values of φ by adjusting the finite number of coefficients. A better approach, leading to greater numerical precision, is to impose those conditions at $2N$

uniformly distributed discrete points $\varphi_n = (2n+1)\pi/(2N)$, where $n = 0, 1, 2, \ldots, 2N-1$ (cf. [6]). Integration over φ then gets replaced with summation over φ_n. Equations (12) and (13) turn into one,

$$2N c_k \, f_{l,\mathcal{E}}(\rho_0) = \mathrm{e}^{\mathrm{i}\alpha_1\pi} \sum_l \frac{\sin(\alpha_1\pi) + (-1)^{l-k}\,\sin(\alpha_2\pi)}{\sin\frac{(l+\alpha_1+\alpha_2-k)\pi}{2N}}\, d_l \, g_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0) \;, \tag{16}$$

as do (14) and (15). Eliminating the c_k's yields

$$\sum_l A_{kl}(\mathcal{E})\, d_l = 0 \;, \tag{17}$$

with the matrix element

$$A_{kl}(\mathcal{E}) = \frac{\sin(\alpha_1\pi) + (-1)^{l-k}\,\sin(\alpha_2\pi)}{2N\sin\frac{(l+\alpha_1+\alpha_2-k)\pi}{2N}} \Big[f_{l,\mathcal{E}}(\rho_0)\, g'_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0) - f'_{l,\mathcal{E}}(\rho_0)\, g_{l+\alpha_1+\alpha_2,\mathcal{E}}(\rho_0) \Big] \;. \tag{18}$$

The l summation may be over any $2N$ values (not even necessarily sequential): any basis can be chosen for expanding the wave function, but the more adequate the choice, the more accurate the levels found. At least for low-lying states, the right choice is to have the values $l + \alpha_1 + \alpha_2$ group as closely around zero as possible.

In the $N \to \infty$ limit, the denominator in Eq. (18) gets replaced with $(l+\alpha_1+\alpha_2-k)\pi$, which is precisely what one would get if Eqs. (12)–(15) were integrated over φ rather than summed over φ_n.

The numerical procedure is simply to scan a desired interval of energy, for given α_1, α_2, and ρ_0, to find the values that nullify the determinant of $||A_{kl}||$.

There is an evident fourfold symmetry in the (α_1, α_2) space. Apart from the $(\alpha_1, \alpha_2) \mapsto (\alpha_2, \alpha_1)$ invariance, there is P-symmetry (reversal of signs of both α's) as well as periodicity $(\alpha_j \mapsto \alpha_j + 1)$. Taken together, these imply invariance with respect to $(\alpha_1, \alpha_2) \mapsto (1-\alpha_2, 1-\alpha_1)$. Hence, the spectrum is symmetric with respect to both diagonals of the square $0 \le \alpha_{1,2} \le 1$, and it is enough to confine oneself to any one of the four triangles formed by those diagonals.

A big improvement in precision can be gained by finding one and the same level at different values of N and then extrapolating to $N \to \infty$. In fact, comparing the results for different N is the only reliable way to estimate the error caused by the truncation. Convergence in N is better for wave functions that are less singular at impurity positions, since it is difficult to represent singular functions with finite Fourier series. The leading-term behavior of a generic wave function near an impurity of strength α $(0 \le \alpha \le 1)$, with the distance from the impurity $r \to 0$, is $r^{1/2-|\alpha-1/2|}$. Convergence, therefore, is expected to be the best at $\alpha = 1/2$ and the worst near the endpoints $\alpha = 0$ and $\alpha = 1$.

This is indeed what is observed. The finite-N data, for N not too small, are found to be quite well described by an empiric formula

$$\mathcal{E}(N) = \mathcal{E} + c\, N^{-\nu} \;, \tag{19}$$

with the exponent ν depending rather weakly on ρ_0, but strongly on the α's (Table 1).

α_1, α_2	$\rho_0 = 0.75$			$\rho_0 = 1.5$		
	$\mathcal{E}$	ν	c	$\mathcal{E}$	ν	c
0.1, 0.1	1.147	0.10	-0.153	1.027	0.09	-0.030
0.3, 0.2	1.280	0.41	-0.357	1.043	0.41	-0.077
0.5, 0.5	1.442	1.01	-0.773	1.060	0.99	-0.272
0.7, 0.0	1.135	0.67	-0.039	1.023	0.82	-0.029
0.9, 0.3	1.195	0.33	-0.200	1.032	0.38	-0.051

Table 1: The extrapolated ground state energy and the convergence rate, from a fit to Eq. (19). The values of $N = 40$, 80, 160, 320, 640 were used for the fitting.

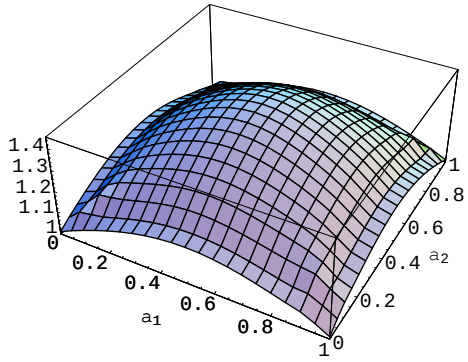
The same technique was used in Ref. [6] in the treatment of the three-anyon problem, the whole numerical algorithm being rather similar to the present one. The convergence there is much better close to the fermionic end $\alpha = 1$, where the wave functions are less singular; a certain symmetry between α and $1 - \alpha$ enabled one to altogether escape the region $0 < \alpha < 1/2$ with poor convergence. The trick does not work here, however: for all four values of (α_1, α_2) equivalent due to symmetry, convergence is about the same.

4 Results and discussion

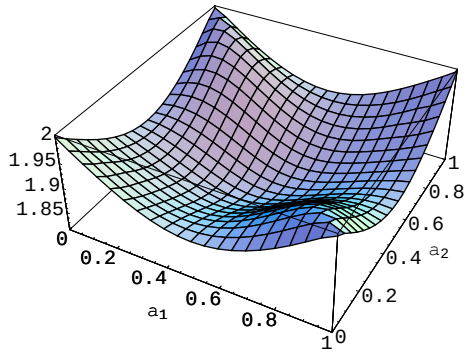
Shown on Fig. 2 are the energies of the three lowest states as functions of the impurity strengths at a fixed value of distance between impurities. The values $N = 80$, 160, 320, 640 were used for the extrapolation by means of fitting to Eq. (19). By qualitative analogy with the relative motion of two anyons, introducing the impurities with positive strength increases the (algebraic) mean value of the particle's kinetic angular momentum. Therefore, the energy increases if the angular momentum for zero impurity strengths is nonnegative, and decreases if it is negative. (Since in this case, eigenstates of the Hamiltonian are not eigenstates of the angular momentum, neither, in general, are the "correct" basis states at $\alpha_1 = \alpha_2 = 0$, into which the level splits as the impurities are turned on. However, the statement holds as pertaining to the mean value.)

A separate issue is the dependence of the levels on the distance between impurities. At $\rho_0 = 0$, the levels are given by Eq. (7) with $\alpha = \alpha_1 + \alpha_2$. At infinite ρ_0, one has the single-particle oscillator spectrum (6). For very small α_1 and α_2, there is a clear mapping between the two spectra, and with the change of ρ_0, each state will slowly interpolate into its counterpart. As the impurity strengths increase, levels come closer to crossing each other. However, as long as $\alpha_1 \neq \alpha_2$, there can be only avoided crossings, since there is no symmetry in the system. (Reflection with respect to the x axis reverses the signs of the α's.) A generic case is depicted on Fig. 3 (a).

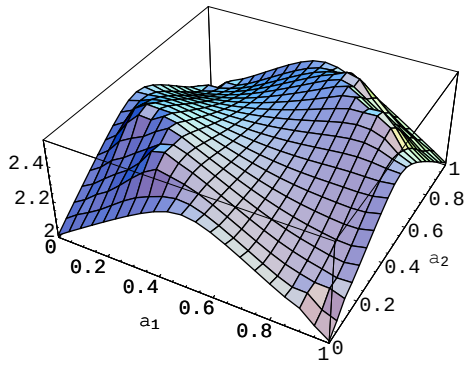
True crossings become possible for $\alpha_1 = \alpha_2$, when there is C_2 symmetry; cf. Fig. 3 (b). These will turn into avoided crossings when that symmetry is broken in any way—say, resulting from a change, no matter how small, in the position or strength of one of the impurities. Continuity is still maintained, however: If the change is small, so will be the minimal distance between the levels, and their wave functions will be mutually "flipping"



(a)



(b)



(c)

Figure 2: The energies of the ground state (a) and of the first two excited states (b,c) as functions of α_1, α_2, at $\rho_0 = 0.75$.

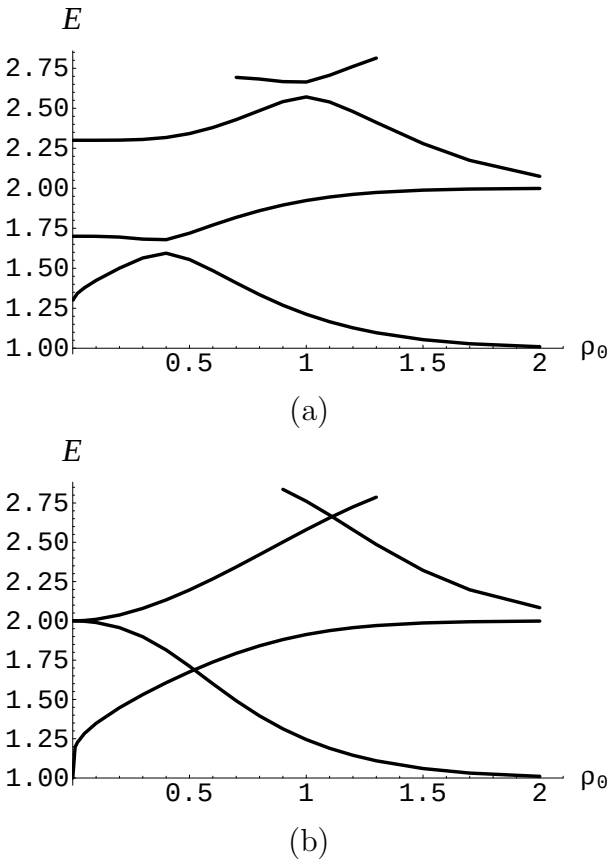


Figure 3: The energies of the ground state and of the first two excited states as functions of ρ_0: (a) $\alpha_1 = 0.4$, $\alpha_2 = 0.3$, (b) $\alpha_1 = \alpha_2 = 0.5$.

in the narrow region near the avoided crossing—so that the overall picture will be little different from a true crossing.

There is one more peculiarity in our second example, which arises whenever $\alpha_1 + \alpha_2$ is an integer—in this case, 1. (The spectrum is then the same at zero and infinite ρ_0.) For small ρ_0, the ground state energy behaves nonperturbatively, $\partial\mathcal{E}_0/\partial\rho_0|_{\rho_0=0}$ turning infinite. This is due to the fact that in this and only this case, the wave function of the ground state (and indeed of all states with zero angular momentum) is not singular for $\rho_0 = 0$ but becomes singular when the two impurities are split up. The same reason is responsible for the breakdown of perturbation theory which has been long known in pertinence to the A-B problem: A direct attempt to treat a weak flux as a perturbation and to build up an expansion in α fails for the ground state, because its singular wave function, r^α with a small α, cannot be obtained from the regular unperturbed wave function, r^0, by perturbation. A special treatment is needed in order to enable perturbation theory to produce the correct answer [8].

States with nonzero angular momentum, on the contrary, have $\partial\mathcal{E}_0/\partial\rho_0|_{\rho_0=0} = 0$, since their wave functions vanish at the origin fast enough.

One final remark is in order concerning the case of big distances. At any $\rho_0 \gg 1$, there will exist states whose wave functions are situated almost totally inside the ρ_0 circle, as well as ones (high enough in the spectrum) whose wave functions are almost totally outside. Thus, while it is true that any given level will, at big enough ρ_0, assume its integer value which it has in the absence of impurities,—at any given ρ_0, no matter how big, there exist infinitely many levels whose energies tend to their $\rho_0 = 0$ values. As is commonly the case when there are two competing parameters, the order of limiting transitions is crucial. In practice, an energy cutoff will be ensured by a finite temperature; and the presence of the impurities will not be felt when the distance between them is much greater than the thermal wavelength.

To conclude, we have construed a numerical algorithm for the solution of the problem of a particle coupled to two magnetic impurities in two dimensions, and found several low-lying states. It would be quite straightforward to generalize this to any number of impurities on a circle: The integrated boundary conditions would still have the form akin to (16), with just the matrix elements modified. Of course, for more than two impurities, placing them all on one circle is a loss of generality (not so for two impurities in the thermodynamic limit, when the center of the harmonic potential ceases to exist). With several impurities not on one circle, the boundary conditions would be more complicated, but in principle still solvable.

Evaluating the partition function of the system considered here and inferring the probability distribution of winding numbers of a particle around two fixed points on a plane is left for future work.

References

[1] Y. Aharonov, D. Bohm, Phys. Rev. 115 (1959) 485; for an earlier description of the same effect, see W. Ehrenberg and R.W. Siday, Proc. Phys. Soc. London, B62 (1949) 8.

[2] J.M. Leinaas, J. Myrheim, Nuovo Cimento 37B (1977) 1; G.A. Goldin, R. Menikoff, D.H. Sharp, J. Math. Phys. 21 (1980) 650; 22 (1981) 1664; F. Wilczek, Phys. Rev. Lett. 48 (1982) 1144; 49 (1982) 957.

[3] R. Laughlin, Phys. Rev. Lett. 60 (1988) 2677.

[4] J. Desbois, C. Furtlehner, S. Ouvry, Nucl. Phys. B[FS] 453 (1995) 759.

[5] A. Comtet, J. Desbois, S. Ouvry, J. Phys. A: Math.Gen. 23 (1990) 3563; for a recent attempt concerning the two-point winding number distribution, see O. Giraud, A. Thain, J.H. Hannay, J. Phys. A: Math.Gen. 37 (2004) 2913.

[6] S. Mashkevich, J. Myrheim, K. Olaussen, R. Rietman, Phys. Lett. B348 (1995) 473; S. Mashkevich, J. Myrheim, K. Olaussen, Phys. Lett. B382 (1996) 124.

[7] For an earlier attempt, see P. Stovicek, Phys. Lett. A142 (1989) 5.

[8] J. McCabe, S. Ouvry, Phys. Lett. B260 (1991) 113; A. Comtet, S. Mashkevich, S. Ouvry, Phys. Rev. D52 (1995) 2594; S. Mashkevich, Phys. Rev. D54 (1996) 6537.

[9] M. Abramowitz, I. Stegun, *Handbook of Mathematical Functions*, Dover, New York (1965).