

Spin tunneling in the *kagomé* antiferromagnet

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The collective tunneling of a small cluster of spins between two degenerate ground-state configurations of the *kagomé*-lattice quantum Heisenberg antiferromagnet is studied. The cluster consists of the six spins on a hexagon of the lattice. The resulting tunnel-splitting energy Δ is calculated in detail, including the prefactor to the exponential $\exp(-\mathcal{S}_0/\hbar)$. This is done by setting up a coherent-spin-state path integral in imaginary time and evaluating it by the method of steepest descent. The hexagon tunneling problem is mapped onto a much simpler tunneling problem, involving only one collective degree of freedom, which can be treated by known methods. It is found that for half-odd-integer spins, the tunneling amplitude and the tunnel-splitting energy are exactly zero, because of destructive interference between symmetry-related (+) instanton and (-) instanton tunneling paths. This destructive interference is shown to occur also for certain larger loops of spins on the *kagomé* lattice. For small, integer spins, our results suggest that tunneling strongly competes with in-plane order-from-disorder selection effects; it constitutes a disordering mechanism that might drive the system into a partially disordered ground state, related to a spin nematic.

I. INTRODUCTION

Consider a Heisenberg antiferromagnet (AFM) with nonrandom but competing exchange interactions. The classical ground state is often nontrivially nonunique, in having a continuous manifold of inequivalent (but degenerate) ground states. However, if one takes account of quantum and thermal fluctuations around the classical ground states, the nontrivial degeneracy may be broken. The effects of fluctuations can generally be represented by an effective "selection" Hamiltonian, which is a function of the classical spin directions and "selects" certain ground states (sometimes having long-range order) in favor of others. Since long-range order can thus be induced out of an apparently disordered manifold of ground states, such selection effects are called "ordering due to disorder".¹

An effect that *competes* with "order-from-disorder" selection effects is tunneling between different ground-state configurations. Tunneling tends to drive the system into a superposition of degenerate states rather than selecting a particular one. Hence, in the regions of parameter space in which tunneling events are important, they could suppress order-from-disorder selection effects.

In this paper we study spin tunneling in a two-dimensional (2D) quantum Heisenberg antiferromagnet on a *kagomé* lattice.²⁻⁵ This is a frustrated spin system with a very large ground-state degeneracy, in which various selection effects have been investigated.⁴⁻⁸ We study tunneling events that involve the rigid simultaneous rotation of small groups of spins (in particular a mode involving only the six spins on a *kagomé* hexagon). We find, rather unexpectedly, that the tunneling amplitudes are zero when the spin s is a half-odd integer, but nonzero when s is integer. This is due to destructive interference between two topologically distinct tunneling paths con-

necting the same initial and final states. The interference occurs when the tunneling amplitudes have different topological phase factors.^{9,10} Therefore there should be interesting integer vs half-odd-integer s effects for that range of s values for which tunneling effects are as strong as or stronger than selection effects: Systems with integer s would have a greater tendency to be disordered because tunneling suppresses selection effects, whereas systems with half-odd-integer s , where tunneling is absent, would tend to be ordered.

Apart from studying the role of tunneling in the *kagomé* lattice, we hope that this paper will provide an instructive example of a rather nontrivial spin-tunneling calculation. As is customary, the tunneling amplitude of interest is calculated by setting up a coherent-spin-state path integral in imaginary time and evaluating it by the method of steepest descent,¹¹ which is an expansion in powers of $1/s$. Our calculation includes a complete evaluation of the prefactor to the exponential $e^{-\mathcal{S}_0/\hbar}$ (\mathcal{S}_0 is the classical action), and a discussion of the integration ranges of the spin-path integral (these ranges are finite originally but need to be extended to infinity to allow an evaluation of the prefactor). Although the calculation of tunneling rates for spin systems has been of interest in various different contexts,¹²⁻¹⁶ we are aware of only one recent paper where such prefactors are calculated explicitly.¹⁶ Moreover, we show explicitly how one may give an exact treatment of the simultaneous collective motion of all the relevant spin degrees of freedom by reducing the problem to one involving only a single, collective degree of freedom. The reduced problem can be treated by methods well known from studying a particle in a double-well potential.

The results of our calculations suggest that for small, integer s , the tunneling amplitude is sufficiently large that tunneling can be regarded as a significant disordering mechanism, that tends to drive the system into a partially

disordered state, related to a spin-nematic state.^{6,17}

This paper is organized as follows: In Sec. II we review ground-state selection effects on the *kagomé* lattice, and describe the hexagon tunneling event that is to be studied in later sections. In Secs. III and IV we study a simple model Lagrangian, chosen such that it will be of use for the subsequent study of the *kagomé* system. Specifically, the calculations of the classical action \mathcal{S}_0 (Sec. III) and the tunnel-splitting energy Δ (Sec. IV) are presented in detail. Section V shows how the full hexagon tunneling problem can be mapped onto the simple model problem studied in earlier sections, and contains the main result of this paper, Eq. (5.36). In Sec. VI the occurrence of destructive interference during the tunneling of larger sets of spins on the *kagomé* lattice is discussed. There are four appendixes. In Appendix A an estimate is made of the size and shape of the coplanarity potential that we employ in Sec. V to study the hexagon tunneling problem. Appendix C contains a summary of results that are well known for a particle tunneling in a double well and are needed in Sec. IV.

II. THE KAGOMÉ ANTIFERROMAGNET

The *kagomé* lattice is a 2D triangular lattice with lattice constant a_0 , where sites have been removed at all sites of a triangular superlattice, with lattice constant $2a_0$ (see Fig. 1).¹⁸ The quantum Heisenberg AFM on this lattice has the Hamiltonian operator

$$\hat{\mathcal{H}} = J \sum_{\langle i,j \rangle} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j \quad (J > 0), \quad (2.1)$$

where $\hat{\mathbf{s}}_i$ is the spin vector operator for the i th spin and the sum runs over all nearest neighbors. Coherent spin states (see, e.g., Ref. 19) may be used to discuss this system in classical terms. Associate the coherent spin state $|\varphi_i, \theta_i\rangle$ with the i th spin, where the spherical coordinates $(\varphi_i, \theta_i) \equiv \Omega_i$ define a unit vector \mathbf{n}_i [Fig. 2(a)]. The well-known property $\langle \varphi_i, \theta_i | \hat{\mathbf{s}}_i | \varphi_i, \theta_i \rangle = s \mathbf{n}_i$, allows one to interpret \mathbf{n}_i as a “classical spin vector.” Also, a “classical” Hamiltonian \mathcal{H} may be introduced as the coherent-spin-state expectation value $\langle \hat{\mathcal{H}} \rangle$:

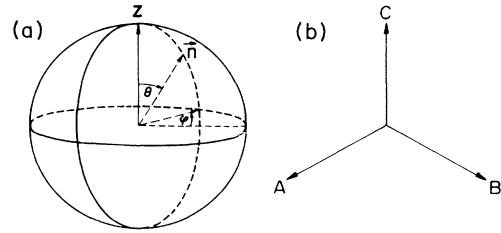


FIG. 2. (a) The unit vector $\mathbf{n} = (\varphi, \theta)$. (b) Types, A , B , and C spins on a triangle of the *kagomé* lattice. The common plane of A , B , and C , i.e., the “reference plane,” defines the $\varphi = 0$ and π directions in (a).

$$\begin{aligned} \mathcal{H} &\equiv \left[\prod_{i \in \otimes} \langle \varphi_i, \theta_i | \right] \hat{\mathcal{H}} \left[\prod_{i \in \otimes} | \varphi_i, \theta_i \rangle \right] \\ &= s^2 J \sum_{\langle i,j \rangle} \mathbf{n}_i \cdot \mathbf{n}_j \quad (J > 0). \end{aligned} \quad (2.2)$$

When referring to the “energy” of a state, we shall always mean this expectation value \mathcal{H} . Likewise, the term “ground state” will not be used to refer to an actual eigenstate of the operator $\hat{\mathcal{H}}$, but to a state that minimizes \mathcal{H} . It is this \mathcal{H} that is used in discussions of the classical *kagomé* antiferromagnet.

The energy is minimized by any configuration in which the total spin on *each* elementary triangle of the lattice is zero.^{2,6} In such states, the spins of any given triangle of the *kagomé* lattice lie in one plane, with relative angles of 120° [see Fig. 2(b)], forming a rigid unit in spin space. Because of the many ways of fitting such triangles together, the distinct classical ground states form a manifold with a dimensionality proportional to the system size.

A. Selection effects

It is convenient to describe the classical ground states with reference to a coplanar ground state, in which all spins lie in the same “reference plane.” All coplanar ground states can be constructed by labeling the sites by letters A , B , and C , such that each triangle has one of each, and then replacing the three kinds of letters by spins in three directions differing by 120° angles² [Fig. 2(b)]; these states correspond one to one to the ground states of a three-state Potts AFM on a *kagomé* lattice.

All noncoplanar classical states can be generated by continuous distortions of coplanar states, henceforth to be called “Potts states,” without crossing energy barriers.⁶ For example, any hexagon of six spins that is labeled only by two letters (e.g., $ABABAB$ in Fig. 1) can be rotated as a rigid unit in spin space by an angle φ around the C direction without any cost in classical energy. We shall refer to this mode as the “rigid-hexagon mode” (it has been discussed by Chandra *et al.*⁴ under the name “weathervane mode”). However, by expanding in spin waves about any given ground state, it has been shown that all noncoplanar states have a larger zero-point energy than the coplanar Potts states. This selection effect can be characterized by a parameter $J_b \sim \mathcal{O}(sJ)$, and ensures that the true ground state will be coplanar.^{4–8}

Further study, using a self-consistent approach, yields

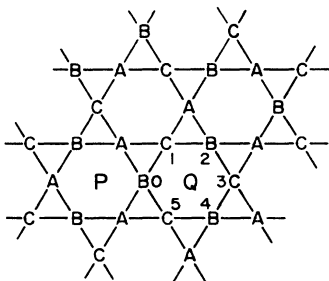


FIG. 1. The $\sqrt{3} \times \sqrt{3}$ ground state of the *kagomé* lattice. The letters A , B , and C represent the spin directions illustrated in Fig. 2(b). The symbols P and Q and the labels 0–5 are the ones used in Appendix A.

a smaller “in-plane” selection energy, of order $J_c \sim O(s^{2/3}J)$, which favors among all possible Potts states a particular state with long-range order, the so-called $\sqrt{3} \times \sqrt{3}$ ground state,^{5,7,8} depicted in Fig. 1. In this state, every hexagon is labeled by just two letters, e.g., *BCBCBC*. To encode the most important effects of this in-plane selection, it is convenient to define a “chirality” variable centered on each triangle, equal to -1 or $+1$ depending on whether the sites take values *ABC* in the clockwise or counterclockwise sense. In the $\sqrt{3} \times \sqrt{3}$ Potts state, the chiralities on neighboring elementary triangles are antiferromagnetically ordered. Another state with long-range order is the so-called $\mathbf{q}=0$ state, in which the spins around every hexagon are arranged in the order *ABCABC*, so that the chiralities on neighboring elementary triangles are ferromagnetically ordered. The selection energy (which is a measure of the energy difference between the $\sqrt{3} \times \sqrt{3}$ and the $\mathbf{q}=0$ states, the former having a lower energy) can be expressed as an effective antiferromagnetic coupling, of strength J_c , say, between the chiralities.

B. Competition between selection effects and tunneling

The above considerations neglected the possibilities of large-scale fluctuations and tunneling between classical ground states. Clearly the smallest object that can tunnel is the rigid-hexagon mode: Consider as initial state $|i\rangle$, the $\sqrt{3} \times \sqrt{3}$ Potts state. If the six spins on an *ABABAB* hexagon rotate by 180° around the *C* direction (take the latter to define the *z* axis), another Potts state, $|f\rangle$, with a *BABABA* hexagon is reached (Fig. 3). In the absence of in-plane selection ($J_c=0$), $|i\rangle$ and $|f\rangle$ would be degenerate. Tunneling between $|i\rangle$ and $|f\rangle$ would tend to drive the system into a superposition $(1/\sqrt{2})(|i\rangle \pm |f\rangle)$, with energy $E_0 \pm \Delta$ (where Δ , the tunnel-splitting energy, is proportional to the tunneling amplitude). Now, in the presence of in-plane selection effects, the energies of $|i\rangle$

and $|f\rangle$ differ by $12J_c$, since the chiralities on all six triangles bordering the hexagon of $|i\rangle$ are opposite to those of $|f\rangle$. If $12J_c > \Delta$, the tunneling amplitude is very small, and the system selects $|i\rangle$, the $\sqrt{3} \times \sqrt{3}$ state. If, on the other hand, $12J_c < \Delta$ and the tunneling amplitude is appreciable, the system can lower its energy by adopting some superposition of $|i\rangle$ and $|f\rangle$ [in the limit $J_c \rightarrow 0$, this superposition would simply be $(1/\sqrt{2})(|i\rangle - |f\rangle)$].

Such a hexagon tunneling event can clearly take place starting from any Potts state $|i\rangle$ that contains an *ABABAB*-type hexagon, not just from the $\sqrt{3} \times \sqrt{3}$ state. Thus, tunneling constitutes a disordering factor that competes with in-plane selection. If such hexagon tunneling events occur with large probability throughout the *kagomé* lattice, a ground state might conceivably result that is at most partially ordered (related to a spin nematic) (see Sec. VII).

C. Effective hexagon Hamiltonian

We shall study the hexagon tunneling event described in the preceding section in the presence of a coplanarity barrier of size J_b , that tends to keep the spins aligned with the reference plane. Our aim is to compute the tunnel-splitting energy Δ in the most direct way possible. In setting up the calculation, we therefore make two essential simplifying assumptions.

(i) We assume that the effects of in-plane selection can be neglected (i.e., take $J_c=0$). At the end of the calculation, we shall compare the order of magnitude of Δ with estimated values of J_c , to check *a posteriori* whether the neglect of J_c was justified or not (see Sec. VII).

(ii) The initial and final states are assumed to be “locally well-ordered,” namely, precisely *ABABAB* and *BABABA* hexagons. Thus we neglect the possibility that, for example, spin waves disorder the ground state so thoroughly that it is impossible to even define distinct tunneling processes.

Both assumptions are made mainly for the sake of simplicity—extending the calculation to more general situations would be beyond the scope of this paper.

Since $J_b \sim sJ$, we have $J_b \ll s^2J$ when $s \gg 1$, and consequently we assume that only the six hexagon spins will move significantly during the hexagon tunneling event. Hence, we take all other spins in the lattice to stay fixed, and adopt the following Hamiltonian for the six-spin hexagon system:

$$\mathcal{H}_{\text{hex}} = \mathcal{H}_{\text{AFM}} + \mathcal{H}_{\text{cop}}, \quad (2.3)$$

where

$$\mathcal{H}_{\text{AFM}} = s^2J \sum_{l=0}^5 [\mathbf{n}_l \cdot \mathbf{z} + \mathbf{n}_{l+1} \cdot \mathbf{z} + \mathbf{n}_l \cdot \mathbf{n}_{l+1} + \frac{3}{2}], \quad (2.4)$$

$$\mathcal{H}_{\text{cop}} = J_b f(\varphi_{\text{av}}),$$

$$\text{where } \varphi_{\text{av}} \equiv \frac{1}{6} \sum_{l=0}^5 [\varphi_l - \varphi_l(\text{initial})]. \quad (2.5)$$

The index l labels the six spins around the hexagon and is

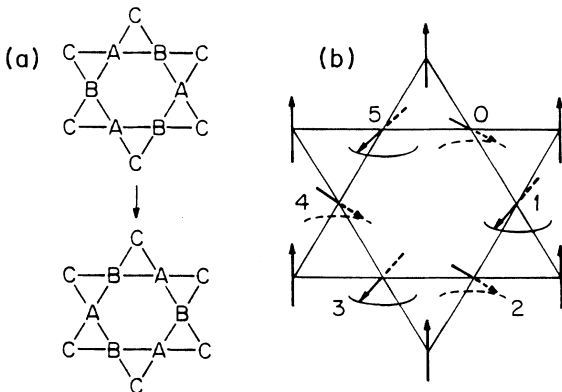


FIG. 3. The rigid-hexagon mode. All six spins on an *ABABAB* hexagon rotate collectively, as a rigid unit in spin space, by 180° around the *C* direction, and end up forming a *BABABA* hexagon. The labels 0–5 correspond to the index l in Eqs. (2.4) and (2.5).

defined modulo 6 [see Fig. (3)]. All spins are written in terms of the same coordinate system, in which the z -axis points in the C direction, the xz plane coincides with the reference plane, and φ is measured from the positive x direction. \mathcal{H}_{AFM} contains simply those terms from Eq. (2.2) that involve the six hexagon spins and their six C -type nearest neighbors. A constant has been added to ensure that $\mathcal{H}_{\text{AFM}}=0$ in the initial and final configurations $|i\rangle$ and $|f\rangle$.

\mathcal{H}_{cop} represents the coplanarity barrier that opposes hexagon tunneling. The function $f(\varphi)$ describes the shape of the barrier; it is of order unity and is sketched schematically in Fig. 4. Its argument in Eq. (2.5), φ_{av} , is a measure of the deviation of the plane of the near-rigid hexagon from the reference plane [in which $\varphi_B(\text{initial})=0$, $\varphi_A(\text{initial})=\pi$].

Symmetry about the reference plane ensures that $f(\varphi)$ has the properties

$$f(m\pi)=0, \quad f(\varphi)=f(-\varphi)=f(\varphi+m\pi) \quad (2.6)$$

for any integer m . At this stage it is not necessary to specify $f(\varphi)$ in more detail. An estimate of the actual form of \mathcal{H}_{cop} is made in Appendix A, and summarized in Eq. (A22). The suitability of using such a barrier is further discussed in Sec. VII.

Intuitively, the six hexagon spins are expected to rotate collectively, almost as a rigid unit, maintaining the mutual coplanarity and relative angles of 120° required to minimize \mathcal{H}_{AFM} . In particular, for each of them $\cos\theta_l \simeq -\frac{1}{2}$ throughout the tunneling event, which is why we have taken \mathcal{H}_{cop} to be independent of θ_l . Also, the expected mutual coplanarity of the tunneling spins is the reason why we have written \mathcal{H}_{cop} as a function only of φ_{av} [and not some more general function of the six φ_l 's (Ref. 20)]. These assumptions are found to be justified in Sec. V B.

Evidently, due to reflection symmetry in the reference plane, two kinds of tunneling events between $|i\rangle$ and $|f\rangle$ are possible. They differ from each other only in the *sense* of rotation about the z axis ($\varphi \leftrightarrow -\varphi$), and we shall call them (+) instantons and (-) instantons.

We shall show in Sec. V how the hexagon tunneling problem defined above can be mapped onto a much simpler model problem. This involves only a single, collective spin degree of freedom with effective spin $6s$. Its

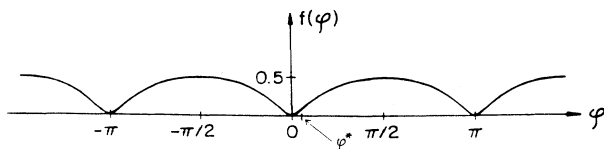


FIG. 4. A typical shape function $f(\varphi)$ for the coplanarity potential \mathcal{H}_{cop} . The function shown here corresponds to the $s=1$ case of the function calculated in Appendix A, Eq. (A22), and used in Secs. IV C and V. The arrow shows the position of φ^* , which marks the crossover of $f(\varphi)$ from quadratic to linear behavior. However, the general discussion of Secs. III and IV, up to Eq. (4.13), is independent of the particular shape of $f(\varphi)$, and only requires the symmetries of Eq. (2.6) to hold.

coordinates, to be denoted by (Φ_0, Θ_0) , are formally defined in Eqs. (5.5) and (5.6) and are suitable averages of the six individual (φ_i, θ_i) 's. The effective Hamiltonian turns out to be [see Eq. (5.22)]:

$$\mathcal{H}_{\text{eff}} = 12s^2 J (\cos\Theta_0 + \frac{1}{2})^2 + J_b f(\Phi_0). \quad (2.7)$$

Rather than proceeding with the mapping of Eq. (2.3) onto Eq. (2.7) right away, in the next two sections we first discuss the simple model problem [based on Eq. (2.7)] in detail, to establish notation and introduce the tools needed to calculate the tunnel-splitting energy Δ .

III. A SIMPLE MODEL SYSTEM

In this section we introduce a simple model problem, which will be used to illustrate how a calculation of the tunnel-splitting energy can be carried through. It is also the system onto which the *kagomé* tunneling problem that is studied in Sec. V can be mapped. We set up the relevant path integral, calculate the classical action and discuss the equations of motion and the typical form of the tunneling path.

A. Model Hamiltonian

The model system is defined by the following Euclidean single-spin Lagrangian:

$$\mathcal{L} = -i\hbar n s \dot{\varphi}(z-1) + \mathcal{H} \quad (3.1)$$

where

$$\mathcal{H} = a(z - z_g)^2 + b f(\varphi) \quad (\text{with } b \ll a), \quad (3.2)$$

and

$$z \equiv \cos\theta. \quad (3.3)$$

This Lagrangian has been written in terms of the imaginary time parameter $\tau = it$ (hence “Euclidean”), since this is convenient for the calculation of tunneling amplitudes. The spherical coordinates $(\varphi, \theta) \equiv \Omega$ define a unit vector \mathbf{n} and label a coherent spin state $|\varphi, \theta\rangle$ for a particle with spin ns . The dot on $\dot{\varphi}$ means ∂_τ (see Ref. 21 for a discussion of the origin of this term). The integer n is introduced in order to accommodate the possibility of a collective degree of freedom with effective spin ns . For the purpose of describing a single spin degree of freedom, take $n=1$.

The “classical” Hamiltonian is the expectation value $\mathcal{H} \equiv \langle \varphi, \theta | \hat{\mathcal{H}} | \varphi, \theta \rangle$ of the quantum operator $\hat{\mathcal{H}}$. Clearly \mathcal{H} has been chosen to have the same form as \mathcal{H}_{eff} of Eq. (2.7); the constants a and b are taken to be of order $s^2 J$ and J_b , respectively [see Eq. (5.23)], with $b \ll a$. The dominant term in \mathcal{H} is an easy-plane anisotropy, which would make every angle on the “latitude line” $z = z_g$ on the unit sphere be degenerate; it mimics \mathcal{H}_{AFM} in Eq. (2.4) (which forced all six hexagon spins to have $\cos\theta_l = -\frac{1}{2}$). In the other term, $f(\varphi)$ is taken to be the same function as that in Eqs. (2.5) and (2.6); it introduces a small anisotropy within the degenerate subspace and mimics \mathcal{H}_{cop} . There are two degenerate ground-state configurations, $|i\rangle = |2m_1\pi, z_g\rangle$ and $|f\rangle = |(2m_2+1)\pi, z_g\rangle$, with m_1 and m_2 arbitrary in-

tegers (the different values of m_1 and m_2 describe the same physical state, of course). Contours of constant \mathcal{H} are shown in Fig. 5.

B. Tunneling amplitude

The tunnel-splitting energy Δ that arises due to tunneling of the spin direction between $|i\rangle$ and $|f\rangle$ is proportional (Ref. 22) to the tunneling amplitude

$$U_{fi} \equiv \langle f | e^{-\hat{H}T/\hbar} | i \rangle = \int \mathcal{D}\Omega e^{-\mathcal{S}/\hbar}, \quad (3.4)$$

where $\mathcal{S} = \int_{-T/2}^{T/2} d\tau \mathcal{L}$ is the Euclidean action, $\mathcal{D}\Omega$ is the path integral measure (discussed in Sec. IV A), and T is a large time. Such an amplitude can be approximately evaluated by the method of steepest descent:

$$U_{fi} = \sum_j \mathcal{N}^{(j)} e^{-\mathcal{S}_0^{(j)}/\hbar} \equiv U_{fi}^{(j)}. \quad (3.5)$$

Here $\mathcal{S}_0^{(j)}$ is the action evaluated along the j th ‘‘tunneling path,’’ which is a solution to the Lagrangian equations of motion and for tunneling problems is in general complex. It will always be denoted by overlined variables, e.g., $(\overline{\varphi}^{(j)}, \overline{z}^{(j)})$. The index j allows for the possibility of different tunneling paths satisfying boundary conditions that differ in the indices m_1 and m_2 (but that all describe physically the same initial and final states) (Ref. 23). The prefactors

$$\mathcal{N}^{(j)} = \int \mathcal{D}\Omega e^{-(\mathcal{S} - \mathcal{S}_0^{(j)})/\hbar} \quad (3.6)$$

are usually evaluated only (if at all) to lowest order in the steepest descent method, by transforming to the fluctua-

tion variables $(\delta\varphi^{(j)}, \delta z^{(j)}) \equiv (\varphi - \overline{\varphi}^{(j)}, z - \overline{z}^{(j)})$ and keeping only the lowest term in the expansion $\mathcal{S} - \mathcal{S}_0^{(j)} = \delta^2 \mathcal{S}^{(j)} + \delta^3 \mathcal{S}^{(j)} \dots$.

In the present case, all tunneling paths connecting $|i\rangle$ at $\tau = -T/2$ to $|f\rangle$ at $\tau = T/2$, can be constructed from two very simple paths, to be denoted by $(\overline{\varphi}^\pm, \overline{z}^\pm)$. The first, for which $\overline{\varphi}^+(\tau) \in [0, \pi]$, we call a (+) instanton, the second, for which $\overline{\varphi}^- = -\overline{\varphi}^+(\tau) \in [0, -\pi]$, a (-) instanton. They differ solely in the sense of φ rotation and are sketched in Fig. 6. All other tunneling paths that approximately satisfy the equations of motion and contribute to Eq. (3.5) are multiple-instanton paths. They consist of n_1 (+) instanton and n_2 (-) instanton events, with $n_1 + n_2 = \text{odd}$, all assumed widely separated (relative to their characteristic width) in time, and following each other in arbitrary order (this is the so-called dilute-gas approximation, see Coleman [22]). In the following, we consider only single-instanton events [i.e., $j \rightarrow \pm$ in Eq. (3.5)]; the effects multiple-instantons are taken into account in Appendix C.

The symmetry $\mathcal{H}(\varphi, z) = \mathcal{H}(-\varphi, z)$ of the Hamiltonian allows one to conclude immediately that $|U_{fi}^+| = |U_{fi}^-|$. This is intuitively obvious, and can be proven to hold exactly to all orders of the steepest descent approximation (i.e., to all orders in $1/s$) (see Sec. IV B). Intuitively speaking, the symmetry of \mathcal{H} ensures that the local neighborhoods of the two tunneling paths $(\overline{\varphi}^+, \overline{z}^+)$ and $(\overline{\varphi}^-, \overline{z}^-)$ are identical for the two paths, so that the local shapes and sizes of the barriers (which determine $\text{Re}[\mathcal{S}_0^{(j)}]$) and the local fluctuations around the tunneling paths (which determine $|\mathcal{N}^{(j)}|$), are identical. However, the amplitudes U_{fi}^\pm can differ by a phase, which may lead to destructive interference between them.

C. Classical action, continuing to complex coordinates

Let us find \mathcal{S}_0^\pm , the classical action for single-instanton events. Since energy is conserved along any path that extremizes the action, $\mathcal{H}(\overline{\varphi}^\pm, \overline{z}^\pm) = 0$. Solving for \overline{z}^\pm as a function of $\overline{\varphi}$, one obtains

$$i\overline{z}^\pm \equiv \overline{z}^\pm - z_g = \pm i\sqrt{b/a} \sqrt{f(\overline{\varphi}^\pm)}, \quad (3.7)$$

with \overline{z}^\pm real. The Euclidean action is easily evaluated along these paths by changing integration variables from τ to $\overline{\varphi}^\pm$ and using $f(\overline{\varphi}^+) = f(\overline{\varphi}^-)$:

$$\begin{aligned} \mathcal{S}_0^\pm &= -i\hbar ns \int_{-T/2}^{T/2} d\tau (\partial_\tau \overline{\varphi}^\pm)(z_g + i\overline{z}^\pm - 1) + 0 \\ &= \mp i\hbar ns \pi(z_g - 1) + \hbar ns \sqrt{b/a} \int_0^\pi d\varphi \sqrt{f(\overline{\varphi}^\pm)}. \end{aligned} \quad (3.8)$$

Note that the quantity $\sqrt{b/a}$ plays the role of an

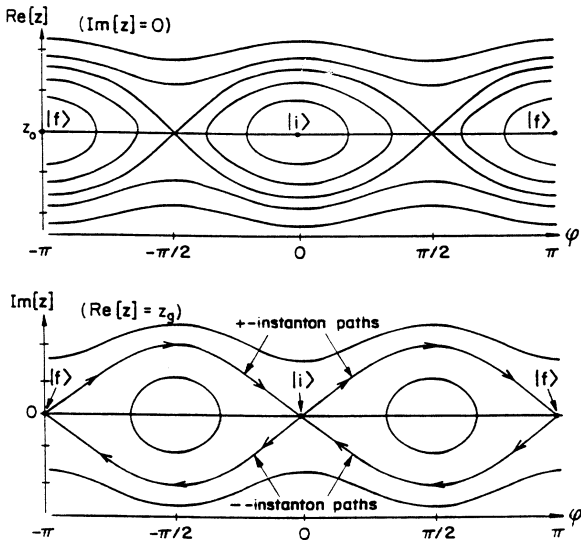


FIG. 5. Contours of constant $\mathcal{H}(\varphi, z)$. In (a), $\text{Im}[z]=0$, and the contours in the $(\varphi, \text{Re}[z])$ plane depict ‘‘valleys’’ centered at $(\varphi, z) = (0 \pmod{\pi}, z_g)$. In (b), $\text{Re}[z] = z_g$, and the contours in the $(\varphi, \text{Im}[z])$ plane show ‘‘ridges’’ centered at $(\varphi, z) = (\pm\pi/2 \pmod{\pi}, z_g)$. The (+) instanton and (-) instanton tunneling paths are contours of $\mathcal{H}=0$ around these ridges.

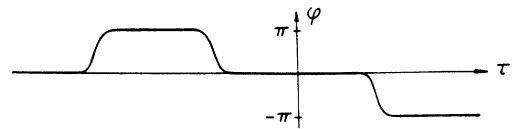


FIG. 6. An (+) instanton $\overline{\varphi}^+(\tau)$ followed by two (-) instantons $\overline{\varphi}^-(\tau)$, where τ is the (imaginary) time parameter.

effective barrier size for the tunneling process. This is intuitively plausible. The barrier height in the φ direction is measured by b . When $(z-z_g)$ is real, a measures the steepness of the valley in the z direction. When $(z-z_g)$ becomes purely imaginary $[(z-z_g)^2 \rightarrow -(z-z_g)^2]$, the z valley turns into a ridge (see Fig. 5). The motion occurs along a constant energy contour around this ridge [see Fig. 5(b)], and $1/a$ measures the width of the ridge. Hence, b/a measures the effective barrier size.

D. Possible cancellation due to phase factors

We show in Sec. IV B that $\mathcal{N}^+ = \mathcal{N}^-$ (under some technical assumptions, explained there). The sum of the two amplitudes U_{fi}^\pm is therefore simply

$$\begin{aligned} U_{fi}^+ + U_{fi}^- &= U_{fi}^+ (1 + e^{(\mathcal{S}_0^+ - \mathcal{S}_0^-)/\hbar}) \\ &= U_{fi}^+ (1 + e^{-i\pi l}), \end{aligned} \quad (3.9)$$

where the constant $l \equiv 2ns(z_g - 1)$ is not necessarily an integer. The relative phase of $e^{-i\pi l}$ between the amplitudes of two tunneling paths that connect the same initial and final states has a well-known geometrical interpretation. It is related to the area enclosed on the unit sphere between the two paths $(\varphi^+(\tau), \text{Re}[\theta^+(\tau)])$ and $(\varphi^-(\tau), \text{Re}[\theta^-(\tau)])$. (See [9] for more comments on this aspect.) Now, if l is an odd integer, the (+) instanton and (-) instanton paths interfere destructively and their amplitudes add to zero: $U_{fi}^+ + U_{fi}^- = 0$.²⁴ Note that as long as the barrier does not violate the symmetry between (+) instantons and (-) instantons, this cancellation does not depend on the particular shape of the barrier, since the shape function $f(\varphi)$ only affects the real part of \mathcal{S}_0 , which cancels out in $\mathcal{S}_0^+ - \mathcal{S}_0^-$.

E. Equations of motion and tunneling path

It was not necessary to solve the equations of motion to obtain the explicit expression Eq. (3.8) for the classical action. For future reference, the equations of motion are

$$-i\hbar n s i \dot{\bar{Z}} = b f'(\bar{\varphi}), \quad (3.10)$$

$$-i\hbar n s \dot{\bar{\varphi}} + 2a i \bar{Z} = 0. \quad (3.11)$$

The prime on f means $\partial/\partial\varphi$. Note how the i of $i\bar{Z}$ and that originating from $\tau=it$ combine to result in consistent equations of motion (this is a direct illustration of why it is useful to employ imaginary time in tunneling calculations). Eliminating \bar{Z} , we get

$$\ddot{\bar{\varphi}} = \frac{1}{2} d^2 f'(\bar{\varphi}), \quad \text{where } d^2 = \frac{4ab}{(\hbar n s)^2}. \quad (3.12)$$

The constant d has the dimensions of inverse time, and $1/d$ characterizes the width of an instanton. To illustrate the nature of the solutions of Eq. (3.12), consider a simple case, namely, $f(\varphi) = \sin^2\varphi$. Then Eq. (3.12) is just the sine-Gordon equation, whose solutions, in the limit $T \rightarrow \infty$, are

$$\begin{aligned} \bar{\varphi}^+(\tau) &= 2 \arctan(e^{d\tau}), \\ \bar{\varphi}^-(\tau) &= -\bar{\varphi}^+(\tau) = \bar{\varphi}^+(-\tau) - \pi. \end{aligned} \quad (3.13)$$

These represent (+) instanton and (-) instanton events and are sketched in Fig. 6. The shape of an instanton changes quantitatively, but not qualitatively, if a different barrier shape function is used.

IV. THE TUNNEL-SPLITTING ENERGY Δ

For integer s , for which the (+) instanton and (-) instanton amplitudes have the same sign and interfere constructively, the resulting tunnel-splitting energy Δ can be calculated from the prefactor of Eq. (3.6):

$$\mathcal{N}^\pm = \int \mathcal{D}\Omega e^{-(\mathcal{S} - \mathcal{S}_0^\pm)/\hbar}. \quad (4.1)$$

In the steepest descent approximation, this can be accomplished via three steps: (i) extending the integration ranges for φ and z in the path integral to infinity, (ii) integrating out the z degree of freedom, and (iii) using standard methods to evaluate the resulting φ -path integral.

Before proceeding, however, there is one issue that needs to be addressed: The steepest descent approximation relies on and exploits the fact that the Lagrangian is proportional to a large parameter. It gives an expansion of the prefactors \mathcal{N}^\pm in inverse powers of this large parameter, which, in our case, is the spin s . However, the Lagrangian of Eq. (3.1) contains terms proportional to both s^2 and s (since $a \sim s^2$ and $b \sim s$). Therefore the question arises whether the steepest descent approximation still is a systematic expansion in powers of $1/s$. The answer to this question is yes, since, loosely speaking, the steepest descent method only requires *some* (not necessarily all) terms in the exponent to be proportional to a large parameter. By examining an integral of the form

$$\int_{-\infty}^{\infty} dx e^{-s[g_1(x) + 1/s g_2(x)]},$$

for example, it can readily be shown that the standard manipulations of the steepest descent method give an expression for the prefactor that is correct at least to the lowest order in $1/s$ (namely, $s^{-1/2}$), since subtleties resulting from the $1/s g_2(x)$ term affect only higher orders of $1/s$.²⁵

A. Extending the integration ranges

The path integral expression Eq. (3.4) for the tunneling amplitude (in real time) can be arrived at by the usual procedure of discretizing time and inserting completeness relations in spin space at each time slice (see, e.g., Refs. 21 and 26). This procedure leads to a formal expression for the measure (appropriate for any spin problem):

$$\int \mathcal{D}\Omega(t) = \lim_{N \rightarrow \infty} \left[\frac{2s+1}{4\pi} \right]^N \prod_{j=1}^N \int_0^{2\pi} d\varphi(\tau_j) \int_{-1}^1 dz(\tau_j), \quad (4.2)$$

where $\varepsilon(N+1) = T$. What distinguishes this measure from the ones usually encountered in particle tunneling problems is the fact that φ and z have finite integration ranges. In a somewhat cavalier fashion, we extend these to $[-\infty, \infty]$ and $[-\infty, \infty]$ and absorb the change in normalization by multiplying by an extra overall normali-

zation factor C (Ref. 27). Thus Eq. (4.2) is replaced by

$$\int \mathcal{D}\Omega(t) = C \lim_{N \rightarrow \infty} \prod_{j=1}^N \int_{-\infty}^{\infty} d\varphi(\tau_j) \int_{-\infty}^{\infty} dz(\tau_j). \quad (4.3)$$

The extension of the range for φ from $[0, 2\pi]$ to $[-\infty, \infty]$ is very natural—it allows for motion in which the spin direction rotates around in the same direction many times. The justification for extending the integration range $[-r, r]$ for z from $r=1$ to $r=\infty$ is more tenuous. The core of the argument is the following assertion, proven in Appendix B: In the presence of a z^2 term in the Hamiltonian, the value of r determines the degree of non-differentiability of the φ paths that result after z has been integrated out. If $r=\infty$, the φ paths are Brownian motion paths; if $r=1$, they are much more ill behaved than Brownian motion paths. Therefore, changing the integration range for z from $r=1$ to $r=\infty$ is equivalent to restricting attention to Brownian motion φ paths instead of a larger class of paths that are much more ill behaved. It is argued that this should not have a noticeable effect, for the following two reasons: If one is interested mainly in the effect of small fluctuations around the classical path (as, for example, when calculating the tunnel-splitting energy), physically, one only expects some *smooth* paths in the immediate neighborhood of the classical path to be important. Also, the additional paths that are formally included in the path integral when the integration ranges are extended from $r=1$ to ∞ are far from the tunneling path and therefore only make an exponentially small contribution to the path integral.

In the course of making a change of variables $(\varphi, z) \rightarrow (\delta\varphi, \delta z)$ in the path integral in order to evaluate \mathcal{N}^{\pm} , the overall constant C will be multiplied by a Jacobian factor J^N , which may be infinite in the limit $N \rightarrow \infty$. To obtain finite answers, we stipulate, as is usual, that C be chosen such that the final path integral for $\delta\varphi$ (after the δz dependence has been integrated out), should have the same normalization as that employed by Coleman in his discussion of instantons,²² the results of which we intend to use. This often-used procedure may seem somewhat arbitrary, but the fact that the path integral is defined as an infinite *product* of integrals, each of which may produce finite prefactors when being manipulated, leaves one no choice but to absorb all infinities in a single appropriately chosen constant C . This much having been said, we henceforth pay no attention to normalization constants or Jacobians.

B. The relative phase of the prefactors \mathcal{N}^+ and \mathcal{N}^-

Before integrating out z , let us investigate the relative phase of \mathcal{N}^+ and \mathcal{N}^- , the (+) instanton and (-) instanton prefactors. The quantity $\mathcal{S} - \mathcal{S}_0$ that appears in the integrands of the prefactors in Eq. (4.1) can be written in terms of the fluctuations around the tunneling path $(\delta\varphi, \delta z) \equiv (\varphi - \bar{\varphi}, z - \bar{z})$ as

$$\mathcal{S} - \mathcal{S}_0 = \int d\tau \left[-i\hbar ns \delta\varphi \delta z + a \delta z^2 + b \sum_{n=2}^{\infty} \frac{1}{n!} \left[\frac{\partial^n}{\partial \varphi^n} f(\varphi) \right]_{\bar{\varphi}} \delta\varphi^n \right]. \quad (4.4)$$

Evidently, because $f(\varphi) = f(-\varphi)$, the following symmetry relations hold (the square brackets denote a functional dependence, “*” denotes complex conjugation):

$$(\mathcal{S} - \mathcal{S}_0)[\bar{\varphi}^-, -\delta\varphi, \delta z] = (\mathcal{S} - \mathcal{S}_0)^*[\bar{\varphi}^+, \delta\varphi, \delta z], \quad (4.5)$$

$$(\mathcal{S} - \mathcal{S}_0)[\bar{\varphi}^-, -\delta\varphi, -\delta z] = (\mathcal{S} - \mathcal{S}_0)[\bar{\varphi}^+, \delta\varphi, \delta z]. \quad (4.6)$$

Now, after the change of variables $(\varphi, z) \rightarrow (\delta\varphi, \delta z)$ in the path integral (4.1), $\delta\varphi$ and δz are dummy variables that are integrated over. Since we extended the integration ranges for φ and z to $[-\infty, \infty]$, the integration ranges for $\delta\varphi$ and δz are symmetric around $\delta\varphi=0$ and $\delta z=0$. Hence the following conclusions follow immediately: (i) relation (4.5) implies that $\mathcal{N}^- = \mathcal{N}^{+*}$ and (ii) relation (4.6) implies that $\mathcal{N}^- = \mathcal{N}^+$.

As discussed in Sec. IV A, the extension of the integration range to $[-\infty, \infty]$ is on somewhat less firm ground for z than for φ . Hence conclusion (ii), which holds only if the δz -integration range is symmetric about $\delta z=0$, is in a sense “weaker” than conclusion (i). However, even if the original z -integration range of $[-1, 1]$ is retained, the error in the relation $\mathcal{N}^+ = \mathcal{N}^-$ is expected to be exponentially small. For example, for the case $z_g = -\frac{1}{2}$, which we shall use in Sec. V, only paths for which $\delta z \in [\frac{1}{2}, \frac{3}{2}]$ break the $\delta z \leftrightarrow -\delta z$ symmetry, and these paths deviate so strongly from the tunneling path (for which $\text{Re}[z] = z_g$) that their contribution to the path integral is exponentially small. (Of course, this argument breaks down when $z_g = \pm 1$.)

Finally, note that within the lowest order of the steepest descent approximation, in which one keeps only the $n=2$ term of the infinite sum in Eq. (4.4) [to be indicated by a superscript (2) in Eq. (4.8) below], the relation $\mathcal{N}^+ = \mathcal{N}^-$ holds, *independent* of the range of z integration. The reason is simply that, since

$$(\mathcal{S} - \mathcal{S}_0)^{(2)} = \int d\tau [-i\hbar ns \delta\varphi \delta z + a \delta z^2 + \frac{1}{2} b f''(\bar{\varphi}) \delta\varphi^2], \quad (4.7)$$

where $f'' = \partial^2 f / \partial \varphi^2$, we have

$$(\mathcal{S} - \mathcal{S}_0)^{(2)}[\bar{\varphi}^+, \delta\varphi, \delta z] = (\mathcal{S} - \mathcal{S}_0)^{(2)}[\bar{\varphi}^-, \delta\varphi, \delta z]. \quad (4.8)$$

C. Calculating Δ

We henceforth restrict attention to the lowest order of the steepest descent approximation, in which $\mathcal{N}^+ = \mathcal{N}^- \equiv \mathcal{N}$. It is straightforward, starting from Eq. (4.7), to perform the Gaussian integral over δz to arrive at

$$\mathcal{N} \propto \int \mathcal{D}\delta\varphi e^{-\int d\tau \delta^2 \mathcal{L}_\varphi / \hbar}, \quad (4.9)$$

where

$$\delta^2 \mathcal{L}_\varphi = \frac{1}{2} b f''(\bar{\varphi}) (\delta\varphi)^2 + \frac{(\hbar ns)^2}{4a} (\delta\dot{\varphi})^2. \quad (4.10)$$

Now note that the $\delta^2 \mathcal{L}_\varphi$ of Eq. (4.10) is also the second variation of the following effective Euclidean Lagrangian for φ :

$$\mathcal{L}_\varphi = \frac{1}{2} \frac{(\hbar ns)^2}{2a} \dot{\varphi}^2 + bf(\varphi). \quad (4.11)$$

The Lagrangian equation of motion resulting from \mathcal{L}_φ is just Eq. (3.12), and hence the \mathcal{S}_0 corresponding to \mathcal{L}_φ will be equal to the $\text{Re}[\mathcal{S}_0]$ found earlier. Consequently, both \mathcal{N} and $\text{Re}[\mathcal{S}_0]$ for the original system are equal to those arising from \mathcal{L}_φ . It follows that Δ , too, can be calculated directly using \mathcal{L}_φ . Furthermore, \mathcal{L}_φ is quadratic in $\delta\dot{\varphi}$ and therefore the methods discussed by Coleman²² can be used to calculate the tunnel-splitting energy.²⁸ Coleman's methods, which are summarized in Appendix C, readily lead to the following expression for Δ [compare Eqs. (C7) and (C10)]:

$$\Delta = 2\varphi_{\text{as}}(\pi ns)^{-1/2} [bf''(0)]^{3/4} (2a)^{1/4} \times (e^{-\mathcal{S}_0^+/\hbar} + e^{-\mathcal{S}_0^-/\hbar}). \quad (4.12)$$

Here the constant φ_{as} is to be read off from the asymptotic behavior of the tunneling paths, which, as Coleman shows, can always be written in the form [compare Eq. (C5)]:

$$\bar{\varphi}^\pm(\tau) \simeq \pm\pi \mp \varphi_{\text{as}} e^{-\omega\tau}, \quad \text{with } \omega \equiv \frac{\sqrt{2abf''(0)}}{\hbar ns}, \quad (4.13)$$

Equation (4.12) is the main result of this section. We emphasize once again that Δ is strictly zero if $S_0^+ - S_0^- = i\hbar l\pi$, with l an odd integer, since then (+) instanton and (-) instanton events interfere destructively.

To find φ_{as} explicitly, one needs some knowledge of the asymptotic behavior of the shape function $f(\varphi)$ of the potential as $\varphi \rightarrow 0$. According to Eqs. (A17), (A18), and (A21) in Appendix D, the form of $f(\varphi)$ that is applicable to the hexagon tunneling problem to be studied in the latter parts of this paper is

$$f(\varphi) = \tilde{f}(\sqrt{(\varphi_{\text{eff}}^2 + \varphi^{*2})} - \tilde{f}(\varphi^*)), \quad (4.14)$$

$$\varphi_{\text{eff}} \equiv \varphi \bmod \pi \in (-\pi/2, \pi/2],$$

where

$$\tilde{f}(\varphi) = |\sin\varphi| (1 + \frac{1}{3}\sin^2\varphi)^{1/2} - \tilde{J} \sin^2\varphi, \quad (4.15)$$

and $\tilde{J} \simeq 0.42$ and $\varphi^* = 0.14s^{-1/3}$, as it turns out. In the limit $s \gg 1$, φ^* can be treated as a small parameter, which characterizes the curvature of the potential at $\varphi=0$, since $f''(0) = (1/\varphi^* - 2\tilde{J})$.

"Energy conservation" along the tunneling path implies for the \mathcal{L}_φ of Eq. (4.11) that

$$\frac{1}{2} \frac{(\hbar ns)^2}{2a} \dot{\bar{\varphi}}^2 - bf(\bar{\varphi}) = 0. \quad (4.16)$$

Integrating this equation gives, for a (-) instanton,

$$\tau\omega(f''(0))^{-1/2} = - \int_{-\pi/2}^{-\pi+\bar{\varphi}_\tau} \frac{d\bar{\varphi}}{[2f(\bar{\varphi})]^{1/2}}, \quad (4.17)$$

where $-\pi + \bar{\varphi}_\tau$ is the angle reached at time τ if $\dot{\bar{\varphi}}=0$ at $\tau=0$. This equation is to be solved for $\bar{\varphi}_\tau$ as a function of τ , in the limit $\bar{\varphi}_\tau \rightarrow 0$. In particular, we take $\bar{\varphi}_\tau < \eta\varphi^*$, where $\eta \ll 1$ is an arbitrary small parameter (e.g.,

$\eta=0.01$). In this limit, we anticipate, by Eq. (4.13), that $\bar{\varphi}_\tau$ will have the form $\varphi_{\text{as}} e^{-\omega\tau}$.

It is convenient to split the integral into two parts by writing

$$\tau\omega(f''(0))^{-1/2} = F(\pi/2) - F(\bar{\varphi}_\tau), \quad (4.18)$$

where

$$F(\varphi) \equiv \int_{\eta\varphi^*}^{\varphi} \frac{d\bar{\varphi}}{[2f(\bar{\varphi})]^{1/2}}, \quad (4.19)$$

and the property $f(\varphi) = f(\varphi + \pi)$ has been exploited. Since $\bar{\varphi}_\tau \ll \eta\varphi^* \ll 1$, one may evaluate $F(\bar{\varphi}_\tau)$ analytically by using the asymptotic form of the integrand, namely,

$$f(\varphi \rightarrow 0) \simeq \varphi^2 (\frac{1}{2}\varphi^* - \tilde{J}),$$

with the result

$$F(\bar{\varphi}_\tau) = \left[\frac{\varphi^*}{1 - 2\tilde{J}\varphi^*} \right]^{1/2} (\ln\varphi - \ln\eta\varphi^*). \quad (4.20)$$

Using this result in Eq. (4.18) and solving for $\bar{\varphi}_\tau$ gives

$$\bar{\varphi}_\tau = \varphi_{\text{as}} e^{-\omega\tau}, \quad (4.21)$$

where

$$\varphi_{\text{as}} = \exp \left[C \left[\frac{1 - 2\tilde{J}\varphi^*}{\varphi^*} \right]^{1/2} \right] \quad (4.22)$$

and

$$C \equiv F(\pi/2) + \left[\frac{\varphi^*}{1 - 2\tilde{J}\varphi^*} \right]^{1/2} \ln\eta\varphi^*. \quad (4.23)$$

The constant C is independent of η , since the η dependence of $F(\pi/2)$ cancels that of the second term. Moreover, C is only very weakly dependent on φ^* and hence on s , and approaches a constant value as $s \rightarrow \infty$. (Numerically it is found that C changes from 1.1 to 2.1 as s changes from 1 to ∞ .) Hence, recalling that $\varphi^* = 0.14s^{-1/3}$, we conclude that in the limit $s \rightarrow \infty$,

$$\varphi_{\text{as}} \simeq e^{5.6s^{1/6}} \quad (4.24)$$

This expression diverges as $s \rightarrow \infty$, but in Eq. (4.12) it premultiplies an expression that tends to zero even faster as $s \rightarrow \infty$ [in Sec. V, we find $\mathcal{S}_0 \sim s^{1/2}$, see Eqs. (5.36) and (5.37)].

V. SPIN TUNNELING IN THE KAGOMÉ LATTICE

The stage has now been set for the study of the hexagon tunneling event on the *kagomé* lattice, for which we adopted the Hamiltonian \mathcal{H}_{hex} defined in Eqs. (2.3) to (2.5). Rewriting \mathcal{H}_{AFM} in terms of φ_l and $z_l \equiv \cos\theta_l$, the Euclidean Lagrangian to be studied is

$$\mathcal{L} = \sum_{l=0}^5 -i\hbar s \dot{\varphi}_l (z_l - 1) + J_b f(\varphi_{\text{av}}) + s^2 J \sum_{l=0}^5 [z_l + z_{l+1} + z_l z_{l+1} + C_l \cos(\varphi_l - \varphi_{l+1}) + \frac{3}{2}], \quad (5.1)$$

where

$$C_l \equiv \sin\theta_l \sin\theta_{l+1} = \{(1-z_l^2)(1-z_{l+1}^2)\}^{1/2}. \quad (5.2)$$

The tunneling event was described in intuitive terms in Sec. II C. The initial and final states are

$$|i\rangle: \varphi_l(-T/2) = (0, \pi, 0, \pi, 0, \pi), \quad z_l(-T/2) = z_g, \quad (5.3)$$

$$|f\rangle: \varphi_l(T/2) = (\pi, 0, \pi, 0, \pi, 0), \quad z_l(T/2) = z_g. \quad (5.4)$$

Here $z_g = \cos 2\pi/3 = -\frac{1}{2}$. The motion of each of the six spins will be roughly analogous to the single-spin motion described in Sec. III E.

A. Collective coordinates

We now introduce a coordinate transformation to a set of collective coordinates, (Φ_l, Z_l) , which ultimately allows us to map the hexagon tunneling problem exactly onto the simple model problem of Sec. III, Eqs. (3.1) and (3.2):

$$z_l - z_l(-T/2) = \sum_{k=0}^5 e^{i\pi k/3} i Z_k, \quad (5.5)$$

$$\varphi_l - \varphi_l(-T/2) = \sum_{k=0}^5 e^{-i\pi k/3} \Phi_k, \quad (5.6)$$

where

$$\Phi_l^* = \Phi_{-l}, \quad Z_l^* = Z_{-l}. \quad (5.7)$$

The conditions (5.7) ensure that $\varphi_l - \varphi_l(-T/2)$ is purely real and $z_l - z_l(-T/2)$ purely imaginary. The reason for the latter requirement is the same as that encountered in the discussion of the model tunneling problem (Sec. III): it would otherwise be impossible to satisfy $\mathcal{H}=0$. Making $z_l - z_l(-T/2)$ imaginary flips the sign of the z^2 terms, thus turning the z valley into a ridge around which the tunneling path can proceed along a constant energy contour.

The new coordinates are essentially discrete Fourier transforms of the original ones with respect to l . [Indices such as l and k will be used interchangeably both as ‘‘position’’ labels (for φ and z) and as Fourier labels (for Φ and Z .)] The zeroth ones, (Φ_0, Z_0) , are just the average

values of the old coordinates and can be thought of as the coordinates of a collective degree of freedom (of spin $6s$, as it turns out). They will be referred to as the *tunneling coordinates*, since Φ_0 tunnels from 0 at $\tau = -T/2$ to $\pm\pi$ at $\tau = T/2$, and iZ_0 is its conjugate momentum. The other coordinates (Φ_l, Z_l) , $l=1, \dots, 5$, will be called *transverse coordinates*, since they will be shown to be strictly zero along the tunneling path, and hence describe fluctuations that are orthogonal to the tunneling path.

In order to calculate the tunnel-splitting energy Δ , one needs the classical action $\mathcal{S}_{0\pm}$ and the prefactor \mathcal{N}^\pm . In the following two sections, we show that both these quantities can be obtained from a rather simple *effective* Lagrangian $\hat{\mathcal{L}}_0$, which depends *only* on the tunneling coordinates (Φ_0, Z_0) , so that the problem is substantially simplified. This Lagrangian, defined in Eq. (5.21) and given explicitly in Eq. (5.22), turns out to have just the form of the Lagrangian introduced in Sec. III A, with (Φ_0, Z_0) corresponding to (φ, z) there.

B. Classical action (*kagomé* lattice)

The classical action is completely determined by the tunneling path, for which, as in Sec. III, we again use overlined variables, $(\bar{\varphi}_l, \bar{z}_l)$ or $(\bar{\Phi}_l, \bar{Z}_l)$. This path is determined by the equations of motion, which, by the chain rule, can be written in terms of the new coordinates as

$$\partial_\tau \left[\frac{\partial \mathcal{L}}{\partial \dot{\varphi}_l} \right]_t \left[\frac{\partial \dot{\varphi}_l}{\partial \dot{\Phi}_k} \right]_t = \left[\frac{\partial \mathcal{L}}{\partial \varphi_l} \right]_t \left[\frac{\partial \varphi_l}{\partial \Phi_k} \right]_t, \quad (5.8)$$

$$\left[\frac{\partial \mathcal{L}}{\partial z_l} \right]_t \left[\frac{\partial z_l}{\partial Z_k} \right]_t = 0, \quad (5.9)$$

with boundary conditions $\bar{\Phi}(-T/2) = 0$ and $\bar{Z}(-T/2) = 0$. The parentheses $()_t$ indicate that the derivatives are to be evaluated along the tunneling path. These equations can be solved by the following ‘‘tunneling path ansatz’’:

$$(\bar{\Phi}_l, \bar{Z}_l) \equiv (0, 0) \quad \text{for } l = 1, \dots, 5. \quad (5.10)$$

To see that this ansatz works, consider Eqs. (5.8) and (5.9) term by term:

$$\partial_\tau \left[\frac{\partial \mathcal{L}}{\partial \dot{\varphi}_l} \right]_t \left[\frac{\partial \dot{\varphi}_l}{\partial \dot{\Phi}_k} \right]_t = -i \hbar s \dot{z}_l e^{-i\pi k/3}, \quad (5.11)$$

$$\left[\frac{\partial \mathcal{L}}{\partial \varphi_l} \right]_t \left[\frac{\partial \varphi_l}{\partial \Phi_k} \right]_t = \{s^2 J [-C_l \sin(\bar{\varphi}_l - \bar{\varphi}_{l+1}) + C_{l-1} \sin(\bar{\varphi}_{l-1} - \bar{\varphi}_l)] + \frac{1}{6} J_b f'(\varphi_{av})\} e^{-i\pi k/3}, \quad (5.12)$$

$$\left[\frac{\partial \mathcal{L}}{\partial z_l} \right]_t \left[\frac{\partial z_l}{\partial Z_k} \right]_t = \left\{ s^2 J \left[\bar{z}_{l+1} + \bar{z}_{l-1} + 2 + \sum_{m=0}^5 \left[\frac{\partial C_m}{\partial z_l} \right]_t \cos(\bar{\varphi}_m - \bar{\varphi}_{m+1}) \right] - i \hbar s \dot{\varphi}_l \right\} i e^{i\pi k/3}, \quad (5.13)$$

with

$$\left[\frac{\partial C_m}{\partial z_l} \right]_t = -\frac{1}{C_m} [\bar{z}_m (1 - \bar{z}_{m+1}^2) \delta_{ml} + \bar{z}_{m+1} (1 - \bar{z}_m^2) \delta_{m+l}]. \quad (5.14)$$

Now express $(\bar{\varphi}_l, \bar{z}_l)$, wherever they occur, in terms of $(\bar{\Phi}_l, \bar{Z}_l)$. Using the tunneling path ansatz (5.10) repeatedly, it readily follows that

$$\bar{z}_l = i\bar{Z}_0 + z_g \equiv \bar{Z}_c, \quad \bar{\varphi}_l = \bar{\Phi}_0 + \varphi_0(-T/2), \quad (5.15)$$

whence

$$\varphi_{av} = \bar{\Phi}_0, \quad \bar{\varphi}_l - \bar{\varphi}_{l+1} = \pi, \quad (5.16)$$

$$\sum_{m=0}^5 \left[\frac{\partial C_m}{\partial z_l} \right]_t = -2\bar{Z}_c. \quad (5.17)$$

This means that Eqs. (5.11)–(5.13) depend on the index l only through the factors of $e^{\pm i\pi l k/3}$. Since $\sum_{l=0}^5 e^{\pm i\pi l k/3} = 6\delta_{k0}$, these equations simplify considerably to become

$$-i\hbar s i \bar{Z}_0 \delta_{0k} = \frac{1}{6} J_b f'(\bar{\Phi}_0) \delta_{0k}, \quad (5.18)$$

$$i\hbar s \bar{\Phi}_0 \delta_{0k} = 4s^2 J_i \bar{Z}_0 \delta_{0k}. \quad (5.19)$$

where $z_g = -\frac{1}{2}$ has been used. Evidently, the equations of motion for the transverse coordinates ($k \neq 0$) trivially reduce to zero, and only the tunneling coordinates $\bar{\Phi}_0$ and \bar{Z}_0 have nontrivial behavior.

This allows us to introduce a considerable simplification. Write $\hat{\mathcal{L}}$ for the function that results when \mathcal{L} is expressed in terms of the new coordinates:

$$\hat{\mathcal{L}}(\Phi_0, Z_0; \dots; \Phi_5, Z_5) \equiv \mathcal{L}(\varphi_k(\{\Phi_l\}), z_k(\{Z_l\})). \quad (5.20)$$

Define an *effective* Lagrangian $\hat{\mathcal{L}}_0$, that depends only on

the tunneling coordinates, (Φ_0, Z_0) , by the relation

$$\hat{\mathcal{L}}_0(\Phi_0, Z_0) \equiv \hat{\mathcal{L}}(\Phi_0, Z_0; 0, 0; \dots; 0, 0). \quad (5.21)$$

Now, the behavior of the tunneling coordinates $\bar{\Phi}_0$ and \bar{Z}_0 can be found directly via the effective Lagrangian $\hat{\mathcal{L}}_0$, instead of the full $\hat{\mathcal{L}}$. This follows because the equations of motion for $\hat{\mathcal{L}}_0$ are exactly Eqs. (5.18) and (5.19), essentially by definition, since $(\partial \hat{\mathcal{L}} / \partial Z_0)_t$, evaluated according to the tunneling path ansatz Eq. (5.10), is *identically* equal to $(\partial \hat{\mathcal{L}}_0 / \partial Z_0)_t$, with similar comments holding for $(\partial \hat{\mathcal{L}}_0 / \partial (\partial_z \Phi_0))_t$ and $(\partial \hat{\mathcal{L}}_0 / \partial \Phi_0)_t$. Furthermore, since \mathcal{S}_0 depends solely on the tunneling path, it too can be calculated directly from $\hat{\mathcal{L}}_0$. The effective Lagrangian $\hat{\mathcal{L}}_0$ can be found from Eq. (5.21) to be

$$\begin{aligned} \hat{\mathcal{L}}_0(\Phi_0, Z_0) = & -i\hbar 6s(\dot{\Phi}_0)(Z_c - 1) \\ & + 12s^2 J(Z_c - z_g)^2 + J_b f(\Phi_0). \end{aligned} \quad (5.22)$$

It is from this expression that \mathcal{H}_{eff} of Eq. (2.7) was obtained. Evidently $\hat{\mathcal{L}}_0$ has just the form of the Lagrangian of Eq. (3.1), with

$$n = 6, \quad a = 12s^2 J, \quad b = J_b, \quad z_g = -\frac{1}{2}. \quad (5.23)$$

Consequently, all the results from Sec. III are applicable. The classical action, from Eq. (3.8), is

$$\mathcal{S}_0^\pm = \pm 9i\hbar s \pi + \hbar s \sqrt{3J_b/J_s^2} \int_0^\pi d\varphi \sqrt{f(\bar{\varphi}^+)}. \quad (5.24)$$

From the above expression for the classical action one can immediately read off the most striking result of this paper:

$$e^{-\mathcal{S}_0^+/\hbar} + e^{-\mathcal{S}_0^-/\hbar} = \begin{cases} -2 \exp[-\sqrt{3J_b/J} \int_0^\pi d\varphi \sqrt{f(\bar{\varphi}^+)}] & \text{if } s = \text{integer} \\ 0 & \text{if } s = \text{half-odd integer} \end{cases}. \quad (5.25)$$

Thus, if s is a half-odd integer, the (+) instanton and (−) instanton amplitudes interfere destructively, and the total tunneling amplitude is zero (for a discussion and extension of this result, see Sec. VI).

C. The prefactor (*kagomé* lattice)

The calculation of the prefactor involves the evaluation of the path integral

$$\int \prod_{l=0}^5 \mathcal{D}\Omega_l e^{-\int d\tau \delta^2 \mathcal{L} / \hbar} \quad (5.26)$$

where the second variation of the action is

$$\delta^2 \mathcal{L} = \frac{1}{2} \left[\frac{\partial^2 \mathcal{L}}{\partial z_m \partial z_n} \right]_t \delta z_m \delta z_n + \left[\frac{\partial^2 \mathcal{L}}{\partial \dot{\varphi}_m \partial z_n} \right]_t \delta \dot{\varphi}_m \delta z_n + \left[\frac{\partial^2 \mathcal{L}}{\partial \varphi_m \partial z_n} \right]_t \delta \varphi_m \delta z_n + \frac{1}{2} \left[\frac{\partial^2 \mathcal{L}}{\partial \varphi_m \partial \varphi_n} \right]_t \delta \varphi_m \delta \varphi_n. \quad (5.27)$$

The deviations around the tunneling path, defined by

$$\delta z_l \equiv z_l - \bar{z}_l \equiv e^{i\pi l k/3} \delta Z_k, \quad (5.28)$$

$$\delta \varphi_l \equiv \varphi_l - \bar{\varphi}_l \equiv e^{-i\pi l k/3} \delta \Phi_k, \quad (5.29)$$

are taken to be purely real (it is only the tunneling path itself that has to become complex to minimize the action). Thus, their Fourier transforms obey the conditions $\delta \Phi_l^* = \delta \Phi_{-l}$ and $\delta Z_l^* = \delta Z_{-l}$.

Now, it can be verified that

$$\left[\frac{\partial^2 \mathcal{L}}{\partial \dot{\varphi}_m \partial z_n} \right]_t = -i\hbar s \delta_{mn}, \quad \left[\frac{\partial^2 \mathcal{L}}{\partial \varphi_m \partial z_n} \right]_t = 0, \quad (5.30)$$

$$\frac{1}{2} \left[\frac{\partial^2 \mathcal{L}}{\partial z_m \partial z_n} \right]_t = \frac{1}{2} J s^2 \left\{ 2\delta_{mn} \frac{1}{1-\bar{Z}_c^2} + (\delta_{mn+1} + \delta_{m+1n}) \left[1 - \frac{\bar{Z}_c^2}{1-\bar{Z}_c^2} \right] \right\}, \quad (5.31)$$

$$\frac{1}{2} \left[\frac{\partial^2 \mathcal{L}}{\partial \varphi_m \partial \varphi_n} \right]_t = \frac{1}{2} \frac{1}{36} J_b f''(\bar{\Phi}_0) + \frac{1}{2} s^2 J (1-\bar{Z}_c^2) [2\delta_{mn} - \delta_{m+1n} - \delta_{mn+1}]. \quad (5.32)$$

Obtaining the actual numerical coefficients in Eqs. (5.31) and (5.32) is somewhat tedious; however, the fact that the m, n dependence enters only via δ functions of the form δ_{mn+k} , which is all that is needed for the following argument, can be anticipated directly from the fact that the original \mathcal{L} of Eqs. (5.1)–(5.2) is “translationally invariant” (i.e., invariant under $l \rightarrow l+1$). Now, when writing $\delta^2 \mathcal{L}$ of Eq. (5.27) in terms of the Fourier transform variables $(\delta\Phi_l, \delta Z_l)$ of Eqs. (5.28) and (5.29), one may utilize the relation

$$\sum_{mn=0}^5 \delta_{mn+k} \delta z_m \delta z_n = 6 \sum_{l=0}^5 e^{i\pi l k / 3} \delta Z_l \delta Z_{-l}, \quad (5.33)$$

which is essentially a consequence of the convolution theorem for discrete Fourier transformations. Using Eqs. (5.30)–(5.33) in Eq. (5.27), it follows directly that the variables $(\delta\Phi_0, \delta Z_0)$ decouple completely from the others in $\delta^2 \mathcal{L}$.²⁹ Hence the path integral (5.26) factorizes into a product, say $I_1 I_2$, of two independent path integrals. I_1 depends only on $(\delta\Phi_0, \delta Z_0)$, the variations of the tunneling coordinates around their tunneling path values:

$$I_1 = \int \mathcal{D}(\delta\Omega_0) e^{-\int d\tau \delta^2 \hat{\mathcal{L}}_0 / \hbar}. \quad (5.34)$$

In writing this equation, another shortcut has been employed: $\delta^2 \hat{\mathcal{L}}_0$ is the second variation of the simple Lagrangian $\hat{\mathcal{L}}_0$ of Eq. (5.21), namely,

$$\delta^2 \hat{\mathcal{L}}_0 = -i\hbar 6s \delta\dot{\Phi}_0 \delta Z_0 + 12s^2 J \delta Z^2 + \frac{1}{2} J_b f''(\bar{\Phi}_0) \delta\Phi_0^2. \quad (5.35)$$

This simple form may be used, since $(\partial^2 \hat{\mathcal{L}} / \partial^2 Z_0)_t$, evaluated according to the tunneling path ansatz (5.10), is *identically* equal to $(\partial^2 \hat{\mathcal{L}}_0 / \partial^2 Z_0)_t$, with similar comments holding for the other second derivatives $\hat{\mathcal{L}}_0$ with respect to the Φ_0 and Z_0 .

The other path integral I_2 depends only on $(\delta\Phi_l, \delta Z_l)_{l \neq 0}$, the variations of the transverse coordinates around their zero values along the tunneling path. These fluctuations are exactly harmonic oscillators in the limit $J_b / s^2 J \rightarrow 0$, since then all time dependence drops out of the coefficients in Eqs. (5.31)–(5.32) (recall that $\bar{Z}_c = i\bar{Z}_0 + z_g$, with $i\delta Z_0 \propto \sqrt{b/a} \propto \sqrt{J_b / s^2 J}$). More generally, the fluctuations of the transverse coordinates will shift the ground-state energy by an amount proportional to their characteristic frequencies. However, they will *not* make a contribution to the tunnel-splitting energy Δ .

Thus, for the calculation of Δ , only the path integral I_1 is relevant. Since this depends only on \mathcal{L}_0 , the demonstration that only $\hat{\mathcal{L}}_0$ is important for the calculation of Δ is complete.

It follows that Δ may be directly obtained from the effective Lagrangian $\hat{\mathcal{L}}_0$ of Sec. IV, Eq. (5.22), inserted into the results of Sec. IV C. Substituting the values of Eqs. (5.23) and (5.24) into Eq. (4.12) gives

$$\Delta = \begin{cases} 4 \left(\frac{2}{3}\right)^{1/4} \pi^{-1/2} \varphi_{\text{as}} (J_b f''(0))^{3/4} J^{1/4} \exp \left[-\sqrt{3} J_b / J \int_0^\pi d\varphi \sqrt{f(\varphi)} \right] & \text{if } s = \text{integer}, \\ 0 & \text{if } s = \text{half-odd integer}. \end{cases} \quad (5.36)$$

This is the main result of this paper—an explicit expression for the tunnel-splitting energy in a nontrivial setting.

Expression (5.36) can be evaluated numerically [see the last paragraph of Appendix A for the definition of J_b and $f(\varphi)$, and Eqs. (4.22), (4.23), and (4.20) for φ_{as}]. The results for Δ , in units of J , for some values of s are tabulated in Table I. It should be remarked, though, that strictly speaking and for several reasons, our methods are only applicable in the limit of $s \gg 1$. Collecting the s dependencies of φ_{as} , $f''(0)$, and J_b gives

$$\Delta \propto s J \exp[5.6s^{1/6} - 5.6s^{1/2}] \quad \text{for } s \gg 1. \quad (5.37)$$

VI. DESTRUCTIVE INTERFERENCE

It is quite striking that the tunnel-splitting energy and the tunneling amplitude [see Eqs. (5.25) and (5.36)] are exactly zero if s is a half-odd integer. This is a consequence of destructive interference of the (+) instanton and (−) instanton amplitudes in Eq. (5.25). Actually, this result can be arrived at without the need for a detailed calculation (see also Ref. 9). All that is needed is the fact that $\text{Re}[\mathcal{S}_0^+] = \text{Re}[\mathcal{S}_0^-]$ and $\mathcal{N}^+ = \mathcal{N}^-$, which is guaranteed by symmetry (under some technical assumptions, explained in Sec. IV B), and knowledge of the phase

TABLE I. Numerical values of Δ/J as a function of s , as calculated from Eq. (5.36).

| s | 1 | 2 | 3 | 4 | 5 | 6 | 10 | 20 |
|------------|-----|------|------|------|------|------|-------|--------------------|
| Δ/J | 2.3 | 0.83 | 0.32 | 0.13 | 0.06 | 0.02 | 0.001 | 5×10^{-6} |

of the classical action, Eq. (5.24). In fact, a similar result holds for a much larger class of tunneling problems on the *kagomé* lattice.

Consider the simultaneous tunneling of larger sets of spins on the *kagomé* lattice. Take, for example, any closed “loop” of spins such that all the spins on the loop alternate between types *A* and *B* around the loop. It is proven in Appendix D that all such loops contain $4n + 2$ spins (with n some integer). Now consider the rigid-rotation tunneling mode of this loop (a generalization of the rigid-hexagon mode to loops that are not hexagons), i.e., tunneling between configurations $|i\rangle$ and $|f\rangle$ that differ from each other only through $\varphi_l \rightarrow \varphi_l + \pi$ for each spin on the loop (i.e., in that all *A* and *B* spins on the loop are interchanged). This rigid-rotation tunneling mode does not cost any classical exchange energy, but selection effects provide a coplanarity barrier that has to be tunneled through. Under the (admittedly somewhat tenuous) assumption that during the tunneling motion of the $4n + 2$ spins all other spins will remain fixed, the following assertions can be made: The absolute values of the tunneling amplitudes of the (+) instanton and (−) instanton events are equal, and the relative phase between them is $i2\pi s(4n + 2)(-\frac{3}{2})$. Hence, for half-odd integer s , *destructive* interference between (+) instantons and (−) instantons occurs again.

Only when two loops, with a total number of $4n$ spins, tunnel simultaneously and synchronously will there be *constructive* interference between all the $4n$ spins. The smallest group of spins for which this is conceivable is the six-spin inner loop of a hexagon, nested inside a larger loop of 18 spins. These two loops would tend to tunnel synchronously because of the coplanarity forces between the triangles connecting them. Thus, the smallest tunneling event that has a nonzero amplitude involves a double loop of altogether 24 spins.

The fact that destructive interference happens for half-odd-integer s is noteworthy, since s is half-odd integer for the two experimental realizations of the *kagomé* lattice that have been proposed. These are the magnetoplumbite $\text{SrCr}_{8-x}\text{Ga}_{4+x}\text{O}_{19}$ ($s = \frac{3}{2}$) (Refs. 30–32) and the second layer of He^3 atoms on a graphite substrate ($s = \frac{1}{2}$).^{33,34}

VII. DISCUSSION

A. Discussion: Comparison of energy scales

In this paper, the tunneling barrier was taken as a fixed potential, given by \mathcal{H}_{cop} in Eq. (2.5), although the original Hamiltonian (2.2) had *no* “coplanarity forces.” In what follows, we argue that this approach can be justified in the limit of large s .

Our estimate of \mathcal{H}_{cop} in Appendix A is based on the

following strategy: The tunneling hexagon is frozen at a given point along its tunneling path, at which its plane is tilted by φ relative to the reference plane. Then the frequencies $\omega_l(\varphi)$ of the zero-point modes of the spins on neighboring hexagons are calculated as a function of φ . The coplanarity barrier is then taken to be proportional to $\sum_l \frac{1}{2} \hbar(\omega_l(\varphi) - \omega_l(0))$.

This procedure is reasonable if the tunneling process is “adiabatically” slow, i.e., if the duration of an instanton, say τ_{in} , is indeed long compared to the typical oscillation periods $\omega_l^{-1}(\varphi)$ of the zero-point modes on the surrounding hexagons. In this case, we are effectively “integrating out” in a crude way the fast modes of a complicated many-spin problem. However, if for some zero-point modes one has $\omega_l^{-1}(\varphi) \gtrsim \tau_{\text{in}}$, these modes are slower than the instanton and do not have time to affect the barrier. In that case, the effective barrier should be smaller than the one we used, since the contributions of slow modes to \mathcal{H}_{cop} should not be counted.

Now, in Appendix A, the behavior of the zero-point modes of the hexagons surrounding the tunneling hexagon is found to be as follows: There are both ordinary and soft modes (corresponding to $\rho_{l \neq 3}^\alpha$ and $\rho_{l=3}^\alpha$, respectively, in Appendix A). For the ordinary modes, we find $\hbar\omega_l(\varphi) \sim sJ$, as is usual for antiferromagnets. The soft modes are rigid-hexagon fluctuations; for $\varphi \approx 0$, we find $\hbar\omega_{\text{soft}}(\varphi) \sim s^{2/3}J$, while for large φ , one has $\hbar\omega_{\text{soft}}(\varphi) \sim sJ$. If one were to consider fluctuations on the entire lattice (instead of only on the neighboring hexagons of the tunneling hexagon), these soft modes would translate to an entire branch of soft modes, for which one would also expect $\hbar\omega_{\text{soft}} \sim s^{2/3}J$. This, indeed, is the result found by Chubukov [8], using a method based in Fourier space.

The duration of an instanton event, on the other hand, scales with s according to $\tau_{\text{in}} \sim 1/d \sim \hbar/(Js^{1/2})$, according to Eqs. (3.12) and (5.23). Thus, in the limit of $s \gg 1$, one has $\tau_{\text{in}} \gg \omega_l^{-1}$ for all zero-point modes, both ordinary and soft. In this limit, the instanton is thus indeed slow compared to the zero-point fluctuations, justifying the use of a coplanarity barrier \mathcal{H}_{cop} for sufficiently large s .

How does the calculated tunnel-splitting energy Δ compare to the in-plane selection energy (of order J_c) mentioned in Sec. II A, that tends to lift the degeneracy between $|i\rangle$ and $|f\rangle$, and hence to suppress tunneling? To obtain an estimate of J_c , we note that Chubukov⁸ has calculated the spin-wave velocities for the $\sqrt{3} \times \sqrt{3}$ and $\mathbf{q} = 0$ states (described in Sec. II A), and found them to differ by only about 5%. Since J_c is a measure of the energy difference between the $\sqrt{3} \times \sqrt{3}$ and $\mathbf{q} = 0$ states, it is a natural inference from this small difference in spin-wave velocities that J_c is only a small fraction of the zero-point soft-mode energy, i.e., $J_c \sim \eta Js^{2/3}$, with $\eta < 0.05$ [see also Ref. 5, Eq. (52)]. Since we found

$J_b = 5/2J_s$ [see Eq. (A22)], neglecting J_c relative to J_b seems justifiable. This is the justification for not adding an in-plane selection term to \mathcal{H}_{hex} in Eq. (2.3) in the same way that we added the coplanarity selection term \mathcal{H}_{cop} . However, it should be noted that for small tunneling angles φ , for which $\mathcal{H}_{\text{cop}} \sim J_s^{2/3}$, the inclusion of in-plane selection effects, which are also of order $J_s^{2/3}$, would probably affect some of our results. For example, our calculation of φ_{as} in Sec. IV C would be affected if $J_s \varphi^* \ll J_c \ll J_b$.

Finally, let us compare Δ to J_c . From Table I, it follows that for physically realizable (i.e., small) spin values, we have $\Delta \gtrsim J_c$. This has two implications: First, it is an *a posteriori* justification for taking $J_c = 0$ in our calculation [compare comment (i) in Sec. II C] because Δ does turn out to be substantially larger than J_c . Second, it implies that tunneling effects are at least as important as in-plane selection effects in determining the true nature of the ground state. Unfortunately, these conclusions are at best qualitatively correct, since in the domain of small s the steepest descent approximation that we use so extensively ceases to be reliable quantitatively.

For large s , where the steepest descent approximation is assumed to work well, Table I shows that $\Delta \lesssim J_c$. Thus, in this limit, the neglect of J_c in our calculation becomes questionable. A more sophisticated calculation, that would include from the beginning the effects of in-plane selection, would be beyond the scope of this paper. However, a reasonable conclusion would be that tunneling is suppressed and hence unimportant in this regime.

Because of the abovementioned problems, our calculation gives at best an order-of-magnitude estimate of Δ . However, this estimate does suggest that for small (integer) s , tunneling should be regarded as a significant disordering mechanism competing with order-from-disorder selection effects.

In a quantum Potts model of the entire *kagomé* system, the Hamiltonian would have matrix elements proportional to Δ between any two pairs of states, which differed by the exchange $A \leftrightarrow B$ along a single six-spin hexagon loop (or more generally, there would be matrix elements for any larger closed loop of alternating AB spins). Then a superposition of Potts states, which takes advantage of the resonance between different hexagons (or larger loops), would have a lower energy (at small s) than the $\sqrt{3} \times \sqrt{3}$ state, which is favored by the J_c term.

Two possible kinds of such ground states suggest themselves: The first is a “totally disordered” Potts state; it can be idealized by a trial wave function, which is an equal superposition of all the Potts ground states, which is known to be disordered (it has only algebraically decaying correlations³⁵). The second kind of ground state is a “partially disordered” $\sqrt{3} \times \sqrt{3}$ state; an idealized trial wave function has, say, all C spins fixed, as in the usual $\sqrt{3} \times \sqrt{3}$ state, but each $ABABAB$ hexagon is replaced by an equal superposition of the $ABABAB$ and $BABABA$ configurations (with no correlation between one hexagon and another). Such a state would still have long-range order with respect to the C spins but would be disordered with respect to the A and B spins. We call this a “ferrimagnetic” ground state, since the expectation

value of \mathbf{n}_z is $+1$ on the C sublattice, and $-\frac{1}{2}$ on the other two sublattices.

Both these candidate states have considerably less order than the long-range-ordered $\sqrt{3} \times \sqrt{3}$ state. On the other hand, they are more ordered than the “spin-nematic” state, which has been previously proposed for this system.^{6,17} In the “spin nematic,” all spins lie in the same plane, but all directions in a given plane are equally likely, i.e., $\langle e^{i\theta(\mathbf{r})} \rangle = 0$. The states described by quantum Potts models have either an A , B , or C spin at each site, so that $\langle e^{i3\theta(\mathbf{r})} \rangle \neq 0$.³⁶

For the half-odd integer s , of course, hexagon tunneling is absent (the smallest tunneling event with nonzero amplitude involves the synchronous turning of 24 spins), as discussed in Sec. VI. Therefore, one would expect the long-range order of the usual $\sqrt{3} \times \sqrt{3}$ state to persist, at least to much smaller values of s than for integer spins.

B. Possible extension and other applications

A more fundamental approach for treating coplanarity selection effects, that should be trustworthy also for small s , would be as follows: Write down a functional integral for the entire N -spin system, starting from the Heisenberg Hamiltonian, Eq. (2.2), without an explicit coplanarity term such as Eq. (2.5). Adopt a tunneling path in which only the six spins of the tunneling hexagon move. The tunneling coordinates would be essentially the same as the collective coordinates (Φ_0, Z_0) introduced in Sec. V. However, one would then have of order $N - 1$ transverse modes, instead of only 5. Integrating these out would result in an effective potential for (Φ_0, Z_0) , which could, in principle, be nonlocal in time (since it encodes the effect of changing (Φ_0, Z_0) at time τ on the transverse modes, which, if these modes are slow, will in turn influence the potential felt by (Φ_0, Z_0) at later times).

We briefly mention a possible application of tunneling calculations in the context of finite-size systems. Consider some frustrated antiferromagnetic system whose ground states have spin order with nontrivial discrete symmetry. For small system sizes, the eigenvalue spectrum can be found by exact diagonalization of the Hamiltonian. Tunneling calculations could be useful in obtaining better interpretations of such an eigenvalue spectrum. For example, the $J_1 - J_2$ square antiferromagnet (for $J_2 > 0.5J_1$) has classical ground states in which the even sublattice has alternating spins of one staggered magnetization and the odd sublattice has an independent, arbitrary staggered magnetization. When quantum fluctuations are taken into account, spin-wave theory gives an effective “collinearity” force [analogous to the coplanarity term in Eq. (2.5) in the present paper]. This lines up the staggered magnetizations along the same axis, in either sense,^{37,38} so that classically there are two ground states related by a discrete symmetry and separated by a barrier. Consequently, the two lowest eigenstates of a large system should both be spin singlets, namely, the symmetric and antisymmetric combinations of the two classical ground states (which are also spin singlets) that have been mixed by quantum tunneling. [This behavior contrasts to that of ordinary antiferromagnets; there the smallest gap is associated with $E \simeq s(s+1)/2\chi$, where χ

is the susceptibility, so that the first excited state is a triplet.] The classical path expected (in a small system) has all spins of a given sublattice rotating together during the tunneling event, so it should be possible to map the $J_1 - J_2$ tunneling problem to a four-spin problem, in the same fashion that we mapped a six-spin problem to a one-spin problem.

C. Summary

We have presented a detailed calculation of the tunnel-splitting energy Δ that arises because of the tunneling of six hexagon spins between two degenerate ground-state configurations on a *kagomé* lattice. This was done by introducing a set of collective coordinates and thus mapping the problem onto a much simpler model problem that can be treated by standard methods. These involve the method of steepest descent to evaluate a coherent-spin-state path integral in imaginary time and integrating out the $\cos\theta$ degree of freedom to obtain an effective Lagrangian \mathcal{L}_φ , involving only the coordinate φ . The tunnel-splitting energy for \mathcal{L}_φ can then be found by using well-known methods developed for the tunneling of particles through a double-well barrier.

The most striking aspect of our final result, Eq. (5.36), is that when s is half-odd integer, the tunneling amplitude and the tunnel-splitting energy Δ are strictly zero, due to destructive interference between (+) instanton and (-) instanton paths. This destructive interference is argued to occur also for larger loops of AB spins tunneling between two degenerate configurations. For small, integer s , we find that the tunnel-splitting energy Δ is at least of the same order of magnitude as the in-plane selection energy J_c found by other authors; this implies that tunneling constitutes an important mechanism competing with order-from-disorder selection effects, which might tend to drive the system into a partially disordered ground state.

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APPENDIX A

In this appendix we obtain an estimate for the form of the shape-function $f(\varphi)$ and the magnitude J_b of the coplanarity potential \mathcal{H}_{cop} introduced in Sec. II C, Eq. (2.5).

1. Estimate of zero-point energy

In principle, \mathcal{H}_{cop} has to be calculated as follows: Start from a $\sqrt{3} \times \sqrt{3}$ coplanar ground state, and for a given hexagon, say P , turn all six spins (of types A and B , say), around the C direction (which we take to define the \mathbf{z} axis), by an angle φ . This rigid-hexagon rotation has no cost in classical energy. However, if one allows all spins in the lattice to execute zero-point fluctuations around their classical ground-state directions (characterized by a set of unit vectors $\{\mathbf{n}_i^{(0)}\}$), and calculates the associated zero-point energy $E_0(\varphi)$, as a function of φ , it is found

that $E_0(\varphi)$ has its minimum at $\varphi=0$.⁴⁻⁸ Hence $E_0(\varphi)$ acts as a barrier that opposes rigid-hexagon rotations.

To obtain a crude estimate of $E_0(\varphi)$, we shall only calculate the effect of turning P on the zero-point energy of one of its nearest-neighbor hexagons, say Q (see Fig. 1), arguing that the effects of turning P should have an increasingly weak effect on more distant hexagons. Let the six spins of Q be labeled by $l=0, \dots, 5$ (where the index l is defined modulo 6). Thus, we allow these six spins (including the $l=0$ spin, which is shared by Q and P), to fluctuate,

$$\mathbf{n}_l = \mathbf{n}_l^{(0)} + \sum_{\alpha=x,y,z} \sigma_l^\alpha \mathbf{e}_l^\alpha, \quad (\text{A1})$$

while all other spins in the lattice are kept fixed at their respective $\mathbf{n}_i^{(0)}$. Here we have introduced a (right-handed) set of local basis vectors \mathbf{e}_l^α ($\alpha=x,y,z$) for each spin, with $\mathbf{e}_l^z \equiv \mathbf{n}_l^{(0)}$. We consider only *small* deviation amplitudes $\sigma_l^\alpha \ll 1$, and require that $|\mathbf{n}_l| = 1$. At the end of the calculation, we shall estimate the effects of allowing all six (as opposed to only one) nearest-neighbor hexagons of P to fluctuate simultaneously.

Given Eq. (A1), perform the standard expansion of the classical Hamiltonian (2.2) around $\mathbf{n}_i^{(0)}$, to quadratic order in σ_l^α :

$$\begin{aligned} \mathcal{H} - \mathcal{H}^{(0)} &= s^2 J \sum_{\langle i,j \rangle} [\mathbf{n}_i \cdot \mathbf{n}_j - \mathbf{n}_i^{(0)} \cdot \mathbf{n}_j^{(0)}] \\ &= s^2 J \sum_{l=0}^5 \left[\sigma_l^x{}^2 + \sigma_l^y{}^2 \right. \\ &\quad \left. + \sum_{\alpha,\beta \in \{x,y\}} \sigma_l^\alpha \sigma_{l+1}^\beta \mathbf{e}_l^\alpha \cdot \mathbf{e}_{l+1}^\beta \right]. \end{aligned} \quad (\text{A2})$$

No linear terms occur, because the $\mathbf{n}_i^{(0)}$ directions minimize \mathcal{H} ; this is true even when P has been turned relative to Q , since rigid-hexagon twists do not cost any classical energy.

Now, for each l , the variable ($-\hbar\sigma_l^\alpha$) plays the role of a canonically conjugate momentum to the variable $s\sigma_l^\alpha$. Suppose that it is possible to find a transformation to a new set of pairs of canonically conjugate variables, $\{s\bar{p}_l^\alpha, \hbar\bar{p}_l^\alpha\}$, in terms of which $\mathcal{H} - \mathcal{H}^{(0)}$ is diagonal:

$$\mathcal{H} - \mathcal{H}^{(0)} \equiv J \sum_{l=0}^5 \left[\frac{1}{2} \frac{s^2 (\hbar\bar{p}_l^x)^2}{m_l} + \frac{1}{2} k_l (s\bar{p}_l^y)^2 \right]. \quad (\text{A4})$$

This is just another way of writing the usual spin wave theory—the \bar{p}_l^α are magnons. The zero-point energy of the system can then be written simply as

$$E_0(\varphi) \equiv \sum_{l=0}^5 \frac{1}{2} \hbar [\omega_l(\varphi) - \omega_l(0)], \quad (\text{A5})$$

where the frequencies ω_l and root-mean-square (rms) amplitudes of $s\bar{p}_l^\alpha$ are given, respectively, by

$$\omega_l = s \sqrt{k_l/m_l} \quad \text{and} \quad \langle (s\bar{p}_l^\alpha)^2 \rangle^{1/2} = \left[\frac{\hbar}{2m_l \omega_l} \right]^{1/2}, \quad (\text{A6})$$

In attempting to transform Eq. (A3) into the form Eq. (A4), we proceed as follows. Make the transformations

$$\begin{aligned}
-\sigma_l^x &\equiv 6^{-1/2} \sum_{k=0}^5 e^{-i\pi k/3} \rho_k^x, \\
\sigma_l^y &\equiv 6^{-1/2} \sum_{k=0}^5 e^{i\pi k/3} \rho_k^y,
\end{aligned} \tag{A7}$$

where $\rho_{-k}^\alpha = (\rho_k^\alpha)^*$. Also make the following choices for the vectors \mathbf{e}_l^α [here $R(\mathbf{n}, \varphi)$ denotes a rotation by an angle φ around the \mathbf{n} direction]:

$$\begin{aligned}
\mathbf{e}_{1,3,5}^x &= (1, 0, 0), \quad \mathbf{e}_{1,3,5}^y = (0, 1, 0), \quad \mathbf{e}_{1,3,5}^z = (1, 0, 1), \\
\mathbf{e}_{2,4}^x &= \frac{1}{2}(-1, 0, -\sqrt{3}), \quad \mathbf{e}_{2,4}^y = (0, 1, 0), \\
\mathbf{e}_{2,4}^z &= \frac{1}{2}(\sqrt{3}, 0, -1),
\end{aligned} \tag{A8}$$

$$\begin{aligned}
\mathbf{e}_0^x &= R(\mathbf{e}_0^z, -\varphi)R(\mathbf{z}, \varphi)\mathbf{e}_{2,4}^x \\
&= \frac{1}{2}(-1 - \sin^2\varphi, \cos\varphi\sin\varphi, -\sqrt{3}\cos\varphi), \\
\mathbf{e}_0^y &= R(\mathbf{e}_0^z, -\varphi)R(\mathbf{z}, \varphi)\mathbf{e}_{2,4}^y \\
&= \frac{1}{2}(-\cos\varphi\sin\varphi, 2 - \sin^2\varphi, \sqrt{3}\sin\varphi), \\
\mathbf{e}_0^z &= R(\mathbf{z}, \varphi)\mathbf{e}_{2,4}^z = \frac{1}{2}(\sqrt{3}\cos\varphi, \sqrt{3}\sin\varphi, -1).
\end{aligned} \tag{A9}$$

In the definition of \mathbf{e}_0^α , the $R(\mathbf{z}, \varphi)$ rotation is introduced to account for the rigid rotation of hexagon P relative to \mathcal{Q} . The additional rotation $R(\mathbf{e}_0^z, -\varphi)$ for \mathbf{e}_0^x and \mathbf{e}_0^y is introduced merely for convenience—it allows one to minimize the effect of $\mathbf{e}^x \cdot \mathbf{e}^y$ cross terms in Eq. (A3).

By straightforward calculations one readily arrives at

$$\mathcal{H} - \mathcal{H}^{(0)} = \mathcal{H}_{xx} + \mathcal{H}_{yy} + \mathcal{H}_{xy}, \tag{A10}$$

$$\begin{aligned}
\mathcal{H}_{xx} &= s^2 J \left[\sum_{l=0}^5 (1 - \frac{1}{2} \cos l\pi/3) |\rho_l^x|^2 \right. \\
&\quad \left. - \frac{1}{12} \sin^2\varphi \sum_{k,l=0}^5 (e^{i\pi k/3} + e^{i\pi l/3}) \rho_k^x \rho_{-l}^x \right],
\end{aligned} \tag{A11}$$

$$\begin{aligned}
\mathcal{H}_{yy} &= s^2 J \left[\sum_{l=0}^5 (1 + \cos l\pi/3) |\rho_l^y|^2 \right. \\
&\quad \left. - \frac{1}{12} \sin^2\varphi \sum_{k,l=0}^5 (e^{-i\pi k/3} + e^{-i\pi l/3}) \rho_k^y \rho_{-l}^y \right],
\end{aligned} \tag{A12}$$

$$\mathcal{H}_{xy} = \frac{1}{12} s^2 J \sin 2\varphi \sum_{k,l=0}^5 [\cos k\pi/3 - \cos l\pi/3] \rho_k^x \rho_l^y. \tag{A13}$$

Evidently, $\mathcal{H} - \mathcal{H}^{(0)}$ is not yet diagonal. However, one can obtain an estimate of the zero-point energy $E_0(\varphi)$ by adding up the frequencies of the six individual “pure” modes and neglecting the coupling between different modes (to obtain a pure l mode, take $\rho_k^\alpha = 0$ for all k except for $k=l$ and $k=-l$).³⁹ For pure modes, $\mathcal{H}_{xy} = 0$, and the frequency ω_l can be found from Eq. (A6). The smallest frequency is that of the mode ρ_3^α , which corre-

sponds to rigid-hexagon fluctuations of the spins of \mathcal{Q} , and costs zero energy when $\varphi=0$. From Eq. (A10), one finds

$$[\mathcal{H} - \mathcal{H}^{(0)}]_{l=3} = s^2 J [(\rho_3^x)^2 (\frac{3}{2} + \frac{1}{6} \sin^2\varphi) + (\rho_3^y)^2 \frac{1}{6} \sin^2\varphi] \tag{A14}$$

$$\hbar\omega_3 = sJ |\sin\varphi| (1 + \frac{1}{9} \sin^2\varphi)^{1/2}. \tag{A15}$$

Since $\omega_3(\varphi=0) = 0$, this is a soft mode. The frequencies for the other five pure modes have the form

$$\hbar\omega_l = sJ [(c_{1l} + c_{2l} \sin^2\varphi_l)(1 + c_{3l} \sin^2\varphi_l)]^{1/2}, \tag{A16}$$

where c_{1l} , c_{2l} , and c_{3l} are constants that can be obtained with some more work. It turns out that $c_{1l} \neq 0$ for $l \neq 3$, so that, as expected, these modes are not soft. Also, we find that their joint contribution to $E_0(\varphi)$ [in which $\omega_l(\varphi=0)$ is subtracted off] can be mimicked, to within 1% accuracy, by the expression $-0.21sJ \sin^2\varphi$. Using this result and Eq. (A15) in Eq. (A5), we conclude that the total zero-point energy of the fluctuations of hexagon \mathcal{Q} when its neighbor, hexagon P , is turned by φ , is $E_0(\varphi) = \frac{1}{2} J s \tilde{f}(\varphi)$, where

$$\tilde{f}(\varphi) \simeq |\sin\varphi| (1 + \frac{1}{9} \sin^2\varphi)^{1/2} - \tilde{J} \sin^2\varphi \tag{A17}$$

and $\tilde{J} = 0.42$.

Now we have to estimate the zero-point energy when *all* six neighboring hexagons of hexagon P are fluctuating simultaneously. To do an extended version of the above calculation seems forbiddingly tedious. Roughly, we estimate that the total zero-point energy will be $\mathcal{H}_{\text{cop}} \simeq 5E_0(\varphi)$. We have two arguments, both rather crude, for using a factor 5 and not 6: Firstly, there are 30 (not 36) independent spins in the six hexagons surrounding P . Secondly, there exists one particular superposition of the six soft rigid-hexagon modes (i.e., modes for modes which only $\rho_3^\alpha \neq 0$) of the six neighboring hexagons of P , which results in a mode that is totally unaffected by turning hexagon P . (In this mode, only the six spins of hexagon P and the 18 spins on the outer perimeter of the six neighboring hexagons are fluctuating, at no cost in energy, while the six spins between the inner and outer loops of fluctuating spins remain fixed.)

2. Self-consistency of zero-point fluctuation amplitude

In the above calculation, the zero-point motion of hexagon P itself about its orientation at fixed φ has been ignored. This is reasonable if φ is not small. However, if $\varphi \lesssim \varphi^*$, where $\varphi^* \equiv \langle \varphi^2 \rangle^{1/2}$ is the rms amplitude of the zero-point fluctuations of a hexagon around the coplanar ($\varphi=0$) orientation, the zero-point motion of P itself can no longer be neglected. It has the effect of rounding out the effective potential $f(\varphi)$ at the bottom of the well from a linear to a quadratic φ dependence. Arguing that even if $\varphi=0$ for a given hexagon, to its neighbors it will actually seem to have $\varphi \simeq \pm\varphi^*$ because of its zero-point fluctuations, we incorporate this effect into $f(\varphi)$ by using an effective shape function defined by

$$\begin{aligned}
f(\varphi) &= \tilde{f}(\sqrt{\varphi_{\text{eff}}^2 + \varphi^{*2}}) - \tilde{f}(\varphi^*), \\
\varphi_{\text{eff}} &\equiv \varphi \bmod \pi \in (-\pi/2, \pi/2],
\end{aligned} \tag{A18}$$

where $\tilde{f}(\varphi)$ is given by Eq. (A17). Thus the cusp in the shape function at $\varphi=0$ is rounded out (see Fig. 4), while for large φ , we essentially have $f(\varphi) \simeq \tilde{f}(\varphi)$.

The rms amplitude φ^* has to be determined self-consistently: Calculate the rms value φ^* for hexagon P , fluctuating about the coplanar ($\varphi=0$) configuration, under the assumption that all its neighbors are turned by $\varphi=\varphi^*$ from the coplanar configuration, and solve the resulting self-consistency condition for φ^* . Since φ^* is expected to be small, in this estimate we take into account only the rigid-hexagon fluctuations on P , characterized by ρ_3^α . Expression (A14) gives the effective Hamiltonian for the rigid-hexagon mode of P when P is coupled to just one neighboring hexagon (turned by φ), while the other five neighbors of P are kept fixed at $\varphi=0$. When all six neighbors are turned by roughly φ^* , the effective Hamiltonian for the rigid-hexagon mode of P is therefore roughly

$$s^2 J [(\bar{\rho}_3^x)^2 (\frac{3}{2} + \frac{1}{6} \sin^2 \varphi^*) + (\bar{\rho}_3^y)^2 6 \frac{1}{6} \sin^2 \varphi^*]. \quad (\text{A19})$$

(Note that only the ‘‘stiffness’’ [coefficient of $(\bar{\rho}_3^y)^2$] gets a factor of 6, not the ‘‘mass’’ [coefficient of $(\bar{\rho}_3^x)^2$].) Using expressions (A6) and (A19), one therefore finds the following self-consistency relation:

$$s \bar{\rho}_3^{y*} = \langle (s \bar{\rho}_3^{y*})^2 \rangle^{1/2} = \sqrt{s/2} \left[\frac{3J}{2J\varphi^{*2}} \right]^{1/4}. \quad (\text{A20})$$

Tracing the transformations from $\bar{\rho}_3^y$ back to φ , one finds that the deviation $\bar{\rho}_3^{y*}$ corresponds to hexagon P being turned by $\varphi^* = \sqrt{2/3} \bar{\rho}_3^{y*}$. Using this in Eq. (A20) and solving for φ^* one readily finds

$$\varphi^* = \frac{1}{9} \sqrt{3/2} s^{-1/3} = 0.14 s^{-1/3}. \quad (\text{A21})$$

Note that $\varphi^* \rightarrow 0$ as $s \rightarrow \infty$. The $s^{-1/3}$ dependence here is in agreement with the work of Chubukov.⁸ He has used a self-consistent theory, which is similar in structure to our arguments in this appendix but based in Fourier space [and taking into account cubic terms of the form $\sigma^x(\sigma^y)^2, (\sigma^x)^3$], to calculate zero-point frequencies and amplitudes of fluctuations.

The various frequencies $\omega_l(\varphi)$ scale as follows with s : For the soft mode ($l=3$), Eqs. (A18) and (A15) show that $\hbar\omega_3(\varphi) \sim sJ\varphi^2/\varphi^*$ as $\varphi \rightarrow 0$, so that, by Eq. (A21), one has $\hbar\omega_3 \sim s^{2/3}J$ for $\varphi \lesssim \varphi^*$. For $\varphi \gg \varphi^*$, one has $\hbar\omega_3(\varphi) \sim sJ$. For the five nonsoft modes ($l \neq 3$), Eq. (A16) shows that $\hbar\omega_l(\varphi) \sim sJ$, for all φ .

To summarize the results of this appendix, the co-

$$I' = \left[\frac{4\pi}{2\varepsilon' + r^{-2}} \right]^{1/2} \int_{-\infty}^{\infty} d\varphi_j \exp - \left[\frac{s^2 \Delta\varphi_j^2}{2(2\varepsilon' + r^{-2})} + (\varepsilon'/s)f(\varphi_j) \right]. \quad (\text{B5})$$

The process of integrating out z_j has thus generated a Gaussian cutoff for φ_j :

$$\varphi_j - \varphi_{j+1} \propto \sqrt{2\varepsilon' + r^{-2}}/s. \quad (\text{B6})$$

If $r = \infty$, the φ paths are Brownian-motion paths, since

planarity potential has the form

$$\mathcal{H}_{\text{cop}} = 5E_0(\varphi) = J_b f(\varphi), \quad (\text{A22})$$

with $J_b = \frac{5}{2}Js$. The functions and $f(\varphi)$ and $\tilde{f}(\varphi)$ are defined in Eqs. (A18) and (A17), respectively, and $f(\varphi)$ depends on $\varphi^* \sim s^{-1/3}$. $f(\varphi)$ is plotted in Fig. 4 for the case $s=1$. Our crude estimates are expected to be reliable to within a factor of 2.

APPENDIX B

In this appendix, which is a complement to Sec. IV A, we investigate the way in which the integration range $[-r, r]$ for z influences the degree of non-differentiability of the φ -paths that result after z has been integrated out, for a Hamiltonian containing a z^2 term. It is shown that for $r=1$, the resulting φ paths are highly nondifferentiable, much more pathological than Brownian motion paths. For $r = \infty$ they are Brownian motion paths.

To see the difference between $r=1$ and $r = \infty$, consider the simplest Lagrangian that illustrates the point we wish to make:

$$\mathcal{L} = -i\hbar s \dot{\varphi} z + s^2 z^2 + s f(\varphi), \quad (\text{B1})$$

where $z = \cos\theta$ and $f(\varphi)$ is some function of φ . A typical z_j integral appearing at the j th time slice in the discretized-time version of the path integral $\int d\Omega e^{-S/\hbar}$ has the form

$$I = \int_{-\infty}^{\infty} d\varphi_j \int_{-r}^r dz_j \exp - [-i\Delta\varphi_j z_j s + \varepsilon' z_j^2 + (\varepsilon'/s)f(\varphi_j)], \quad (\text{B2})$$

where

$$\begin{aligned} \dot{\varphi}_j &= (\varphi_j - \varphi_{j+1})/\varepsilon = \Delta\varphi_j/\varepsilon, \\ \varepsilon' &= s^2 \varepsilon/\hbar, \quad \varepsilon = T/(N+1). \end{aligned} \quad (\text{B3})$$

To shed light on the significance of r in Eq. (B2), let us replace the sharp cutoff at $\pm r$ by a Gaussian cutoff of width $2r$ (the resulting change in normalization is not relevant to our argument). Thus we replace I by

$$I' = \int_{-\infty}^{\infty} d\varphi_j \int_{-\infty}^{\infty} dz_j \exp - \left[\left[\varepsilon' + \frac{1}{2r^2} \right] z_j^2 - i\Delta\varphi_j z_j s + (\varepsilon'/s)f(\varphi_j) \right]. \quad (\text{B4})$$

Performing the Gaussian z_j integral, one readily obtains

then $\varphi_j - \varphi_{j+1} \propto \sqrt{\varepsilon}$. However, if $r=1$, then in the limit $\varepsilon \rightarrow 0$, one has $\varphi_j - \varphi_{j+1} \sim 1/s$. The coordinates on neighboring time slices therefore can differ by an amount that is larger than infinitesimal, so that these paths are exceedingly ill behaved.

Instead of using a Gaussian cutoff for the z_j integral in

Eq. (B4), one could also use a sharp window function $w(r)=\theta(r-|z_j|)$ as cutoff. Then the new expression [corresponding to Eq. (B4)] would be exactly equal to the old Eq. (B2). The z_j integral can then be performed by first writing $w(r)$ as the Fourier integral of $\sin r q_z / \pi q_z$. The calculation is more tedious, but the results are qualitatively the same.

APPENDIX C

This appendix concerns two points: (i) The identification of the prefactors of the exponentials in the amplitude for a single tunneling event between neighboring minima of a periodic potential. The relevant path integral (4.9) need not be computed *ab initio*, since one can use standard results for a particle tunneling in a double-well potential, as presented by Coleman.²² (ii) Performing a summation over time histories with multiple instantons, to verify that the tunnel splitting is precisely proportional to the single-instanton amplitude.

1. Single-instanton prefactor

Our starting point is Eq. (4.11) of Sec. IV C:

$$\mathcal{L}_\varphi = \frac{1}{2} m \dot{\varphi}^2 + V(\varphi), \quad (C1)$$

where

$$m \equiv (\hbar ns)^2 / 2a, \quad V(\varphi) = bf(\varphi). \quad (C2)$$

In the parlance of Rajaraman,⁴⁰ φ is the coordinate of "a particle on a unit circle," i.e., all points $\varphi + 2\pi m$ (m is any integer) are physically indistinguishable. The potential $V(\varphi)$ is periodic and symmetric about both $\varphi = 0$ and $\varphi = \pi/2$ [compare Eq. (2.6)]:

$$\begin{aligned} V(m\pi) &= 0, \\ V(\varphi) &= V(-\varphi) = V(\varphi + m\pi) \end{aligned} \quad (C3)$$

for any integer m , with minima at $\varphi = \pi m$ (see Fig. 4). A "particle" moving in this potential will execute zero-point motion, with frequency

$$\omega = \sqrt{k/m}, \quad \text{where} \quad \left. \frac{\partial^2 V}{\partial \varphi^2} \right|_{\varphi = m\pi} = k, \quad (C4)$$

around a minimum of $V(\varphi)$ for most of the time, and will occasionally tunnel via a single-instanton event to a neighboring minimum. Since φ lives on a circle, $V(\varphi)$ has only two physically distinguishable minima, namely, $|0\rangle \equiv \{|2m\pi\rangle\}$ and $|\pi\rangle \equiv \{|(2m+1)\pi\rangle\}$. They can be associated with the two minima of a symmetric double well, since single-instanton tunneling between neighboring minima of a periodic potential is analogous to single-instanton tunneling in a symmetric double-well potential.

Consider first the single-instanton tunneling events from $|0\rangle$ to $|\pi\rangle$. If the initial state is, say, $|2m\pi\rangle \in |0\rangle$,

then $|\pi\rangle$ can clearly be reached by either a (+) instanton or a (-) instanton. The corresponding tunneling paths $\bar{\varphi}^\pm(\tau)$ lead from $|2m\pi\rangle \in |0\rangle$ at $\tau = -T/2$ to $|(2m\pm 1)\pi\rangle \in |\pi\rangle$ at $\tau = T/2$. Asymptotically, they have the form

$$\bar{\varphi}^\pm(\tau \rightarrow T/2) \simeq (2m\pm 1)\pi \mp \varphi_{as} e^{-\omega\tau}. \quad (C5)$$

The value of the constant φ_{as} depends on the entire shape of $V(\varphi)$, but is usually not too hard to obtain (see Sec. IV C).

Coleman shows that to lowest order in the steepest descent approximation, the tunneling amplitude for a single (\pm) instanton event has the following form:⁴¹

$$\begin{aligned} \langle (2m\pm 1)\pi | e^{-\mathcal{H}T/\hbar} | 2m\pi \rangle \\ = \left[\frac{m\omega}{\pi\hbar} \right]^{1/2} e^{-T\omega/2} TK e^{-\mathcal{S}_0^\pm/\hbar}, \end{aligned} \quad (C6)$$

where

$$K = \frac{\varphi_{as}}{(\pi\hbar)^{1/2}} \left[\frac{k^3}{m} \right]^{1/4}. \quad (C7)$$

(Without loss of generality, the phases of the initial and final states have been chosen such that K is real.) For the Lagrangian (C1), $\mathcal{S}_0^+ = \mathcal{S}_0^-$; however, in Secs. III and IV of this paper, \mathcal{S}_0^+ and \mathcal{S}_0^- have different imaginary parts, hence we keep the distinction between them in Eq. (C6). The factor K has dimensions of inverse time and can be interpreted as an attempt frequency. Note that it is not necessary to make a distinction between K_+ and K_- , because to lowest order in the steepest descent approximation, $K_+ = K_-$ (compare Sec. IV B).

The total single-instanton tunneling amplitude from $|0\rangle$ to $|\pi\rangle$ or from $|\pi\rangle$ to $|0\rangle$ is simply the sum of the two amplitudes in Eq. (C6):

$$\begin{aligned} \langle 0 | e^{-\mathcal{H}T/\hbar} | \pi \rangle &= \langle \pi | e^{-\mathcal{H}T/\hbar} | 0 \rangle \\ &= \left[\frac{m\omega}{\pi\hbar} \right]^{1/2} e^{-T\omega/2} TK (e^{-\mathcal{S}_0^+/\hbar} \\ &\quad + e^{-\mathcal{S}_0^-/\hbar}). \end{aligned} \quad (C8)$$

2. Sum of multiple-instanton paths

The total amplitude for tunneling from $|0\rangle$ to $|\pi\rangle$ can be written as an infinite series, the n th term of which represents a string of n single-instanton events, widely separated in time from each other (the "dilute gas approximation"). Letting the initial and final states be separated by a time interval T , with $T \rightarrow \infty$, the net amplitude is²²

$$\begin{aligned} \langle \pi | e^{-\mathcal{H}T/\hbar} | 0 \rangle &= \left[\frac{m\omega}{\pi\hbar} \right]^{1/2} e^{-T\omega/2} \sum_{n=\text{odd}} \frac{1}{n!} [TK (e^{-\mathcal{S}_0^+/\hbar} + e^{-\mathcal{S}_0^-/\hbar})]^n \\ &= \left[\frac{m\omega}{\pi\hbar} \right]^{1/2} e^{-T\omega/2} (e^{T\Delta/(2\hbar)} - e^{-T\Delta/(2\hbar)}), \end{aligned} \quad (C9)$$

where

$$\Delta/2 = \hbar K (e^{-s_0^+/\hbar} + e^{-s_0^-/\hbar}). \quad (\text{C10})$$

In the limit $T \rightarrow \infty$, the lowest energy eigenvalues can be read off from the general expression

$$\langle \underline{\pi} | e^{-\hat{H}T/\hbar} | \underline{0} \rangle = \sum_n e^{-E_n T/\hbar} \langle \underline{\pi} | n \rangle \langle n | \underline{0} \rangle. \quad (\text{C11})$$

This gives

$$E_{\pm} = \hbar\omega/2 \pm \Delta/2 \quad (\text{C12})$$

for the energies of the lowest two energy states of the double-well problem. The first term is obviously the usual zero-point energy.

Substituting Eqs. (C7) and Eq. (C2) into Eq. (C10) gives Eq. (4.12), as was to be shown.

APPENDIX D

In this appendix we prove a result that is used in Sec. VI.

Theorem. Consider any coplanar classical ground-state configuration of the *kagomé* antiferromagnet. Choose any closed loop of alternating *AB* spins. The total number of spins on such a loop is always of the form $4n + 2$, where n is an integer.

Proof. The Bravais lattice of the *kagomé* net, which has one site located at the center of every *kagomé* hexagon (marked *X* in Fig. 7), forms a triangular “superlattice” (SL). Our proof is formulated in terms of the SL, and is divided into four steps.

1. Tiling by rhombi

In any coplanar classical ground state, every *kagomé*-triangle must contain exactly one spin of each of the types *A*, *B*, and *C*. This can be used to construct a tiling of the *kagomé* lattice by decorated rhombi, according to the following scheme: At the center of every “bond” connecting two SL nearest neighbor sites (i.e., *kagomé* vacancies) there is a *kagomé* spin, and every *kagomé* spin is at the center of a SL bond. Any SL rhombus made up of two neighboring SL triangles thus is decorated by a bowtie of five spins, one at its center and four at the centers of its four sides. These five spins form two head-to-head *kagomé* triangles. It is clear that for any given classical ground state, the SL can be tiled by decorated rhombi according to the following matching rules: (a) On

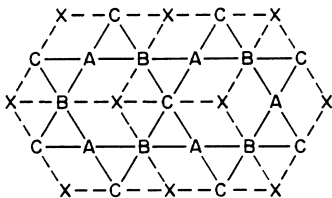


FIG. 7. The centers of *kagomé* hexagons (marked *X*) form a triangular superlattice (SL). Connecting these by the dashed lines divides the plane into (large) rhombi, each with, say, an *A*-spin at its center, surrounded by four other sites.

every rhombus, the two head-to-head spin-bowtie-*kagomé* triangles must each contain exactly one spin of each of the types *A*, *B*, and *C* (see Fig. 7). (b) The shared side of any two neighboring rhombi must have matching spins.

2. Definition of cluster

Associate a connected “cluster” of SL bonds with the given *AB* loop by connecting all SL-sites on the inside of the *AB* loop to their nearest neighbors (Fig. 8). The smallest cluster possible is just a single SL site; the associated *AB* loop surrounding it is the hexagon of six spins studied in this paper. The next-smallest cluster consists of two SL sites connected by a SL bond; the associated *AB* loop has ten spins.

A cluster that cannot be separated into two disconnected clusters by cutting a single SL bond will be called nonseparable. The smallest nonseparable cluster possible is just a single SL site. The next-smallest is a SL hexagon (a SL triangle is not allowed by the tiling rules). A large cluster may contain many nonseparable clusters, say m , connected to each other by $m - 1$ single bonds, to be called “cutting links” (Fig. 8). At the center of each cutting link there will necessarily always be a *C* spin (because both sides of the cutting link are lined by *AB*'s).

3. Reducing clusters to nonseparable clusters

To count the number, say M , of *AB*'s of the original loop that surrounds (and defines) the cluster, we systematically cut cutting links to break down the cluster into disconnected nonseparable clusters: Cut a cutting link, thus separating the mother cluster into two disconnected daughter clusters. Close the *AB* loop around each daughter cluster by replacing the *C* spin of the freshly cut cutting link by an *A* spin for one daughter and a *B* spin

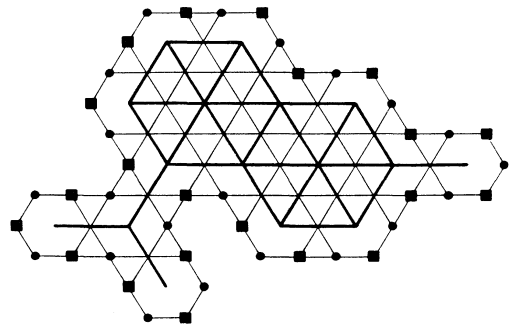


FIG. 8. An *AB* loop surrounding a cluster of bonds (heavy lines) on the superlattice. *A* and *B* spins on this loop are represented by heavy dots and squares, respectively. There is one large nonseparable cluster at the center, whose interior is divided into the twelve large triangles. Each of the four outside vertices is a nonseparable cluster consisting of just one SL site (they are the vertices with just one or three neighbors), and each of the four outside bonds (which connect these nonseparable clusters to each other and to the large nonseparable cluster) is a cutting link. The (perimeter) of the large nonseparable cluster has eight inward and two outward turns.

for the other, whichever is appropriate to maintain the alternation of A 's and B 's around each daughter (the reason that one can replace one C spin by two different spins (A and B) is that the two daughter clusters are considered to be separated from each other once the link has been cut). Then we have $M = D_1 + D_2 - 2$, where M , D_1 and D_2 are the number of AB spins surrounding the mother cluster and the two daughter clusters, respectively. By repeating this process until all cutting links have been cut, we are left with m "disconnected nonseparable clusters," each surrounded by an AB loop containing, say, B_i spins, where $i = 1, \dots, m$. Thus,

$$M = \sum_{i=1}^m B_i - 2(m-1). \quad (\text{D1})$$

4. Perimeter of nonseparable clusters

Next we show that B_i always has the form $B_i = 4n + 2$. The smallest disconnected nonseparable cluster, namely, the single SL site, has $B = 6$. Any larger disconnected nonseparable cluster can be tiled by decorated rhombi, in

such a way that there are only C spins at the centers of the bonds that form the perimeter of the nonseparable cluster, because the disconnected nonseparable cluster is surrounded by a loop of AB spins. Any closed shape tiled by rhombi always has an even number, say $2S_i$, of perimeter bonds, and hence of perimeter SL sites. Any perimeter SL site can be associated with either one, two, or three AB spins on its outside, depending on whether the perimeter turns outward, keeps straight or turns inward at that site (Fig. 8). There are exactly six more inward-turning than outward-turning turns around the perimeter of any nonseparable cluster (because at each turn the direction of the perimeter changes by 60° , since 120° turns are not allowed by the tiling rules). Therefore, the net number of AB spins around a nonseparable cluster always has the form $B_i = 2(2S_i) + 6$. Inserting this result into Eq. (D1), we find

$$M = 4 \left[\sum_{i=1}^m S_i + 1 \right] + 2. \quad (\text{D2})$$

This proves the theorem.

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²¹E. Fradkin, *Field Theories of Condensed Matter Systems*

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²²S. Coleman, *Aspects of Symmetry: Selected Erice Lectures* (Cambridge University Press, Cambridge, England, 1985), p. 274.
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²⁴This result persists when multiple (+) and (-) instanton events are considered (see Appendix C).
²⁵For other examples where the steepest descent approximation has been applied and prefactors have been calculated for problems where different terms in the Lagrangian contain different powers of s , see Ref. 21, and in particular Ref. 16, Sec. III.
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⁴⁰R. Rajaraman, *Solitons and Instantons* (North-Holland, New York, 1982), p. 315.

⁴¹See in particular Appendix 2, p. 341 of Ref. 22.