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Path integral calculation of the writhe for circular semiflexible polymers

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Abstract. Earlier obtained numerical and analytical (non-path-integral) results for the writhe of a circular polymer are reproduced exactly employing the available path integral models for the semiflexible chains. It is confirmed analytically that the average writhe scales with the root of the chain length. We also briefly discuss related topological problems (e.g. knotting of circular polymers), which could be formulated and solved with the use of path integrals.

1. Introduction

Recently [1–3] there have appeared a number of papers which analyse the writhe of self-avoiding polygons placed on three-dimensional ($\mathbb{R}^3$) lattices. Both, analytical and Monte Carlo results were reported with the purpose of gaining some insight into the entanglement complexity of the self-avoiding polymers in solution. The entanglement complexity is believed to affect the coil-soluble transition [4, 5], as well as the rheological properties [6, 7] of polymer solutions. To estimate the effects of entanglement complexity, the following procedure is suggested [8, 9]. Generate numerically a knotted ring. Consider its projection into some arbitrary two-dimensional ($\mathbb{R}^2$) plane. Then count the number of crossings (over and under) along the contour of the projected image of a circle in the plane. Repeat the same procedure for other planes and take an average of the obtained numbers (i.e. make an average over the possible orientations of the plane). The so obtained entanglement complexity number $\langle C\rangle$ for a 'polymer' chain of length N follows a scaling law and was estimated to be

$$\langle C\rangle \propto N^{\alpha_c} \tag{1.1}$$

where $1 < \alpha_c < 2$. Monte Carlo calculations performed in [2] produce $\alpha_c \simeq 1.222 \pm 0.005$.

Unfortunately, an analytical expression for $\langle C\rangle$ is unknown and, hence, we must rely, so far, only on the Monte Carlo data. A more accessible quantity is the average writhe number which is closely related to $\langle C\rangle$. It can be defined in precise analytical terms such that the average writhe can be computed analytically. The present work provides an attempt to perform such a calculation. The writhe of a curve can be defined as follows [1, 2, 10, 11]. We assign a direction to a $\mathbb{R}^3$ curve and project it into a $\mathbb{R}^2$ plane specified by the unit vector $\boldsymbol{n}$ normal to this plane. The projection of a curve in this plane also carries a direction inherited from its 3D pre-image. We also count crossings, as before, but this time we assign $+1$ (or -1) for each over (under) crossing. The obtained result should also be averaged over

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all $\boldsymbol{n}$ directions. If, in addition, the averaging over directions along the curve is performed, then the average writhe $\langle W_r \rangle$ is zero by symmetry. The writhe is defined as

$$W_r = \frac{1}{4\pi} \oint_C \oint_C \mathrm{d}\boldsymbol{r}(\tau) \times \mathrm{d}\boldsymbol{r}(\tau') \frac{(\boldsymbol{r}(\tau) - \boldsymbol{r}(\tau'))}{|\boldsymbol{r}(\tau) - \boldsymbol{r}(\tau')|^3} \tag{1.2}$$

where C is the contour of the path and $\boldsymbol{r}(\tau)$ the location of a point on the curve C at contour position τ. To obtain the non-zero result for the writhe we have either to consider $\langle |W_r| \rangle$, as is done in [1], or to consider the average writhe for the fixed orientation of the curve. In the last case the quantity $\langle W_r \rangle$ could be both positive and negative. Taking the absolute value of this quantity (or using $\langle |W_r| \rangle$ instead), the averaged expression for the writhe is expected to behave as

$$\langle |W_r| \rangle \propto N^{\alpha} \tag{1.3}$$

where α is numerically found to be [2] $\geqslant 0.5$. This result is in excellent agreement with an earlier obtained analytic estimate of the exponent α [1] which provides $\alpha = 0.5$. Since the analytic result of [1] was obtained without any use of the existing polymer models, it is of interest to analyse this result using known path integral models of polymers. In this paper we provide an explicit calculation based on the path integral formulation for semiflexible polymers which we have already discussed earlier in [12].

2. Description of the model and statement of the problem

In order to provide an analytical theory for the scaling of the writhe with the length N of the path, we define the partition function for a semiflexible ring polymer by

$$\begin{aligned} Z &= \int \mathrm{d}\boldsymbol{u}\, G(\boldsymbol{u}_{\mathrm{i}} = \boldsymbol{u}_{\mathrm{f}} = \boldsymbol{u}; N) \\ &= \int \mathrm{d}\boldsymbol{u} \int_{\boldsymbol{u}_{\mathrm{i}}(0) = \boldsymbol{u}_{\mathrm{f}}(N)} D[\boldsymbol{u}(\tau)] \prod_{\tau} \delta(\boldsymbol{u}^2(\tau) - 1) \exp\left[-\frac{1}{2}\gamma \int_0^N \mathrm{d}\tau \left(\frac{\partial \boldsymbol{u}}{\partial \tau} \right)^2 \right] \end{aligned} \tag{2.1}$$

where $\boldsymbol{u}$ is the tangent vector, $\boldsymbol{u} = \mathrm{d}\boldsymbol{r}/\mathrm{d}\tau$ with $\boldsymbol{r}(\tau)$ having the same meaning as in (1.2). The coupling constant γ represents the bending rigidity modulus of the chain [12–14], so that the exponent in the path integral represents the integration over the contour of the square of the local curvature of the polymer chain, i.e. the total bending energy. The path integral (2.1) is known in the polymer literature [12] to represent a Kratky–Porod (KP) chain with bending energy γ [13].

To compute the average of the writhe W_r, we introduce a generating functional

$$Z(g) = \int D[\boldsymbol{u}(\tau)] \prod_{\tau} \delta(\boldsymbol{u}^2(\tau) - 1) \exp\left[-\frac{1}{2}\gamma \int_0^N \left(\frac{\partial \boldsymbol{u}}{\partial \tau} \right)^2 \mathrm{d}\tau + \mathrm{i}g W_r[\boldsymbol{u}(\tau)] \right] \tag{2.2}$$

and obtain the averaged writhe

$$\langle W_r \rangle = \frac{1}{\mathrm{i}} \frac{\partial \ln Z(g)}{\partial g}. \tag{2.3}$$

The imaginary i-factor is introduced here for convenience to show the correspondence to the analogous quantum problem. Thus defined average writhe is non-zero only for the fixed

orientation of the curve, as we have mentioned in section 1. Alternatively, by using the identity

$$\exp(-|x|) = \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}y\, \frac{\exp(\mathrm{i}xy)}{1+y^2} = \Theta(x)\mathrm{e}^{-x} + \Theta(-x)\mathrm{e}^{x} \tag{2.4}$$

where $\Theta(x)$ is a step function, we could calculate $\langle |W_r| \rangle$. This time the imaginary i-factor would occur quite naturally. Use of (2.4) in (2.2) will, nevertheless, not affect the logic and the technical evaluation of the mathematical expressions involved in the rest of our calculations. Therefore, we prefer to work directly with equation (2.2). Equation (2.2) can be related to the exactly solvable quantum mechanical problem. In our previous work [15] we have emphasized that the real three-dimensional curve should be described by the curvature and the torsion. The torsion term can be formally added to the exponent of (2.1) in a variety of ways (as discussed later in section 4). We, however, will choose only one way of incorporating the torsion term. Following Polyakov [16] and our earlier work [12], we replace the KP path integral (2.2) by the integral of the following form:

$$\begin{aligned} Z &= \int \mathrm{d}u\, G(\boldsymbol{u}_{\mathrm{i}} = \boldsymbol{u}_{\mathrm{f}} = \boldsymbol{u}; N) \\ &= \int \mathrm{d}\boldsymbol{u} \int D[\boldsymbol{u}(\tau)] \prod_{\tau} \delta(\boldsymbol{u}^2 - 1) \\ &\quad \times \exp\left\{ -\frac{\gamma}{2}\int_0^N \mathrm{d}\tau \left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\tau}\right)^2 + \mathrm{i}\Theta \int_0^N \mathrm{d}\tau\, C[\boldsymbol{u}(\tau)] \right\} \end{aligned} \tag{2.5}$$

where $C[\boldsymbol{u}(\tau)]$ is the torsion of the curve, which is related to the self-linking number Ψ of the same curve according to the White theorem [10, 11] as

$$\Psi = T_W + W_r \tag{2.6}$$

and θ is a coupling constant related to g (see below). In view of the results obtained in [17], the twisting number T_W is defined by

$$T_W = -\frac{1}{2\pi}\int_0^N \mathrm{d}\tau\, C[\boldsymbol{u}(\tau)]. \tag{2.7}$$

Combining the last two equations, we obtain

$$W_r = \Psi - T_W. \tag{2.8}$$

In addition, using the results of [12, 16] we can write

$$\int_0^N \mathrm{d}\tau\, C[\boldsymbol{u}(\tau)] \stackrel{\circ}{=} \int_0^N \mathrm{d}\tau \int_0^N \mathrm{d}\tau'\, \boldsymbol{u}\cdot\left(\frac{\partial \boldsymbol{u}}{\partial \tau}\times\frac{\partial \boldsymbol{u}}{\partial \tau'}\right) \tag{2.9}$$

where $\stackrel{\circ}{=}$ indicates equality up to, for the present purpose, an unimportant number (in our case Ψ is just a pure number [18]) which can be discarded.

We have discussed in some detail the treatment of the path integral given by (2.2) (together with (2.9)) in a previous work [12], therefore here we only provide the results needed directly for the present calculations. Combining equations (2.5) and (2.9) produces a propagator which describes formally the Dirac monopole in quantum mechanics. In appendix A we provide details which furnish some of the basic properties of such path integrals and their implications. Here, we only state that the Schrödinger-like equation for the propagator given by (2.5) can be solved *exactly* [19, 20] and has been recently discussed in [12, 21, 22]. We shall utilize its known solution in the next section (and appendix B)

while here we only notice that the coupling constant $g = 2\pi\Theta$ in the quantum case cannot be arbitrary. It has been shown in detail [20–23] that in the quantum case 2Θ should be an integer $2\Theta = 0, \pm 1, \pm 2, \ldots$. In the present polymer problem, an arbitrary value for g is used to calculate the average writhe. Therefore, we assume first that g is continuous, as was done earlier in [24]. Then we can formally use (2.3) to calculate the average writhe. After this procedure we restore the discreteness of g as required.

To compare the results of our calculations with the Monte Carlo results of [1–3], we would like to notice that, according to earlier obtained results [12], the non-zero values of g influence considerably the stiffness of the polymer chain. Since, in the reported numerical calculations, only the self-avoidance constraint was implemented, this means that the effective rigidity of the chain was sufficiently low. Under these conditions we can *formally* rewrite (2.3) as

$$\langle W_r(R)\rangle = \lim_{g\to 0} \frac{1}{\mathrm{i}} \frac{\partial}{\partial g} \ln Z(g, N). \tag{2.10}$$

Some care must be taken when the actual calculations in this limit are made as it will become clear in the next section. At the same time we would like to notice that, because the partition function (2.5) can be calculated exactly, there is no need to require $g = 0$ in general. Notice that in the Monte Carlo (MC) simulations random walk chains are used. In the present work we model the polymers by semiflexible chains. We then have two additional parameters, i.e. γ and g, which can be accounted in the future MC simulations. Equation (2.10) represents a kind of 'linear response', i.e. a Kubo-like result, where the average is made over the unperturbed 'equilibrium' system.

3. Calculation of the averaged writhe

By the explicit use of the results presented in appendix A, as well as those from [12, 16], it is easy to recognize that for $g = 0$ the partition function $Z(g, N)$ is just that for quantum rotator [25] and, whence, can be written at once in terms of the corresponding eigenvalues:

$$Z(g = 0, N) = \sum_{j=0}^{\infty} (2j + 1) \exp\left\{-\frac{N}{2\gamma} j(j + 1)\right\}. \tag{3.1}$$

It is well known that this sum cannot be calculated in the closed form. However, we can approximately formally replace the summation by the integration in (3.1). This leads to the following semiclassical approximation [25]:

$$Z(g = 0, N) \approx \int_0^{\infty} \mathrm{d}x\, 2x \exp\left\{-\frac{N}{2\gamma} x^2\right\} = \frac{2\gamma}{N}. \tag{3.2}$$

In the case of finite g, i.e. for the corresponding Dirac monopole problem, we have an expression similar to (3.1). Indeed, it was shown that the energy levels are given by [22]

$$E_j = \frac{1}{2\gamma}[j(j + 1) + |g|(2j + 1)] \tag{3.3}$$

which is just a combination of the rigid rotator and the harmonic oscillator energy levels. This observation is very important for the present problem as we shall demonstrate shortly. The energy level E_j is degenerate. Its degeneracy is given by

$$\text{degeneracy}(j\text{th level}) = 2|g| + 2j + 1. \tag{3.4}$$

The use of (3.3) and (3.4) allows us to compute the generating function for finite g (Dirac monopole) as

$$Z(g, N) = \sum_{j=0}^{\infty} (2|g| + 2j + 1) \exp\{-N E_j\} \tag{3.5}$$

where the E_j are given by (3.3). Obviously, the new partition function is reducible to that given by (3.1) as required.

With the help of (3.5), the average writhe can now be formally calculated according to (2.3) (or (2.10)). However, we immediately run into the following problem. Equations (2.3) and (2.10) both contain an imaginary i-factor, while the partition function given by (3.5) is manifestly real, so that if we use (3.5) for calculation of $\langle W_r \rangle$ we obtain formally an imaginary result. This fact is *not* a mistake in our arguments and it does have a deep physical meaning. We provide an explanation of this point in appendix B. Here, we only state that the imaginary i-factor in equations (2.3) and (2.10) is an artifact of the formal manipulations with the path integrals. More careful analysis performed in [22] (and outlined in appendices A and B) allows us just to ignore the i-factor in these equations. This is true if the sign of g in (2.2) is fixed in the rest of our calculations. If it is not fixed *a priori*, then equation (2.3) should be used in combination with equation $|x| = \Theta(x)x - \Theta(-x)x$ in (3.5) and the imaginary i-factor reappears. Use of the modulus sign in (3.5) leads to non-analyticity of this partition function at $g = 0$ so that formally equation (2.10) cannot be used in combination with (3.5). To remove this problem, we have to make a decision about the sign of g at the very beginning of our calculations, e.g. in equation (2.2). The choice of the sign has some physical meaning, as will be explained shortly. If we choose $g > 0$, for example, then we obtain

$$\langle |W_r| \rangle = \frac{1}{Z(g, N)} \left[2 \sum_{j=0}^{\infty} \exp\{-N E_j\} + \sum_{j=0}^{\infty} (2j + 1)(2g + 2j + 1) \exp\{-N E_j\} \right]. \tag{3.6}$$

If we now let $g \to 0^+$ and replace the summation in (3.6) by the integration in the same fashion as in (3.2), we obtain formally

$$\langle |W_r| \rangle = \frac{N}{2\gamma} \left[\sqrt{\frac{2\gamma\pi}{N}} + \text{const} \frac{\gamma^{3/2}}{N^{3/2}} \right] \propto \sqrt{\frac{N}{\gamma}} + \text{O}\left(\frac{1}{\sqrt{N}} \right). \tag{3.7}$$

which is the central result of our paper, i.e. the average writhe $\langle |W_r| \rangle$ scales with the square root of the chain length, $\sqrt{N}$.

On the other hand, if we select $g < 0$, then (2.10) we get, instead of (3.7), $\langle |W_r| \rangle \propto -\sqrt{N}$. Therefore the algebraic sum of (3.7) and this result would lead to zero, which is in complete agreement with our discussion in section 1 about the average writhe. The choice of sign for g, thus, is equivalent to the choice of orientations of our closed curve. The obtained results are in complete agreement with earlier obtained numerical and analytic results of [1–3].

4. Discussion

In summary, we have succeeded in calculating the scaling behaviour of the writhe for semiflexible polymers by using the path integral methods. Several questions remain to be discussed. Recently, there appeared several papers dealing with supercoiling of DNA, which employ the classical mechanics formalism [14, 30–34] for the calculation of the elastic energy and the conformations for (super)coiled DNA. Therefore, the question arises

of how one can use the results of these works in order to calculate the average writhe. Unfortunately, we cannot provide a complete answer to this question. Instead, we only notice that the classical models discussed in these papers cannot be straightforwardly quantized using the canonical formalism as discussed in appendices A and B. Accordingly, the corresponding Schrödinger-like equations would be much harder to obtain and to solve. Since the calculations presented in section 3 are effectively performed at the semiclassical level, it would be of interest to reobtain the spectrum, e.g. similar to that given by (3.3), using semiclassical methods.

In the simulations of [1–3] dependence of the obtained results on the solvent quality have been investigated. The results indicate that the scaling of the average writhe does not depend on the solvent quality (i.e. good or bad solvent). So far, our calculations have been carried out without any excluded volume interactions (see equations (2.1)–(2.3)). However, we do not expect any changes when these interactions are taken into account, because the topological quantities do not couple strongly to the monomer densities, e.g. in our earlier work [35] it was demonstrated that the contribution of coupling terms between the density (excluded volume) and the tangent vector, i.e.

$$\int_0^N \langle \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}(\tau)}(\boldsymbol{u}(\tau)\cdot\boldsymbol{k})\rangle \,\mathrm{d}\tau$$

are negligible.

We also indicate what other topological properties of polymers could be calculated by use of path integral methods. To this purpose, let us consider the problem of knot formation. In the physical literature this problem was formulated first by Delbrück [36] and is known as 'Delbrück conjecture' [37]. Delbrück had conjectured that for $N \to \infty$ the probability P_N of knot formation is asymptotically close to one. More precisely, if we generate random walks of N steps on the regular $\mathbb{R}^3$ lattice, then among those walks which are closed and have a large number of steps N, only a fraction of measure zero will be unknotted. The analytic form of N-dependence for P_N was recently obtained by Sumners and Whittington [38] and, independently, by Pippenger [39] as discussed in [37], where some refinements of these important results are presented also.

Nevertheless, the problem of knot formation was discussed by mathematicians much earlier in somewhat different terms. We have found these alternative formulations are much better suited for treatment in terms of path integrals.

As has already been noticed in [37], Milnor made two remarkable and related discoveries [40]. Firstly, he proved that 'if the curve is knotted, there must be a plane which intersects in at least six points'. This fact can help to detect knots generated by Monte Carlo methods. Second, if $k(\tau)$ is the local curvature, then the contour integral is

$$\int_0^N \mathrm{d}\tau\, |k(\tau)| > 4\pi \tag{4.1}$$

if the closed curve is knotted and

$$4\pi > \int_0^N \mathrm{d}\tau\, |k(\tau)| \geqslant 2\pi \tag{4.2}$$

if the curve is unknotted [41, 42]. More recent related results could be found in [43–45]. Connections between the Alexander polynomial and these differential geometric results have already been made in Milnor's work [41] where he also provided an estimate for the combination

$$S = \int_0^N \mathrm{d}\tau\, |k(\tau)| + \int_0^N \mathrm{d}\tau\, |C(\tau)| \geqslant 2\pi n \tag{4.3}$$

where n is a positive integer (for unknot $n = 1$) and $C(\tau)$ is the torsion of the curve (e.g. see equation (2.5)). The path integrals with the action S given by (4.3) have recently been discussed by particle physicists [46] and in polymer physics [47, 48] in connection with the problem of ionic strength dependence of the electrostatic persistence length for polyelectrolyte chains. It remains to use these path integrals in order to check the results of (4.1) and (4.2) quantum mechanically.

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Note added in proof. After this paper had been accepted for publication we found that Yor [49], using stochastic calculus, had also obtained results which indirectly lead to our equation (3.7) (for example, see theorem 7.5 of [49]). This method of derivation is completely different from that used in [1] and in this work. Recently we have also succeeded in calculating (1.1) analytically and calculating the topological persistence length (i.e. the minimal number of steps on the lattice needed to form the first non-trivial knot) using Milnor's inequalities (4.1) and (4.2) [50].

Appendix A. Classical mechanics of the Dirac monopole problem and its quantum analogue

According to (2.5) the classical actions for the monopole problem can be written as

$$S[\boldsymbol{u}] = \frac{\gamma}{2}\int_0^N \mathrm{d}\tau \left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\tau}\right)^2 + \mathrm{i}\Theta\int_0^N \mathrm{d}\tau\, C[\boldsymbol{u}(\tau)] \tag{A1}$$

where the end of the vector $\boldsymbol{u}$ is lying on the unit sphere $\boldsymbol{u}^2 = 1$. Instead of adding the Lagrange multiplier to S, which accounts for this constraint, it is more convenient to rewrite S in the form which obeys this constraint from the very beginning. For this purpose we can re-express the vector $\boldsymbol{u}$ as follows [12, 13]:

$$\boldsymbol{u} = (Z^+\boldsymbol{\sigma}Z) \tag{A2}$$

where $\boldsymbol{\sigma}$ are Pauli matrices, $\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \sigma_3\}$ and Z is a two-component vector. Because $\sigma_i^2 = \mathbf{I}$ where $\mathbf{I}$ is the unit matrix ($i = 1$–3) we should require

$$\boldsymbol{u}^2 = |Z_1|^2 + |Z_2|^2 = 1. \tag{A3a}$$

Furthermore, let $Z_1 = x_1 + \mathrm{i}x_2$ and $Z_2 = x_3 + \mathrm{i}x_4$, then

$$u_1 = (x_1 - \mathrm{i}x_2, x_3 - \mathrm{i}x_4)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}x_i + \mathrm{i}x_2\\ x_3 + \mathrm{i}x_4\end{pmatrix} = 2(x_1x_3 + x_2 - x_4) \tag{A3b}$$

and, analogously,

$$u_2 = 2(x_1x_4 - x_2x_3) \tag{A4}$$

$$u_3 = x_1^2 + x_2^2 - x_3^2 - x_4^2 \tag{A5}$$

so that the constraint (A3) becomes

$$x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1. \tag{A6}$$

Now, if

$$Z_1 = \mathrm{e}^{\mathrm{i}\chi}\cos(\theta/2) \qquad Z_2 = \mathrm{e}^{\mathrm{i}(\varphi+\chi)}\sin(\theta/2) \tag{A7}$$

then we obtain with the help of (A3)–(A5) more familiar results:

$$\begin{aligned} u_1 &= \sin\theta\cos\varphi \\ u_2 &= \sin\theta\sin\varphi \\ u_3 &= \cos\theta. \end{aligned} \tag{A8}$$

With such parametrization, let us consider the term $(\mathrm{d}\boldsymbol{u}/\mathrm{d}\tau)^2$ in (A1). It is shown in [26] that

$$\frac{1}{2}\left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\tau}\right)^2 = 2\dot{Z}^\dagger\dot{Z} - 2a^2 \tag{A9}$$

where $\dot{Z} = \mathrm{d}Z/\mathrm{d}\tau$, etc and

$$a = \mathrm{i}Z^\dagger\dot{Z}. \tag{A10}$$

With the help of the above results the action S given by (A1) can be written as

$$S = 2\int_0^N \mathrm{d}\tau\,[\gamma\{\dot{Z}^\dagger\dot{Z} - a^2\} - 2\Theta a] \tag{A11}$$

where $2\Theta = 0, \pm 1, \pm 2$, if the system is to be quantized.

Now let

$$\mathbf{S} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}(\alpha+\delta)/2}\cos(\beta/2) & \mathrm{e}^{\mathrm{i}(\delta-\alpha)/2}\sin(\beta/2) \\ -\mathrm{e}^{-\mathrm{i}(\delta-\alpha)/2}\sin(\beta/2) & \mathrm{e}^{\mathrm{i}(\alpha+\delta)/2}\cos(\beta/2) \end{pmatrix} \tag{A12}$$

where α, β, δ are the Euler's angles. It can be shown (26) that

$$\mathrm{tr}(\dot{\mathbf{S}}^+\dot{\mathbf{S}}) = 2\dot{Z}^\dagger\dot{Z} \tag{A13}$$

and

$$a = \tfrac{1}{2}\,\mathrm{tr}(\sigma_3\mathbf{S}^{-1}\dot{\mathbf{S}}). \tag{A14}$$

Using these relations it is possible to write

$$\mathrm{tr}(\dot{\mathbf{S}}^+\dot{\mathbf{S}}) = \tfrac{1}{2}\dot{\beta}^2 + \tfrac{1}{2}(\dot{\delta} + \dot{\alpha}\cos\beta)^2 + \tfrac{1}{2}\dot{\alpha}^2\sin^2\beta. \tag{A15}$$

The above expression coincides exactly with that for the kinetic energy of the symmetric top (e.g. see [27], equation (4.83), and choose the moments of inertia $I_1 = I_3 = I = 1$ in this equation). Combining these results with (A11) we obtain an equation for the asymmetric top, e.g. see [12] and appendix B. The quantum mechanics for the symmetric top can now be developed in a usual way [27] via the Hamiltonian formalism with subsequent replacement of the classical commentators by the quantum mechanical ones. The same procedure for the asymmetric top produces the corresponding Schrödinger equation for the Dirac monopole. What is important for us, however, is that the action S given by (A11) *does not* contain an imaginary i-factor discussed in the main text. This fact will be further explained in appendix B.

Appendix B. Geometry of the quantum Dirac monopole problem

Following [18] and our earlier work [28] it can be shown that

$$\Theta \int_0^N \mathrm{d}\tau\, C[\boldsymbol{u}(\tau)] = \int_0^N \mathrm{d}\tau\, \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\tau} \cdot \boldsymbol{A}[\boldsymbol{u}(\tau)] \tag{B1}$$

where the vector potential $\boldsymbol{A}$ is given by (22)

$$\boldsymbol{A} = \left(-\frac{g u_2}{1+u_3}, \frac{g u_1}{1+u_3}, 0 \right) \tag{B2}$$

with u_1, u_2 and u_3 being given in (A8).

Once we recognize that such a vector potential representation is possible, we can immediately use the quantum mechanical correspondence rules [29] which imply that the Schrödinger-like equation should look like

$$\mathrm{i}\frac{\partial \Psi}{\partial t} = \frac{1}{2}(-\mathrm{i}\nabla - \boldsymbol{A})^2 \Psi \equiv \hat{H}\Psi \tag{B3}$$

where we have rescaled all variables to absorb the dimensional constants. In view of the discussion presented in section 3 and in appendix A, the Hamiltonian $\hat{H}$ should respect the spherical symmetry of the problem. Explicit calculation [22] produces

$$2\hat{H} = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{2\mathrm{i}g}{1+\cos\theta}\frac{\partial}{\partial\varphi} + g^2\left(\frac{1-\cos\theta}{1+\cos\theta}\right). \tag{B4}$$

The Schrödinger-like equation with such a defined Hamiltonian was solved long ago [20] by Tamm. However, the solution which he obtained is not illuminating. To make it more transparent, use of the stereographic projection is the most helpful. This projection converts initially a three-dimensional problem to that in the plane. We have demonstrated earlier [7], that in the plane, use of complex variables is most convenient. In the present case we introduce the complex variable Z and its conjugate $\bar{Z}$ so that the stereographic projection is achieved by writing

$$\begin{aligned} Z &= \sqrt{2g}\mathrm{e}^{\mathrm{i}\varphi}\tan\left(\frac{\theta}{2}\right) \\ \bar{Z} &= \sqrt{2g}\mathrm{e}^{-\mathrm{i}\varphi}\tan\left(\frac{\theta}{2}\right). \end{aligned} \tag{B5}$$

In terms of such introduced complex variables the Hamiltonian $\hat{H}$ acquires the following form:

$$\hat{H}/g = -\left(1+\frac{|Z|^2}{2g}\right)\bar{\partial}\partial - \frac{1}{2}\left(1+\frac{|Z|^2}{2g}\right)(Z\partial - \bar{Z}\bar{\partial}) + \frac{1}{4}|Z|^2 \tag{B6}$$

where $\partial = \partial/\partial Z$, $\bar{\partial} = \partial/\partial\bar{Z}$, $|Z|^2 = Z\bar{Z}$, etc.

In the limit $g \to \infty$ the right-hand side of (B6) coincides exactly with the Landau Hamiltonian for a non-relativistic particle in a constant magnetic field, which we have discussed extensively in [7] (e.g. see (2.9) of [7]). This explains why the monopole spectrum given by (3.3) contains the harmonic oscillator part. In the opposite limit, $g \to 0$, the oscillator-like term (i.e. $\frac{1}{4}|Z|^2$) vanishes and we obtain the rigid rotator problem. The path integral based on the Hamiltonian (B6) will not contain an imaginary i-factor (e.g. see (6.8) of [18]) and, hence, there is no need to use 1/i-factors in equations (2.3) and (2.10) if the corresponding path integrals are written with explicit account of the existing geometrical constraints.

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