O(n) quantum rotors close to n=2 and d=1

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We investigate the role of topological defects in the zero-temperature transition in an *n*-component quantum rotor with ferromagnetic interaction on a *d*-dimensional lattice close to d=1, n=2. The topological defects in the present problem are identified with higher-dimensional classical defects arising in the imaginary time classical action of the quantum rotor. In the same spirit as in Cardy and Hamber [Phys. Rev. Lett. **45**, 499 (1980)], we use the analyticity of the renormalization-group equations. In the (d,n) plane, there is a line passing through (1,2) across which the critical exponents are nonanalytic. As expected a clear $d \rightarrow (d+1)$ correspondence is seen between the quantum and equivalent classical transitions.

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Long ago. Cardy and Hamber¹ discussed the critical behavior of the classical *n*-vector model in *d* spatial dimensions in the vicinity of the special d=n=2, which corresponds to the Kosterlitz-Thouless (KT) transition² point. The physical interpretation of defects is ambiguous when $(n,d) \neq (2,2)$, but they argued that it is connected with the compactness of the O(n) space. Cardy and Hamber assumed the analyticity of the renormalization-group equations in n and d and their analysis suggests that there exists a line in the (d,n) plane $[d=d_c(n)]$ that passes through the point (n,d)=(2,2) and has the following property: for n > 2, d > 2, the topological defects play a crucial role in determining the nature of the phase transition if $d \ge d_c(n)$, and they are unimportant for $d \leq d_c(n)$. The calculations predict the slope of the line d $=d_c(n)$ near (n,d)=(2,2) to be $4/\pi^2$. Later, Kohring *et al.*,³ numerically investigated the role of vortex strings in the order-disorder transition of a three-dimensional (3D) XY model and concluded that the vortex strings are responsible for the phase transition. They also studied the phase structure for a generalized planar model with vortex suppression that has the unusual feature of long-range order in a ground state with finite, disordering entropy. The prediction of Cardy and Hamber implies that the point corresponding to the 3D classical Heisenberg systems in the *n*-*d* plane (i.e., d=n=3) lies in the region where topological defects are important and thus defects should explicitly be taken into consideration when describing the critical behavior of the 3D Heisenberg model. The real-space renormalization-group calculations⁴ on the O(n) model for $1 \le n \le 2$ and $1 \le d \le 2$ support the prediction of Cardy and Hamber regarding the importance of defects in the n = d = 3 case. Lau and Dasgupta⁵ numerically explored the role of topological point defects, namely, hedgehogs in the critical behavior in the above case and found out that configurations containing defect pairs are necessary for the transition from the ferromagnetic to the paramagnetic phase. The suggestion^{1,6} is that the singular defects are not properly taken into consideration in a O(3) nonlinear sigma model and hence exponents obtained from an extrapolation of the ϵ expansion do not agree well with those obtained from the series results.

In this paper, we study the role of topological defects in the quantum phase transition^{7,8} of *d*-dimensional,

n-component quantum rotors (with ferromagnetic interaction) close to the special point d=1, n=2 that corresponds to the quantum Kosterlitz-Thouless transition.⁷ The topological defects in the present problem can be visualized by writing the quantum rotor Hamiltonian in the imaginary time path-integral formalism and they clearly correspond to higher-dimensional classical defects. We employ similar arguments as in Ref. 1 to investigate the role of these topological defects on the transition behavior of quantum rotors. We assume the analyticity of renormalization-group (RG) equations in *n* and *d* and using the corresponding RG equations we locate the boundary in the (n,d) plane across which the exponents are nonanalytic and topological defects dominate.

The RG equations in the classical case¹ are simply the extension of Kosterlitz equations² in $d=2+\epsilon$ and $n=2+\delta$ and reduce to the RG equations for the classical nonlinear-sigma model (CNL σ)⁹ when topological defects are neglected whereas for n=2, they reduce to the RG equations of the XY model in $d=2+\epsilon$ dimensions.¹⁰ The analysis of the fixed-point structure as discussed already, clearly indicates a region where topological defects are dominant.

To develop the similar renormalization-group equations in the quantum case, let us look at the quantum rotor Hamiltonian in the quantum nonlinear-sigma-model (QNL σ) approach. The effective imaginary time Euclidean action of a *d*-dimensional QNL σ model at a finite temperature *T* is written as¹¹

$$\frac{S_{\rm eff}}{\hbar} = \frac{\rho_s^0}{2\hbar} \int_o^{\beta\hbar} d\tau \int d^d x \left[\left| \nabla \hat{n}(x,\tau) \right|^2 + \frac{1}{c_o^2} \left| \frac{\hat{n}(x,\tau)}{\partial \tau} \right|^2 \right],$$
(1)

with $|\hat{n}(x,\tau)|^2 = 1$. Here, $\hat{n}(x,\tau)$ is the *n*-component vector order-parameter field, ρ_s^o is the bare stiffness, c_o the bare spin-wave velocity, and the spatial integrals have a short-distance cutoff Λ^{-1} . The renormalization-group equations to the one-loop order are given as

$$\frac{dg}{dl} = (1-d)g + (n-2)\frac{K_d}{2}g^2 \coth\left(\frac{g}{2t}\right), \qquad (2)$$

$$\frac{dt}{dl} = (2-d)t + (n-2)\frac{K_d}{2}gt \operatorname{coth}\left(\frac{g}{2t}\right), \qquad (3)$$

where $t = (k_B T \Lambda^{d-2})/\rho_s^o$ and $g_o = (\hbar c \Lambda^{d-1})/\rho_s^o$ are dimensionless temperature and coupling scales and e^l is the length rescaling factor $K_d^{-1} = 2^{d-1} \pi^{d/2} \Gamma(d/2)$. We shall now analyze these RG flow Eqs. (2) and (3) in $d = 1 + \epsilon$. Clearly Eq. (2) then suggests that there is a quantum critical point at T = 0 at $g_c = (2/K_d)(d-1)/(n-2)$; but for $d = 1 + \epsilon$, the RG Eq. (3) shows that thermal fluctuations will grow and the system will eventually flow to the infinite temperature fixed point and thus one does not expect a thermal critical behavior. We shall henceforth look at the quantum critical behavior in $d = 1 + \epsilon$ and employ the flow equation for the coupling given as

$$\frac{dg}{dl} = -\epsilon g + \frac{(n-2)}{2\pi}g^2, \qquad (4)$$

with $g_c = 2\pi\epsilon/(n-2)$, which separates the quantum ferromagnetic phase from the quantum paramagnetic state. Comparing with RG flow equations of the CNL σ model,^{9,12} one finds that Eq. (4) really corresponds to a classical thermal phase transition in d+1 dimensions.

It is clear that $g_c = 0$ for d = 1 and it is undetermined for d=1 and n=2, when the system undergoes a quantum KT transition.⁷ The continuum spin-wave theory discussed above does not take into consideration the local topological defects [i.e., the vortices in the equivalent two-dimensional (2D) classical picture] that arise due to the lattice and thus fails to capture the essential physics of the KT transition. The quantum rotor model with d=1 and n=1 in the naive continuum limit is described by a massless theory that yields a powerlaw behavior of equal-time correlation functions. But the continuum limit as already discussed does not take into consideration tunneling events or the vortices (in the 2D classical picture) and the lattice Hamiltonian allows for 2π vortices. Considering these local defects, the quantum rotor Hamiltonian is described by a sine-Gordon action in the presence of a $\cos(2\phi)$ potential where ϕ is the dual field. The corresponding action takes the same form as Eq. (1)with an additional topological term $y \cos(2\phi)$. The corresponding renormalization-group equations are written as⁷

$$\frac{dy}{dl} = \left(2 - \frac{\pi}{g}\right)y,\tag{5}$$

$$\frac{dg}{dl} = -Ay^2,\tag{6}$$

where g is the coupling as discussed in the QNL σ model and y is the topological term that can be identified with the fugacity field of the vortices in the equivalent 2D classical picture. Clearly Eqs. (5) and (6) exhibit a quantum KT transition from a gapless (power-law equal-time correlation behavior) to a gapped phase (exponential equal-time correlation behavior) at $g = \pi/2$ and y = 0.

In the same spirit as Cardy and Hamber, we shall now assume the analyticity of the RG equations written above in *d* and *n*. The resultant RG equations thus obtained for quantum rotors in $d=1+\epsilon$ and $n=2+\delta$ are

$$\frac{dg}{dl} = -\epsilon g + (n-2)f(g) + 4\pi^3 y^2, \tag{7}$$

$$\frac{dy}{dl} = \left(2 - \frac{\pi}{g}\right)y. \tag{8}$$

These equations readily reduce to the RG equations of quantum KT for n=2 and yield the QNL σ -model results [Eq. (4)] with $f(g)=g^2/(2\pi)$ when y=0, as discussed already. Let us now explore the fixed-point structure of the above RG equations. The fixed points and the corresponding eigenvalues are fixed-point I:

$$\frac{f(g_c)}{g_c} = \frac{\epsilon}{n-2}; \quad y^* = 0,$$
$$\lambda_I = -\epsilon + (n-2)f'(g_c) + \cdots,$$
$$\lambda_I' = 4 - \frac{2\pi}{g_c} + O(\epsilon).$$

fixed-point II:

y

$$g = \frac{\pi}{2} + O(\epsilon),$$

$$^{2} = \frac{\Delta}{4\pi^{3}} + O(\epsilon^{2}), \quad \Delta = \frac{\epsilon\pi}{2} + (2-n)f\left(\frac{\pi}{2}\right),$$

$$\lambda_{II} = \left(\frac{8\Delta}{\pi}\right)^{1/2} + O(\epsilon),$$

$$\lambda_{II}' = -\left(\frac{8\Delta}{\pi}\right)^{1/2} + O(\epsilon).$$

Let us now assume that f(g)/g is a monotonic function of g. For $\epsilon < 0$ (i.e., d < 1) and n < 2 neither of the fixed points is stable and as expected from the Mermin-Wagner theorem¹² no transition occurs. For n < 2, only the fixedpoint II is real and this determines the nature of the transition so that we find that the transition is topological for n < 2. For n > 2 if Δ happens to be negative. If is unphysical and the critical behavior determined by fixed-point I is not of a topological nature. This is the region where the QNL σ -model results seem to hold true. For n > 2 and $\Delta > 0$, both the fixed points are real, but I is an unstable one and II determines the critical behavior, which is once again topological in nature. In this region, the QNL σ -model predictions are not valid; rather one has to take into consideration the topological nature of transition. At $\Delta = 0$, the fixed points coincide so that λ'_{I} and λ'_{II} become marginal and $\lambda_{I} = \lambda_{II}$. Across the boundary, $\Delta = 0$; the exponents are continuous but nonanalytic. One can obtain the initial slope of this boundary. In general it will be a curve in the n-d plane as shown in Fig. 1. For d=1 and $n \leq 2$ the leading and subdominant eigenvalues (λ_I



dimension d

FIG. 1. The schematic diagram of different regions in the n-d plane. In region I, results obtained from nonlinear-sigma-model calculations are in good agreement, in region II topological defects drive the quantum phase transition, and in region III quantum phase transitions are forbidden.

and $\lambda'_I I$) correspond to different branches of the same analytic function with a square-root branch point at d=1 and n=2. One can similarly extend the classical Cardy-Hamber conjecture using an exact form of eigenvalues that can be described in terms of the quantity $x = (2/\pi)\cos^{-1}[(2+n)^{1/2}]$,

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which is rational for integer *n* between -2 and +2 and incorporates the branch point. Once again the conjecture is that the exponent $\nu^{-1} = 4x/(1+x)$ (where ν is the correlation length exponent related to the quantum transition) so that we obtain the exact exponent $\nu=1$ for n=1, d=1 (Ref. 8 and $\nu=\frac{1}{2}$ for n=-2 (quantum Gaussian transition).

It is readily seen that the O(3) model in d=2 falls in the region of II, where topological effects are dominant, so the results for the QNL σ model for $d=1+\epsilon$ should not be extrapolated to $\epsilon=1$. One should also note that the boundary originates at n=1 and d=0, since the lower critical dimension of the quantum Ising model is 0 and it has a transition when $d=\epsilon$. Similarly for $1 \le n \le 2$, the lower critical dimension is between $0 \le d \le 1$ and the transition is topological as seen in Fig. 1. For $n \le 1$, λ' is no longer a next-to-leading eigenvalue and thus the transition is not topological. As expected the phase boundary in the n-d plane is in agreement with the standard $d \rightarrow (d+1)$ scenario.

Similar questions may be addressed regarding the finite temperature transition in these quantum models. The finite temperature transition is essentially a *d*-dimensional classical (finite temperature) transition since critical fluctuations are classical.^{7,8} Thus we expect in the finite temperature transition that low-dimensional topological defects will come into play and the classical picture of Cardy and Hamber¹ will be valid.

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