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Avoided critical behavior in a uniformly frustrated system

L. Chayes [a], V.J. Emery [b], S.A. Kivelson [c], Z. Nussinov [c], G. Tarjus [d]

[a] *Department of Mathematics, UCLA, Los Angeles, CA 90095, USA*

[b] *Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA*

[c] *Department of Physics, UCLA, Los Angeles, CA 90095, USA*

[d] *Laboratoire de Physique Théorique des Liquides, Université Pierre et Marie Curie, 75252 Paris Cedex 05, France*

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Abstract

We study the effects of weak long-ranged antiferromagnetic interactions of strength Q on a spin model with predominant short-ranged ferromagnetic interactions. In three dimensions, this model exhibits an avoided critical point in the sense that the critical temperature $T_c(Q = 0)$ is strictly greater than $\lim_{Q\to 0} T_c(Q)$. The behavior of this system at temperatures less than $T_c(Q = 0)$ is controlled by the proximity to the avoided critical point. We also quantize the model in a novel way to study the interplay between charge-density wave and superconducting order.

Keywords: Avoided critical point; Uniform frustration; Spherical spin model

1. Introduction

There are many diverse contexts in which a short-ranged tendency to order is thwarted by a long-ranged frustrating interaction. In particular, recent theories of the glass transition [1] and of the properties of doped Mott insulators [2,3] have lead to the consideration of such models. In the first example, a tendency of the molecules in a supercooled liquid to pack into a locally preferred structure is frustrated by the inability of such structures to tile space; the long-range nature of the induced interaction represents the superextensive growth of strain which would occur if the locally preferred structure were forced to tile space. In the second example, a short-range tendency of holes in an antiferromagnet to phase separation competes with the long-range Coulomb repulsion between holes. In this latter case, effects of quenched disorder and quantum fluctuations may also be important.

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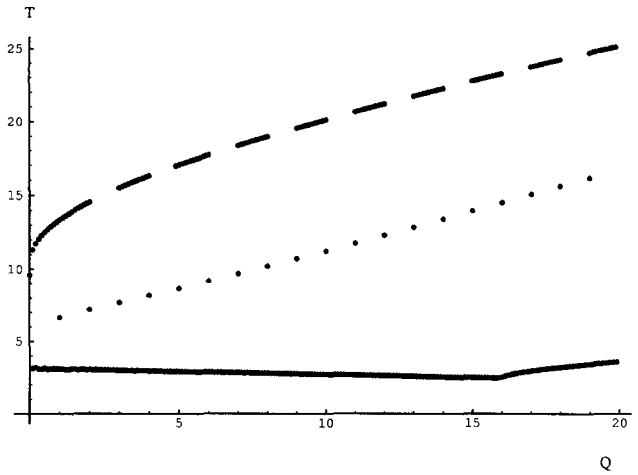

Fig. 1. Phase diagram in the T–Q plane for the classical model in $d = 3$.

It has been argued [1] that the effect of such uniform, long-range frustration is an avoided critical point, leading to a phase diagram of the sort shown in Fig. 1. Here, T is the temperature and Q is the strength of the frustrating interaction. The salient feature of this phase diagram is the discontinuity in T_c in the $Q \to 0$ limit. The presence of the avoided critical point leads to new types of fluctuation phenomena for $Q \ll 1$ and $T \lesssim T_c$ $(Q = 0)$.

To capture the essential physics of these problems, we will consider a spin model on the d-dimensional hypercubic lattice. Our starting point is the classical Hamiltonian

$$H_{\rm cl}[S] = \tfrac{1}{2}J \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} |S_{\boldsymbol{R}} - S_{\boldsymbol{R}'}|^2 + \tfrac{1}{2}Q \sum_{\boldsymbol{R}\neq\boldsymbol{R}'} v(\boldsymbol{R}-\boldsymbol{R}')S_{\boldsymbol{R}}\cdot S_{\boldsymbol{R}'}, \tag{1.1}$$

where J and Q are positive couplings, the sum over $\langle \boldsymbol{R}, \boldsymbol{R}'\rangle$ is over nearest neighbor pairs, and $v(\boldsymbol{R})$ is long-ranged, with asymptotic fall off

$$v(\boldsymbol{R}) \sim |\boldsymbol{R}|^{-x}, \tag{1.2}$$

with $0 < x \leq d$. Specifically, it is most convenient to express the interaction on the lattice in terms of its Fourier transform, which in the simplest cases we will consider here, implies that the Hamiltonian is

$$H_{\rm cl}[S] = \tfrac{1}{2}\sum_{\boldsymbol{k}} \mathcal{J}(\boldsymbol{k})|\tilde{S}_{\boldsymbol{k}}|^2. \tag{1.3}$$

Here $\tilde{S}$ is the Fourier transform of S,

$$\mathcal{J}(\boldsymbol{k}) = J\Delta(\boldsymbol{k}) + Q[\Delta(\boldsymbol{k})]^{-y} + \cdots, \tag{1.4}$$

with $y = (d - x)/2$, and

$$\Delta(\boldsymbol{k}) = \sum_{\alpha=1}^{d} V(k_\alpha) \tag{1.5}$$

is the Fourier transform of the lattice Laplacian, and

$$V(k) = 2[1 - \cos(k)] \approx k^2 \qquad \text{for } k \ll 1. \tag{1.6}$$

In Eq. (1.4), the $\cdots$ refers to additional, short-range terms which are generically present and which will be included for reasons that will become clear shortly. To make our discussion explicit, and because it is typically the case of most physical interest, we will focus on the Coulombic case $y = 1$; the principal results are qualitatively similar for any long-range potential.

This model can be studied with various definitions of the spin variables, S_R. Probably, the most interesting case is the Ising version, [4–6] where $S_R = \pm 1$. The majority of the results in the present paper concern the exactly solvable "mean spherical" version of this model, in which the spins are taken to be real numbers with the mean global constraint

$$N^{-1} \sum_R \langle (S_R)^2 \rangle = 1, \tag{1.7}$$

where N is the number of sites and $\langle\ \rangle$ denotes the thermal average. As is well known, this model is equivalent, in the thermodynamic limit, to the usual spherical model in which this global constraint is enforced configuration by configuration [7] and to the large n limit of the $O(n)$ model [8]. (Ongoing work on the $1/n$ expansion will shed some additional light on the relation of the present results to the properties of the model at finite n [9].)

Since, in the context of doped Mott insulators, quantum effects are important, we also consider a quantum version of this model. In particular, we wish to consider a model with two distinct types of low temperature ordered phases: those with spin (charge) order *and* those with momentum (superconducting) order. These order parameters are canonically conjugate and dual to each other. We are motivated in this choice by an analogy with models of hard-core bosons on a lattice, or equivalently to a spin $s = 1/2$ frustrated quantum Heisenberg-Ising model in which the XY coupling is the particle kinetic energy (and hence associated with the momentum) while the Ising ordering is associated with ordering of the dual fields, (charge ordering) which can either correspond to phase separation or formation of a charge density wave ordered state [10]. With this in mind, we define a quantum model

$$H = H_{\rm cl}[S] + H_{\rm qu}[P], \tag{1.8}$$

where $H_{\rm qu}$ and $H_{\rm cl}$ are appropriate quadratic forms, in which the "momenta", $\{P_R\}$, are cannonically conjugate to the spins, $\{S_R\}$, i.e.

$$[S_R, P_{R'}] = i\hbar\delta_{R,R'}. \tag{1.9}$$

The constraint equation is

$$N^{-1} \sum_R [\alpha_s \langle |S_R|^2 \rangle + \alpha_p \langle |P_R|^2 \rangle] = s^2. \tag{1.10}$$

As long as neither α_s nor α_p is zero, we can, without loss of generality, [11] take $\alpha_s = \alpha_p = 1$. To be concrete, we also confine our considerations to the simplest case in which $H_{\rm qu}$ consists of the simplest, unfrustrated nearest-neighbor ferromagnetic interaction

$$H_{\rm qu}[P] = \tfrac{1}{2}W \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} |P_{\boldsymbol{R}} - P_{\boldsymbol{R}'}|^2. \tag{1.11}$$

Thus, W is the bare superfluid stiffness. It also is necessary to augment the Hamiltonian with a uniform field, K, which favors charge ordering ($\langle S_{\boldsymbol{R}}\rangle \neq 0$) when negative and superconducting ordering ($\langle P_{\boldsymbol{R}}\rangle \neq 0$) when positive,

$$H_{\rm cl} \to H_{\rm cl} + \tfrac{1}{2}K \sum_{\boldsymbol{R}} |S_{\boldsymbol{R}}|^2, \tag{1.12}$$

or, in other words, $\mathcal{J}(\boldsymbol{k}) \to \mathcal{J}(\boldsymbol{k}) + K$.

In the context of quantum spin glasses, Nieuwenhuizen [12] and Hartman and Weichman [13] have considered quantized versions of the spherical model. In both cases, after some manipulation, [12,13] it is possible to write the Hamiltonian in the form of Eqs. (1.8)–(1.11). However, the constraint considered by Hartman and Weichman corresponds to the case $\alpha_s = 0$, while that of Nieuwenhuizen corresponds to $\alpha_p = 0$. As we shall see, this difference has important physical consequences. In particular, to exhibit the two conjugate ordered phases, it is necessary that both α's be non-zero.

Effects of quenched disorder can be included by adding a random field to the Hamiltonian

$$H_{\rm dis} = \sum_j h_j S_j. \tag{1.13}$$

For our purposes, the ensemble of random fields is adequately specified by its second moment,

$$[\tilde{h}_{\boldsymbol{k}}\tilde{h}_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k},-\boldsymbol{k}'} f(\boldsymbol{k}), \tag{1.14}$$

where the [ ] signifies configuration averaging. (We imagine that $[h_j] = 0$, although this is unimportant.) Since the random fields are, presumably, generated by remote quenched charges, we will typically suppose that $f(\boldsymbol{k})$ vanishes as $k \to 0$ as $f(\boldsymbol{k}) \sim k^2$, but is otherwise positive at all other values of $\boldsymbol{k}$. (Note that the two previously cited studies [12,13] considered quantum spherical models with random exchange interactions so as to construct a spherical version of a spin-glass; this problem is interesting but considerably more complex than the one considered here.)

We now return to the additional terms (signified by ...) in Eq. (1.3). The Hamiltonian, as written, depends on $\boldsymbol{k}$ only through $\Delta(\boldsymbol{k})$. It turns out that this implies a degeneracy (that is non-generic for lattice systems) which is a consequence of a lattice version of the rotational symmetry of free space and hence would be exact in a continuum version of the model. We will lift this degeneracy through the inclusion of the term

$$\cdots = \tfrac{1}{2}\lambda \left\{ \sum_{a\neq b} V(k_a)V(k_b) \right\}, \tag{1.15}$$

which in position space corresponds to a second neighbor interaction. This term vanishes like k^4 as $k \to 0$; notice that, to this order, any perturbation consistent with the symmetry of the hypercubic lattice can be written as $\lambda'[\Delta(\boldsymbol{k})]$ plus the term in Eq. (1.15). However, any portion of the perturbation which depends only on the Laplacian does not lift the degeneracy. In this sense, Eq. (1.15) is the unique, leading order term that breaks the "rotational" symmetry of the continuum. For concreteness, we will always consider the model with λ positive, unless otherwise stated.

To summarize, in the rest of the paper we will consider the statistical mechanics of the classical model defined by the Hamiltonian in Eq. (1.3) with

$$\mathcal{J}(\boldsymbol{k}) = J\Delta(\boldsymbol{k}) + Q[\Delta(\boldsymbol{k})]^{-\gamma} + \tfrac{1}{2}\lambda \sum_{a \neq b} V(k_a)V(k_b) + K, \tag{1.16}$$

and with the equation of constraint defined in Eq. (1.7). We will then consider the quantized version of the same model defined by the Hamiltonian in Eq. (1.8) with H_{qu} defined by Eq. (1.11) and the equation of constraint by Eq. (1.10) with $\alpha_s = \alpha_p = 1$. Henceforth, we will work in units such that Planck's constant, Boltzmann's constant, the energy scale J, and the lattice constant are all set equal to 1.

2. Discussion of results

2.1. Classical model

For $Q = 0$, the model described is the usual spherical model. As is well known for this case, $d = 2$ is the lower critical dimension; there is no finite temperature transition in $d = 2$ but the correlation length diverges rapidly, like $\xi_0 = L(\lambda)\exp[2\pi/T]$, as $T \to 0$, which is qualitatively similar to the behavior of the $O(n)$ model for $n > 2$. In $d = 3$, there is a finite temperature transition at a critical temperature $T_c = A(\lambda)$ where $A(\lambda)$ is a strongly varying function of λ with $A(0) \simeq 0.79$, and the correlation length diverges as $\xi_0 = (4\pi/A)[(T - T_c)/T_c]^{-\nu}$ with $\nu = 1$ as the temperature approaches T_c from above. The spherical model is somewhat unsatisfactory for temperatures below T_c where there is a well defined growth of the order parameter, $\langle S_j \rangle = [(T_c - T)/T_c]^{1/2}$, but the (Josephson) correlation length is infinite. (This is one of the problems we hope will be fixed when $1/n$ corrections are included [9].)

For non-zero Q, ferromagnetic order is completely forbidden. However, modulated order of one sort or another is permitted. For small Q, it can be easily seen by minimizing $\mathcal{J}(\boldsymbol{k})$ in Eq. (1.3) with respect to k that the preferred order occurs for $k = q$, where $V(q) = \sqrt{Q}$. Since q is small in this limit, a first approximation to the physics can be obtained by taking a continuum limit, in which only the order k^{-2} and k^2 terms in $\mathcal{J}$ are retained; in particular, this means that the term proportional to λ is neglected since it is smaller by a factor of $\sqrt{Q}$ than the first two terms for $k \sim q$. However, as is well known in the continuum theory of smectic liquid crystals, the transverse fluctuations of such density wave order are sufficient to destroy the long-range order which, in the

Table 1
Values of the three dimensional wave vector, q, that minimize $\mathcal{J}(k)$ in different ranges of Q. This determines the locations of the peaks in the structure factor in the disordered phase and the location of the Bragg peaks in the charge-ordered phase. The value of q labeled "complicated" is given by the solution of $V(q) = v$ where v is the solution of the cubic equation $9v^2 = Q + 18|\lambda|v^3$.

$\lambda > 0$	$0 < Q < 16$	$q = \langle q, 0, 0\rangle$	$V(q) = \sqrt{Q}$
$\lambda > 0$	$16 \le Q \le 16(1+4\lambda)$	$q = \langle \pi, 0, 0\rangle$	–
$\lambda > 0$	$16(1+4\lambda) < Q < 64(1+4\lambda)$	$q = \langle \pi, q, 0\rangle$	$V(q) = \sqrt{Q/(1+4\lambda)} - 4$
$\lambda > 0$	$64(1+4\lambda) \le Q \le 64(1+8\lambda)$	$q = \langle \pi, \pi, 0\rangle$	–
$\lambda > 0$	$64(1+8\lambda) < Q < 144(1+8\lambda)$	$q = \langle \pi, \pi, q\rangle$	$V(q) = \sqrt{Q/(1+8\lambda)} - 8$
$\lambda > 0$	$144(1+8\lambda) \le Q$	$q = \langle \pi, \pi, \pi\rangle$	–
$-1/8 < \lambda < 0$	$0 < Q < 144 - 1152\|\lambda\|$	$q = \langle q, q, q\rangle$	complicated
$\lambda < 0$	$144 - 1152\|\lambda\| \le Q$	$q = \langle \pi, \pi, \pi\rangle$	–

context of the spherical model is equivalent to the destruction of any finite temperature transition. (A power law phase, as in the $2d$ XY model or the $3d$ continuum theory of smectic liquid crystals is impossible for this simple class of models.) In the present context, this is a consequence of the existence of a co-dimension one hypersurface of minimizing wave vectors which implies insufficient stiffness against fluctuations to permit a finite temperature ordering transition in any dimension. As discussed above, this piece of continuum physics is reproduced on the lattice when only the first two terms in $\mathcal{J}$ are retained (even though they are computed to all orders in k). In this case the preferred order occurs at k on the hypersurface $\Delta(k) = \sqrt{Q}$ and therefore as long as $0 < \sqrt{Q} < 4d$, no finite temperature ordering transition is possible. (For larger Q, even if $\lambda = 0$, the lattice asserts itself, and ordering can occur.) Thus we see, trivially, that in the model with $\lambda = 0$, there is an avoided critical point for all dimensions $d > 2$, as in Fig. 1, in which T_c drops from a finite value for $Q = 0$, to zero for $Q \neq 0$.

We now address the question of what happens to this phase diagram when the symmetry-breaking term proportional to λ is introduced. In this case, the minima of $\mathcal{J}(k)$ occur at isolated points in the Brillouin zone, and hence finite-temperature ordering is possible at non-zero Q in all dimensions $d > 2$. For $Q < 16$ and λ positive, there are $2d$ minima which occur at $k = \pm q\hat{e}_a$, for $a = 1, \ldots, d$, with $V(q) = \sqrt{Q}$, and hence correspond to unidirectional striped phases. (The ordering vectors for all Q and all λ are listed in Table 1.) In dimension $d = 3$, as shown in Fig. 1, there remains a finite discontinuity in T_c as $Q \to 0$. Specifically, for positive λ, $T_c(Q = 0) = A_0 + A_1\lambda + \mathcal{O}(\lambda^2)$ with $A_0 = A(0)$ and $A_1 = A'(0) \simeq 0.074$, while

$$\lim_{Q\to 0} T_c(Q) = \frac{\sqrt{\lambda}T_c(0)}{BT_c(0) + \sqrt{\lambda}}, \tag{2.1}$$

with $B \simeq 0.14245$. For $d > 3$, finite λ results in a continuous, although extremely non-analytic behavior of T_c at small Q: $T_c(Q) = T_c(0)[1 - B_d T_c(0)\lambda^{-1/2}(Q)^{(d-3)/4}]$ where B_d is a dimension dependent number of order 1. (For what it is worth, for $2 < d < 3$, there is a finite discontinuity in T_c, and indeed, T_c is finite for $Q = 0$, but tends to zero in the $Q \to 0$ limit as $T_c \sim B_d^{-1}\sqrt{\lambda}(Q)^{(3-d)/4}$.)

In Fig. 1, we show the phase diagram for the three-dimensional classical model as a fuction of Q and T for fixed, positive λ (The solid lines in the figure are the phase boundaries computed for $\lambda = 1/4$, but the qualitative results are insensitive to the value of λ.) There appear two dashed lines in the small-Q region of the figure which signify crossover temperatures discussed below:

• T_1 marks the temperature at which the frustration becomes significant. At $T > T_1$, correlations behave essentially like those of the model with $Q = 0$, while for $T < T_1$, the effect of the frustration is to break the incipient ferromagnetic order into randomly oriented "domains" of typical size, ξ, which at $T \approx T_c(Q = 0)$ has magnitude $\xi \approx (1/Q)^{1/4}$, and which grows slowly as the temperature is lowered.

• T_2 marks the temperature at which lattice effects becomes important. For $T > T_2$, the fluctuations are essentially isotropic, while for $T < T_2$, the correlation length begins to diverge as the ordering temperature is approached, with the same critical exponent as the unfrustrated model, and the correlation functions begin to choose preferred orientations for the domains, corresponding to the onset of stripe ordering. One additional pathology of the spherical model apparent in this phase diagram (which, we expect, is corrected in order $1/n$) is that there is no commensurate lock-in whatsoever for small Q, i.e. there is no preference for stripe ordering wave vectors q which are commensurate with the underlying lattice. In Fig. 2 we show the Fourier transform, $\tilde{G}(k)$, of the spin–spin correlation function,

$$G(R) = \langle S_0 S_R \rangle, \tag{2.2}$$

at various temperatures for a fixed, small value of $Q = 1/2$ and $\lambda = 1/4$. One can clearly see the differences in the structure of the correlations in the different regimes of temperature.

The most dramatic manifestation of avoided critical behavior is the existence of these sharp crossover regimes. For instance, we associate the remarkable properties of supercooled liquids as they become glassy with the behavior of a uniformly frustrated system in the temperature range $T \lesssim T_1$. The structural correlation functions of certain high temperature superconducting materials also exhibit behavior which is strikingly similar to that of the various low temperature regimes of the present model. It seems that avoided critical behavior is surprisingly robust, at least in $d \leq 3$. It occurs naturally in the continuum version of the model, and survives lattice effects. Preliminary results from the $1/n$ expansion [9] show that it persists at finite n. This is a new construct which is likely to find applications in a variety of other arenas.

2.2. *Effects of quantum fluctations*

In the quantum model, there are two distinct types of possible ordered states: charge-ordered states, in which S_R develops a non-zero expectation value, and superconducting states, in which P_R develops a non-zero expectation value. At zero temperature, the ground state will be ordered if s exceeds a parameter-dependent critical value s_c while the ground state is quantum disordered if $s < s_c$. (When factors of $\hbar$ are restored,

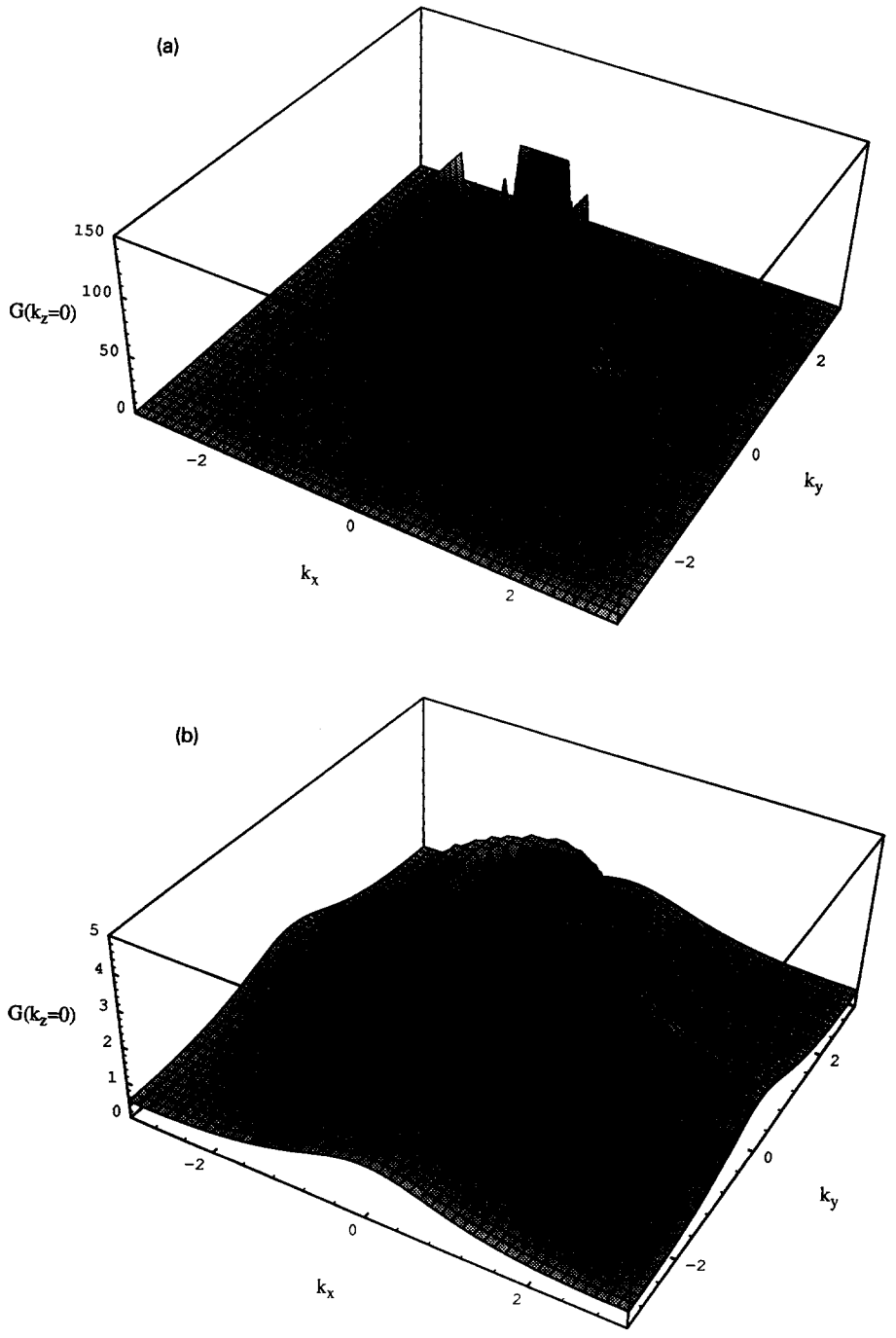

Fig. 2. $\tilde{G}(\boldsymbol{k})$ for $Q = 1/2$ and $\lambda = 1/4$ at different temperatures: (a) $T = T_c$, (b) $T_1 > T = 1.8T_c > t_2$, (c) $t = 3.3T_c$.

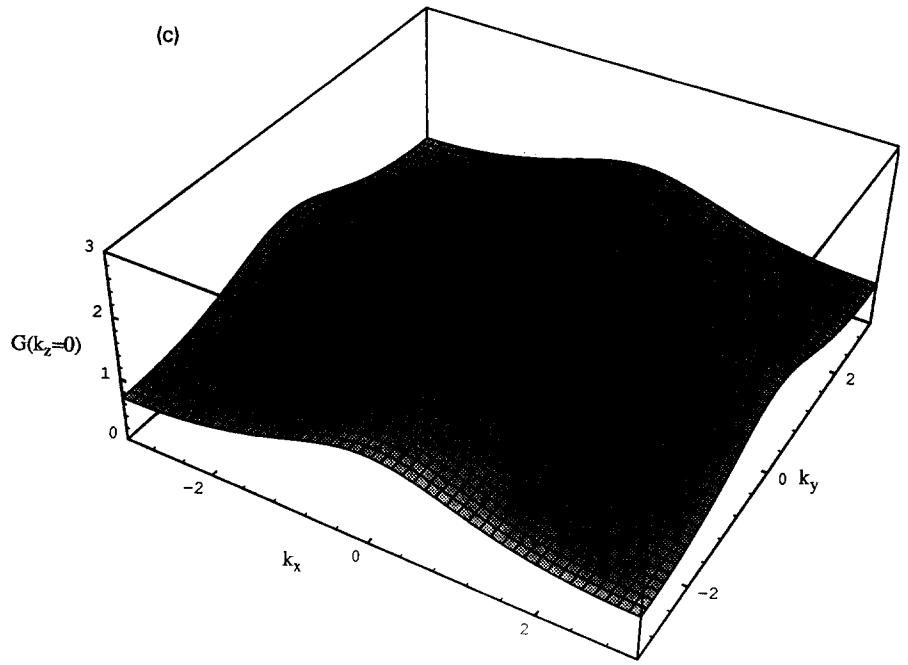

Fig. 2 — continued.

$s^2 \to s^2/\hbar$, in Eq. (1.10) so s^2 is the natural measure of the importance of quantum fluctuations.) The superconducting state can occur only for K greater than a critical value, K_0, while the charge-ordered state can occur only for $K < K_0$; coexistence, i.e. supersolid order, can occur only for the special case of $K = K_0$. (For $Q \leq 16$, $K_0 = -2\sqrt{Q}$; more generally, K_0 is that value of K for which the minimum over all $\boldsymbol{k}$ of $\mathcal{J}(\boldsymbol{k})$ in Eq. (1.16) is equal to 0.) As in the classical model, the transverse quantum fluctuations in the continuum approximation (or for $\lambda = 0$) are sufficient to destroy any possible charge order for small Q, even at zero temperature. However, for non-zero λ, not only is there a finite value of s_c for $d > 1$, but it is a continuous function of Q, even in the limit $Q \to 0$. Indeed, s_c is a rather weak function of all parameters, and is always greater than, but approximately equal to 1. (The dependence of s_c on K and Q for $W = 1$ is shown in Fig. 3.) Thus, at zero temperature and for $s > s_c$, there is a superconducting to charge-density wave transition that occurs as a function of K. Similarly, as a function of decreasing s, there is a superconducting to quantum-disordered transition which occurs for $K > K_0$, and a similar charge-density wave to quantum-disordered phase transition for $K < K_0$.

At finite temperatures, the behavior of the system for $K < K_0$ and $s > s_c$ is similar to that of the classical frustrated model described above, while for $K > K_0$, the superconducting to normal transition occurs in qualitatively the same way as in the ordinary ferromagnetic spherical model. However, as long as $|K - K_0|$ is small, both the normal and superconducting states will exhibit substantial correlations which resemble

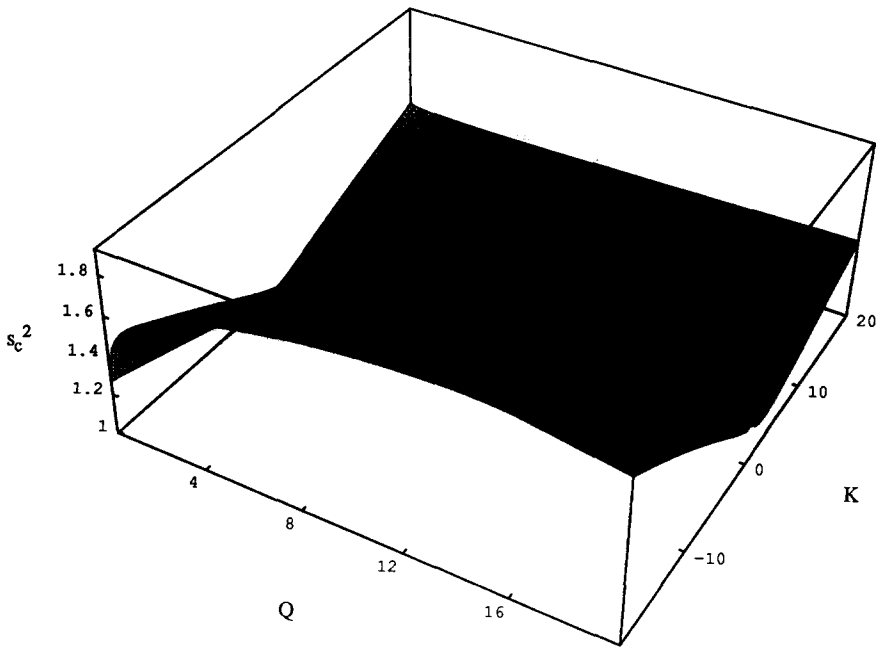

Fig. 3. Contour plot of s_c for fixed $\lambda = 1/4$ and $W = 1$. The line with the arrow is the trajectory through parmeter space referred to in Fig. 4.

the nearby charge-density wave phase. The same two crossover temperatures that appear in the correlation function of the classical model calculations (Fig. 2), but in contrast to that case, the spin correlation length saturates at a long but finite value for $T \leq T_c$ where T_c is the superconducting transition temperature.

2.3. *Effects of disorder*

For $Q > 0$, disorder destroys the possiblity of a charge-ordered state in all dimensions $d \leq 4$. For $K < K_0$, the ground-state in $d \leq 4$ has more or less extended short-ranged charge correlations, depending the strength of the disorder, but no true long-range order. (Indeed, the behavior of the disordered system in dimension d is qualitatively similar to that of the ordered system in dimension $d - 2$, or in other words the disorder produces the standard "dimensional reduction" associated with random field problems [17]) For $Q = 0$, however, the fact that the mean-squared random field, $f(\boldsymbol{k})$, vanishes at small k insures that a finite transition temperature to a charge-ordered (ferromagnetic) state survives up to a critical magnitude of the disorder. Thus, in all dimensions $d \leq 4$, the model has an avoided critical point. By contrast, weak disorder has relatively little effect on the ground state and low-temperature properties of the superconducting state unless $K - K_0$ is quite small. For fixed disorder, and $K > K_0$, the superconducting T_c tends continuously to zero as K is decreased, and always vanishes before $K > K_0$. (Recall that, in the absence of disorder, the superconducting state would have given way to a

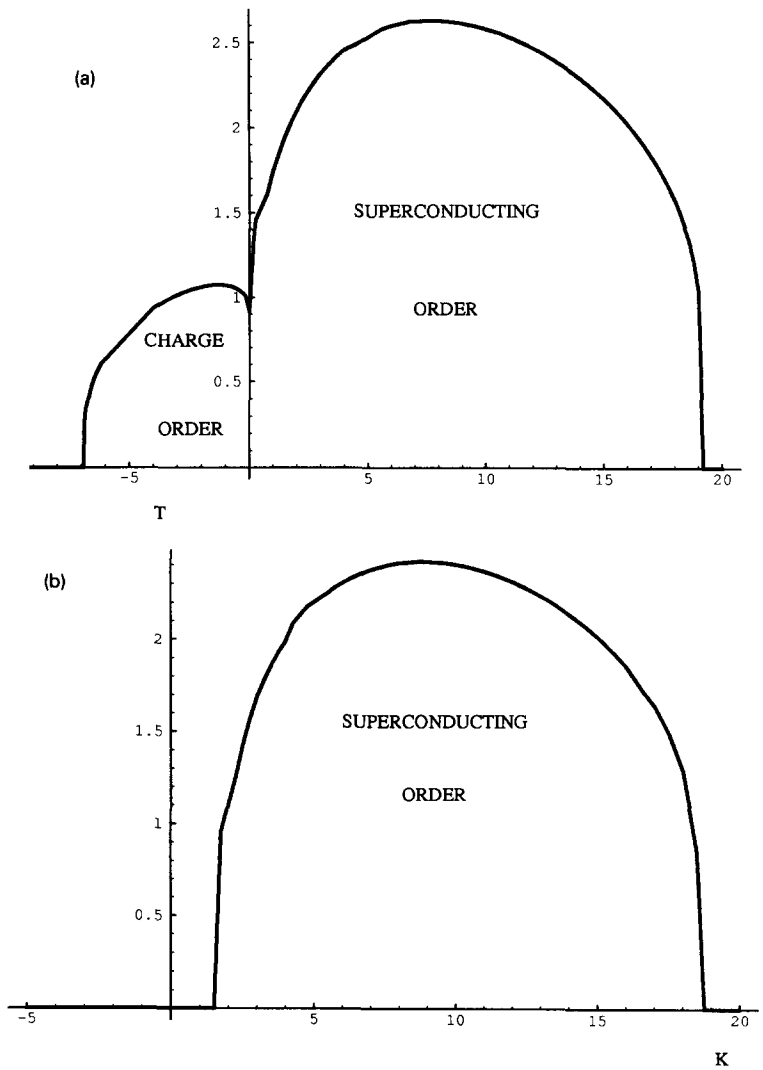

Fig. 4. The phase diagram as a function of temperature and position along the representative trajectory through parameter space $s^2 = 1.4$ and $Q = 20$ both (a) in the absence of disorder, and (b) in the presence of a disorder potential, $f(k) = 2\Delta(k)$.

charge-ordered state, both with finite transition temperatures, at precisely $K = K_0$.)

In Fig. 4, we show the phase diagram as a function of temperature and position along the representative trajectory through parameter space indicated by the arrow in Fig. 3, both in the presence and absence of disorder.

2.4. *Some exact ground-states for the Ising model*

An amusing side benefit of the present analysis is that, for certain ranges of parameters, the exact ground states of the classical spherical model are also the exact ground states

for all n of the $O(n)$ model with the same Hamiltonian, including the $n = 1$ Ising case. (These are listed in Table 1.) The proof is simple: For the spherical model, the ground states are found by minimizing the Hamiltonian with respect to spin configurations, subject to one global constraint. For the Ising model, the same minimization problem must be solved, but now subject to $N - 1$ additional constraints to insure that each spin has length 1. Thus, the ground-state energy of the Ising model must always be greater than or equal to that of the spherical model. If it so happens that the ground state of the spherical model is an Ising state, then this state must be a ground state of the corresponding Ising model. To extend the proof to the $O(n)$ model, we simply consider n copies of the spherical model with one coupled constraint.

In this way, we can prove that there exists a *region* of parameter space for which the corresponding frustrated $O(n)$ model has the spherical model ground state (and is thus independent of n). In three dimensions these states are: (1) a six-fold degenerate width 1 stripe with $\boldsymbol{q} = (\pi, 0, 0)$, (2) a six-fold degenerate columnar state with $\boldsymbol{q} = (\pi, \pi, 0)$, and (3) a two-fold degenerate Néel state with $\boldsymbol{q} = (\pi, \pi, \pi)$. (The degeneracies apply to the Ising model; for $n > 1$, the $O(n)$ models have an additional continuous degeneracy.) In addition, it is possible to prove that there exists at least a *surface* in parameter space on which the ground-state is: (1) a 12-fold degenerate width 2 stripe with $\boldsymbol{q} = (\pi/2, 0, 0)$, (2) a 24-fold degenerate rectangular columnar state with $\boldsymbol{q} = (\pi, \pi/2, 0)$, (3) a 12-fold degenerate rectangular Néel state with $\boldsymbol{q} = (\pi, \pi, \pi/2)$, and 4) a 16-fold degenerate width 2 Néel state with $\boldsymbol{q} = (\pi/2, \pi/2, \pi/2)$. (Surely, for the Ising model there is a commensurability energy which stabilizes these latter states in a finite region of parameter space.) Similar results can straightforwardly be obtained in other dimensions.

3. Method of solution

3.1. The classical model

Consider a model of the form of Eq. (1.3) where for convenience, we add a counter-term as in Eq. (1.12) defined so that the minimum value of $\mathcal{J}$ is zero. The standard version [15] of the spherical model dictates that we integrate over all configurations (S_k) subject to the constraint Eq. (1.7). A simpler solution, that was introduced as early as 1952 [7], employs the method of Lagrange multipliers: The original Hamiltonian is augmented by the term $\frac{1}{2}\mu \sum_k |S_k|^2$ and the integration takes place over *all* finite energy spin configurations. The model is now unconstrained and quadratic, so all quantities can be computed readily. As long as $\mu > 0$, this can be done without apologies and equation of constraint becomes an implicit equation for $\mu(T)$:

$$\frac{1}{T} = \Phi_N(\mu) \equiv \frac{1}{N} \sum_{\boldsymbol{k}} \frac{1}{\mathcal{J}(\boldsymbol{k}) + \mu}, \tag{3.1}$$

or, in the thermodynamic limit,

$$\frac{1}{T} = \Phi(\mu) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{\mathcal{J}(\boldsymbol{k}) + \mu}, \tag{3.2}$$

and the integral is over the first Brillouin zone. If this equation cannot be satisfied for any value of μ, we are at or below criticality. Since Φ is a monotonically decreasing function of μ, T_c is determined according to

$$1/T_c = \Phi(0^+). \tag{3.3}$$

For $T < T_c$, the Lagrange multiplier is set to zero. The total population of the finite modes therefore is deficient, and the remainder is identified as a condensate to be distributed among the zero modes.

It is intuitively clear that at least as far as the equilibrium properties of local observables are concerned, the above procedure is equivalent, in the thermodynamic limit, to the original constrained model. Such results have been established with a large degree of generality – more than sufficient to cover the cases of interest here. See, for example, [16] (in particular Theorem 1) and references therein.

Most of the claims made in the earlier sections thus amount to explicit calculations or elementary analysis of the function $\mathcal{J}(\boldsymbol{k})$. In particular, the internal energy per site U as a function of temperature is simply

$$U = \tfrac{1}{2}[T - \mu(T)], \tag{3.4}$$

and all other thermodynamic quantities can be determined by taking appropriate partial derivatives of this expression. For $T < T_c$, the magnitude, m, of the condensate is simply

$$m^2 = 1 - T\Phi(0) = [T_c - T]/T_c. \tag{3.5}$$

The spin–spin correlation functions can be straightforwardly calculated according to

$$\tilde{G}(\boldsymbol{k}, T) \equiv \langle |S_k|^2 \rangle = T/[\mathcal{J}(\boldsymbol{k}) + \mu(T)], \tag{3.6}$$

as is easily seen using the so called *method of generating functions:* Add small terms to the Hamiltonian (well localized in position or momentum space) and differentiate the free energy with respect to the appropriate coupling. From Eq. (3.6), the inverse of the correlation length may be extracted:

$$\xi_a(T)^{-1} = \min |\mathrm{Im}\{q_a^0\}| \tag{3.7}$$

(in general, ξ may be anisotropic, hence it is labeled by a direction) where $\boldsymbol{q}^0$ is the solution of the implicit equation

$$\mathcal{J}(\boldsymbol{q}^0) + \mu(T) = 0, \tag{3.8}$$

and the minimization in Eq. (3.7) is over the set of solutions with all other components of $\boldsymbol{q}$ real.

Crossover temperatures can, of course, never be determined from a single sharp criterion. However, near the avoided critical point, a crossover occurs in a narrow range

of temperatures, so it is both useful and appropriate to define a crossover temperature explicitly. The crossover temperature, T_1 (below which the frustration becomes "important") is therefore defined as the solution of the implicit equation

$$\mu(T_1) = 2\sqrt{Q}, \tag{3.9}$$

where the factor of 2 is chosen for aesthetic reasons. Notice that for an avoided critical point, $T_1 \to T_c(Q=0)$ as $Q \to 0$. Along a trajectory in the Q–T plane which lies at fixed distance above $T_1(Q)$, the correlation length approaches a finite limit as $Q \to 0$, while below T_1, the correlation length diverges in this limit. The lower crossover temperature T_2 (below which the lattice anisotropy becomes "important") will be defined – with the same degree of arbitrariness as T_1 – as the solution of

$$\mu(T_2) = \lambda Q. \tag{3.10}$$

For small Q and λ and $T_1 \gg T \gg T_2$, the structure factor is dominated by a sharp ridge at $|\boldsymbol{k}| = q$, while for $T_2 > T$, there are six sharp peaks at $|\boldsymbol{k}| = q$ and $\boldsymbol{k}$ along a coordinate axis. With our definition, at $T = T_2$, the modulation in the magnitude of $S(\boldsymbol{k})$ (as a function of angle) with fixed $|\boldsymbol{k}| = q$, is comparable to the height of the ridge.

3.2. *The quantum model*

The quantum model is solved in much the same way as the classical model, through the introduction of a chemical potential to enforce the constraint, which reduces the problem to a set of decoupled harmonic oscillators. Thus, for all temperatures above T_c, μ is implicitly determined from the relation

$$s^2 = \Phi_{\mathrm{qu}}(\mu, T), \tag{3.11}$$

where

$$\Phi_{\mathrm{qu}}(\mu, T) = \frac{1}{2}\int \frac{d^d k}{(2\pi)^d} \times \left[\left(\sqrt{\frac{W\Delta(\boldsymbol{k})+\mu}{\mathcal{J}(\boldsymbol{k})+\mu}} + \sqrt{\frac{\mathcal{J}(\boldsymbol{k})+\mu}{W\Delta(\boldsymbol{k})+\mu}}\right)\left(2n\left(\frac{\omega_k}{T}\right)+1\right)\right], \tag{3.12}$$

$$\omega_k = \{[W\Delta(\boldsymbol{k})+\mu][\mathcal{J}(\boldsymbol{k})+\mu]\}^{-1/2}, \tag{3.13}$$

and $n(x) = (e^x - 1)^{-1}$ is the Bose occupation factor. (The behavior of the dispersion relation as $k \to 0$ is somewhat peculiar, but this has no effect on the present results [14].) Again, Φ is a monotonically decreasing function of μ so, at $T = 0$, the critical value of s is determined from the equation

$$s_c^2 = \Phi(0,0), \tag{3.14}$$

and, when $s > s_c$, the critical temperature T_c is determined according to

$$s^2 = \Phi(0, T_c). \tag{3.15}$$

For $s > s_c$ and $T < T_c$, the magnitude of the condensate, m, is determined according to

$$m^2 = s^2 - \Phi(0,T), \tag{3.16}$$

where, as discussed above, m is the magnitude of the superconducting condensate for $K > K_0$ and the amplitude of the charge-density wave for $K < K_0$. The dynamic spin correlation function (since in quantum mechanics, dynamics and thermodynamics are intimately related, the Fourier transform of the two-time spin correlation function is the fundamental quantity) is easily seen to be

$$\tilde{G}(\boldsymbol{k},\omega) = \frac{1}{2}\sqrt{\frac{W\Delta(\boldsymbol{k})+\mu}{\mathcal{J}(\boldsymbol{k})+\mu}} \times\{[n(\omega_{\boldsymbol{k}}/T)+1]\delta(\omega-\omega_{\boldsymbol{k}}) + n(\omega_{\boldsymbol{k}}/T)\delta(\omega+\omega_{\boldsymbol{k}})\}, \tag{3.17}$$

while the static structure factor,

$$\tilde{G}(\boldsymbol{k}) = \int \frac{d\omega}{2\pi}\tilde{G}(\boldsymbol{k},\omega) = \frac{1}{2}\sqrt{\frac{W\Delta(\boldsymbol{k})+\mu}{\mathcal{J}(\boldsymbol{k})+\mu}}[2n(\omega_{\boldsymbol{k}}/T)+1]. \tag{3.18}$$

The inverse charge-ordering correlation length (which, again, will generally be anisotropic) is

$$1/\xi_a^{\mathrm{ch}}(T) = \min|\mathrm{Im}\{q_a^{\mathrm{ch}}\}|, \tag{3.19}$$

where $\boldsymbol{q}^{\mathrm{ch}}$ is the solution of the implicit equation

$$\mathcal{J}(\boldsymbol{q}^{\mathrm{ch}}) + \mu(T) = 0, \tag{3.20}$$

and the minimization is again performed with all other components of $\boldsymbol{k}$ real. A similar expression for the superconducting correlation function is easily obtained by inverting the term in the square root in Eq. (3.17) and a superconducting correlation length obtained from the solution of the implicit equation

$$W\Delta(\boldsymbol{q}^{\mathrm{sc}}) + \mu(T) = 0. \tag{3.21}$$

Finally, the internal energy per site U as a function of temperature is simply

$$U = U_0(T) - \tfrac{1}{2}s^2\mu(T), \tag{3.22}$$

where

$$U_0(T) = \frac{1}{2}\int \frac{d^d k}{(2\pi)^d}\omega_{\boldsymbol{k}}[2n(\omega_{\boldsymbol{k}}/T)+1] \tag{3.23}$$

is the internal energy of independent harmonic oscillators, and all other thermodynamic quantities can be determined by taking appropriate partial derivatives of this expression.

3.3. The model with disorder

Because of the harmonic nature of the model, the effect of an arbitrary configuration of random fields $\{h_j\}$ can be formally accounted for by shifting all spins according to

$$\tilde{S}_k \to \tilde{S}_k + \tilde{h}_k/[\mathcal{J}(k) + \mu], \tag{3.24}$$

for either the classical or the quantum model. The result is an additive term to the internal energy,

$$U \to U - \frac{1}{2}\int \frac{d^d k}{(2\pi)^d} \frac{|\tilde{h}_k|^2}{[\mathcal{J}(k) + \mu]}, \tag{3.25}$$

and a shift in the implicit equation for μ brought about by the substitution

$$\langle|\tilde{S}_k|^2\rangle \to \langle|\tilde{S}_k|^2\rangle + \frac{\langle|\tilde{h}_k|^2\rangle}{[\mathcal{J}(k) + \mu]^2}. \tag{3.26}$$

Upon configuration averaging, this relation implies

$$\Phi_{\text{dis}}(\mu, T) = \Phi_{\text{qu}}(\mu, T) + \int \frac{d^d k}{(2\pi)^d} \frac{f(k)}{[\mathcal{J}(k) + \mu]^2} \tag{3.27}$$

(and the obvious corresponding equation for the classical model). The spin correlation function in the presence of disorder is altered both by the implicit change produced by the altered temperature dependence of μ, and by the addion of a zero fequency additive contribution

$$\tilde{G}_{\text{dis}}(k, \omega) = \tilde{G}(k, \omega) + \frac{\delta(\omega) f(k)}{[\mathcal{J}(k) + \mu]^2}. \tag{3.28}$$

It is clear from Eq. (3.27) that for $K - K_0$ negative Φ_{dis} diverges as $\mu \to -K_0$ for all dimensions $d \leq 4$, so that no charge ordered state is possible. Moreover, if $K - K_0$ is positive but small, $\Phi_{\text{dis}}(0, T)$ will have a large, additive contribution from the disorder term, from which it follows that the superconducting T_c must always vanish as $K \to K_0 + \Delta K$ where ΔK is a positive, increasing function of the strength of the disorder.

4. Mathematical dump

We now provide the calculational details which underly the various claims made in the previous sections. Our starting point is an elementary calculation concerning the stationary points of $\mathcal{J}(k)$:

Proposition 4.1. Let

$$\mathcal{J}_Q(k) = \sum_a V(k_a) + \tfrac{1}{2}\lambda \sum_{a \neq b} V(k_a) V(k_b) + \frac{Q}{\sum_a V(k_a)} + K, \tag{4.1}$$

with $V(k_a) = 2(1 - \cos k_a)$ and $\lambda \neq 0$. Let p be a stationary point of $\mathcal{J}(k)$ in the first Brillouin zone, $-\pi < k_a \leq \pi$. Then any component of p may be 0 or π but the

components that are not 0 or π are equal in magnitude to each other. In particular, if $\boldsymbol{p}$ is a stationary point then $|p_a| = 0$, π, or $q_{\ell,s}$ with $q_{\ell,s}$ satisfying

$$1 + \lambda[4\ell + (s-1)V(q_{\ell,s})] = \frac{Q}{(4\ell + sV(q_{\ell,s}))^2}, \tag{4.2}$$

where ℓ is the number of components equal to π and s is the number of the remaining components that are non–zero. This theorem applies in arbitary dimension, $d \geq 1$.

Proof. Upon differentiating $\mathcal{J}(\boldsymbol{k})$ we find

$$\left(1 + \lambda \sum_{b \neq a} V(k_b) - \frac{Q}{[\sum_b V(k_b)]^2}\right) \sin k_a = 0. \tag{4.3}$$

This is obviously satisfied if $k_a = 0$ or π. Now suppose that $\boldsymbol{k}$ satisfies Eq. (4.3) with two or more components, k_b and k_c not 0 or π. Then, subtracting, we get

$$\lambda V(k_b) = \lambda V(k_c), \tag{4.4}$$

which implies $|k_b| = |k_c|$. If there are ℓ directions where $|k_a| = \pi$ and s directions where $|k_a|$ is not 0 or π then the magnitude of these remaining components satisfies the stated equation. □

What follows is the starting point for both the analysis of the low temperature behavior in the system as $Q \to 0$ and for the analysis of the ground state space. For the most part, the indices on the q defined above will be understood from context and omitted.

Proposition 4.2. Let $\mathcal{J}(\boldsymbol{k})$ be as described in Proposition 4.1. Then for $\lambda > 0$, and $Q \leq 16$, the minimizing wave vector has a single non–zero component of magnitude q satisfying

$$V(q) = \sqrt{Q}. \tag{4.5}$$

Proof. If $\lambda = 0$, the function has an absolute minimum of $2\sqrt{Q}$ which is achieved if $\sum_a V(k_a) = \sqrt{Q}$. Provided that $\sqrt{Q} \leq 4$, this value can be obtained even if $\lambda > 0$ by a vector with only a single component that has the above stated magnitude. □

We are now ready for our principal result for this section:

Theorem 4.3. In three dimensions, for the model described in Proposition 4.1, there is an avoided critical point at $Q = 0$. In particular, for fixed $\lambda > 0$, let $T_c(0)$ $(= T_c(0; \lambda))$ be the critical temperature for the $(Q = 0)$, ferromagnetic version of the model:

$$\frac{1}{T_c(0)} = \frac{1}{(2\pi)^3} \int_{|k_a| < \pi} \frac{d^3k}{\sum_a V(k_a) + \frac{1}{2}\lambda \sum_{a \neq b} V(k_a)V(k_b)}, \tag{4.6}$$

and $T_c(Q)$ given as in Eqs. (3.2) and (3.3) with $\mathcal{J}_Q(\boldsymbol{k})$ given in Eq. (4.1) with $K = K_0 = -2\sqrt{Q}$. Then

$$\frac{1}{T_c(0)} < \lim_{Q \to 0} \frac{1}{T_c(Q)} = \frac{1}{T_c(0)} + \frac{B}{\sqrt{\lambda}}, \tag{4.7}$$

$$B = \frac{1}{(16\pi^2)} \int d\Omega \, [\sin^4\theta \cos^2\phi \sin^2\phi + \cos^2\theta \sin^2\theta]^{-1/2} \approx 0.14245.$$

Proof. For $Q \ll 1$, let $q \simeq Q^{1/4}$ denote the solution of

$$V(q) = \sqrt{Q}, \tag{4.8}$$

and let Δ be a small number independent of Q, the precise specifications of which will be detailed later. (In most of what is to follow, the distinction between q and $Q^{1/4}$ is practically irrelevant – q may simply be regarded as convenient notation for $Q^{1/4}$.) It is clear that for the large-k portion of the integral, $|\boldsymbol{k}| > \Delta$, as $Q \to 0$, nothing particularly interesting happens to the integrand $[\mathcal{J}_Q^{-1}(\boldsymbol{k})]$. Hence

$$\lim_{Q\to 0} \int_{|\boldsymbol{k}|>\Delta} \frac{d^3k}{\mathcal{J}_Q(\boldsymbol{k})} = \int_{|\boldsymbol{k}|>\Delta} \frac{d^3k}{\mathcal{J}_{Q=0}(\boldsymbol{k})}. \tag{4.9}$$

Notice that, for small Δ, the right hand side is only just shy of $1/T_c(0)$.

Now, let $0 < t < 1$ and define the two constants $A_\pm = 1 \pm q^t$, which have the property that $A_\pm \to 1$ as $Q \to 0$. In terms of these, we break the remaining region of integration in three: (1) A small k region, $\mathcal{R}_1$ with $0 < |k| \le qA_-$; (2) A critical region, $\mathcal{R}_2$ with $qA_- < |k| \le qA_+$; (3) An intermediate k region $\mathcal{R}_3$ with $qA_+ < |k| \le \Delta$. We shall show that, as $Q \to 0$, the contribution from region 1 vanishes, the contibution from region 3 plus the contribution from large k in Eq. (4.9) converge to $1/T_c(0)$, and the contribution from the critical region approaches $B/\sqrt{\lambda}$.

• In $\mathcal{R}_1$, as an upper bound, we will neglect the λ–perturbation in the denominator. Noting that in the specified region, $\sum_a V(k_a) + Q/\sum_a V(k_a)$ is increasing and that, in general, $V(k_a) \le k_a^2$, we have

$$\int_{\mathcal{R}_1} \frac{d^3k}{\mathcal{J}_Q(\boldsymbol{k})} \le \int_{\mathcal{R}_1} \frac{d^3k}{k^2 + Q/k^2 - 2\sqrt{Q}} \le 4\pi q^4 \int_{|k|<qA_-} \frac{dk}{(k - Q^{1/4})^2}. \tag{4.10}$$

The last term is bounded by constants times $q^{(3-t)}$ as $Q \to 0$ and thus the limiting contribution from this region may be neglected.

• Next, consider the intermediate region $\mathcal{R}_3$. Since $\mathcal{J}_Q = \mathcal{J}_0 + Q/\sum_a V(k_a) - 2\sqrt{Q}$ it follows that

$$\int_{\mathcal{R}_3} \frac{d^3k}{\mathcal{J}_Q(\boldsymbol{k})} = \int_{\mathcal{R}_3} \frac{d^3k}{\mathcal{J}_0(\boldsymbol{k})} + \int_{\mathcal{R}_3} \frac{[2\sqrt{Q} - Q/\sum_a V(k_a)]\, d^3k}{\mathcal{J}_0(\boldsymbol{k})\mathcal{J}_Q(\boldsymbol{k})}. \tag{4.11}$$

Now the first term on the right hand side of Eq. (4.11) may be added directly to the right hand side of Eq. (4.9) to obtain, in the small Q limit, exactly $1/T_c(Q=0)$. Let us show that the second term vanishes as $Q \to 0$. In this region, the numerator is positive so we may discard the term involving $\sum_a V(k_a)$. The denominator is made smaller if we set $\lambda = 0$ so let us do that as well. Let D denote any positive constant for which

$V(k_a) \geq Dk_a^2$ holds for all k_a with $|k_a| \leq \pi$. Putting these together, and canceling powers of k the task is to show that

$$\sqrt{Q} \int_{\mathcal{R}_3} \frac{d^3k}{\sum_a V(k_a) - 2\sqrt{Q} + Q/\sum_a V(k_a)} \tag{4.12}$$

vanishes in the $Q \to 0$ limit. For the term $Q/\sum_a V(k_a)$ in the denominator, we may use the bound $V(k_a) \leq k_a^2$ and, further, for the other appearance of $\sum_a V(k_a)$, we may replace this sum with $k^2 - Ek^4$ where E is some constant independent of Q (or Δ). With these estimates in tow, the problem is one dimensional and, were it not for the quartic term, would be entirely trivial. In any case, we are now reduced to showing that

$$\int_{\mathcal{R}_3} \frac{dk\,\sqrt{Q}k^2}{(k^2 - \sqrt{Q})^2 - Ek^6} \tag{4.13}$$

vanishes as $Q \to 0$.

Let us now assert that Δ has been chosen small enough so that (for all q sufficiently small) throughout the range $qA_+ \leq k \leq \Delta$,

$$Ek^6 < \tfrac{1}{2}(k^2 - \sqrt{Q})^2. \tag{4.14}$$

Indeed, provided that q is sufficiently small, the inequality clearly holds at the lower limit and, upon comparison of derivatives, the desired inequality holds throughout the entire range provided that $E\Delta$ is somewhat less than one. What is left after these estimates can, essentially, be done by hand:

$$\int_{\mathcal{R}_3} \frac{\sqrt{Q}k^2\,dk}{(k^2 - \sqrt{Q})} \leq \int_{\mathcal{R}_3} \frac{\sqrt{Q}\,dk}{(k - Q^{1/4})^2} \leq \frac{\sqrt{Q}}{q - Q^{1/4} + q^{(1+t)}} \approx q^{(1-t)}, \tag{4.15}$$

which indeed vanishes as $Q \to 0$.

• Thus we are left with the critical region $\mathcal{R}_2$. In this region, the deviation of k from q is so slight that we are essentially in the position where we can "expand and neglect". In particular, upper and lower bounds may be derived, in this region, by setting various items to their maximum or minimum value. Since the procedure is similar on both sides, we will be content with an explicit derivation of a lower bound on the remaining integral that agrees with the stated formula. As will become apparent, an upper bound can be derived in the same fashion.

In what follows, all constants C_n will be functions of Q with the property that $C_n \to 1$ as $Q \to 0$. It is slightly easier to work with the quantities $V(k_a)$ instead of the k_a hence we define the variables

$$v_a = [V(k_a)]^{1/2}, \tag{4.16}$$

and note that $dv_a = |(\sin k_a)/2\sin(\frac{1}{2}k_a)| \geq C_1\,dv_a$. It is further clear that in the region $|k - q| < q^{1+t}$, we may write $d^3k \geq C_2 q^2\,dv\,d\Omega$. Next, it is noted that the image of the

region $|k-q| < q^{1+t}$, in v-space, also contains a spherical shell of size $C_3 q^{(1+t)}$. We will confine our attentions to this smaller region. Thus,

$$\int_{\mathcal{R}_2} \frac{d^3k}{\mathcal{J}(k)} \geq C_2 q^2 \int_{|u|<C_3 q^{1+t}} \frac{du\, d\Omega}{4C_4 u^2 + \lambda C_5 q^4 R(\Omega)}, \tag{4.17}$$

where $u = v - q$,

$$R(\Omega) = \lim_{q\to 0} \frac{1}{q^4} \frac{1}{2} \sum_{a\neq b} v_a^2 v_b^2 \equiv \sin^2\theta \cos^2\theta + \sin^4\theta \cos^2\phi \sin^2\phi. \tag{4.18}$$

For $R(\Omega) \neq 0$, the u integral is easily preformed to yield

$$\int_{\mathcal{R}_2} \frac{d^3k}{\mathcal{J}(k)} \geq \frac{C_5}{\sqrt{\lambda}} \int \frac{d\Omega \alpha_0}{\sqrt{R(\Omega)}}, \tag{4.19}$$

$$\alpha_0 = \tan^{-1}[2C_3 q^{t-1}/\sqrt{\lambda R(\Omega)}] \to \pi/2. \tag{4.20}$$

Hence, it is seen that

$$\lim_{Q\to 0} \int_{\mathcal{R}_2} \frac{d^3k}{\mathcal{J}(k)} \geq \frac{\pi}{2\sqrt{\lambda}} \int \frac{d\Omega}{\sqrt{R(\Omega)}}, \tag{4.21}$$

as claimed.

An upper bound follows almost the identical derivation with a renaming of the constants C_n. □

Corollary. In dimension $d > 3$, there is a "nearly avoided critical point" for the stated model in the sense that for fixed $\lambda > 0$, as $Q \to 0$,

$$\frac{1}{T_c(Q)} - \frac{1}{T_c(0)} \sim Q^{(d-3)/4} \lambda^{-1/2} B_d, \tag{4.22}$$

$$B_d = (2\pi)^{-d} \int_{\Omega} d\Omega [R_d(\Omega)]^{-1/2}, \qquad R_d(\Omega) = \frac{1}{2} \sum_{a\neq b} x_a x_b \,|_{x^2=1}\,.$$

Proof. If we use the same division of regions and follow step for step the analysis of Theorem 4.3, we see that all the estimated quantities that go to zero are now multiplied by an extra factor of $k^{(d-3)}$ (from the volume element). This always amounts to an extra factor of $q^{(d-3)}$ Similarly, the term that was of primary interest works in a similar way but is multiplied by $q^{(d-3)}$. Everything else that was finite produces $1/T_c(0)$ mutatis-mutandis. In particular, we get

$$\lim_{Q\to 0} Q^{-(d-3)/4} \left(\frac{1}{T_c(Q)} - \frac{1}{T_c(0)} \right) = \lambda^{-1/2} B_d. \tag{4.23}$$

□

Our discussion of the ground state space now picks up where Proposition 4.2 left off. Right now, for $\lambda > 0$ and $Q < 16$ the situation is well under control and these are the

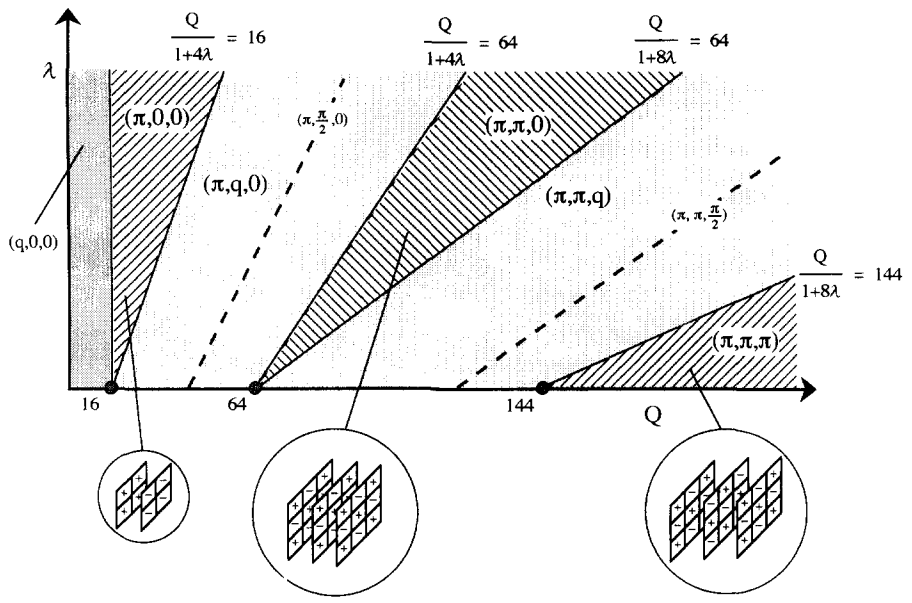

Fig. 5. Pictures of the various ordered phases of the Ising version of the model for positive λ.

sorts of results that we seek throughout the phase plane. For the sake of brevity, we will focus our attention on the cases of principal interest, namely $d = 3$ and $\lambda > 0$.

Proposition 4.1 tells us that in any region, there are only a finite number of possibilities to consider; however, for $d = 3$, this turns out to be eight additional distinct modes (other than $(q,0,0)$) and five new regions. Notwithstanding, we will attempt to be as brief as possible and still lay claim to a rigorous proof; this is most efficiently carried out by writing out five separate sub-propositions. A complete list of the competing modes as well as the regions of interest can be found in Fig. 5. In the up and coming, the various state (or modes) will not be distinguished from their reflection or coordinate axis exchange equivalents. Thus, e.g. Proposition 4.4.1 below really pertains to six ground (equivalent) states.

Proposition 4.4.1. In the region $\lambda > 0$, $Q > 16$ and $Q < 16(1 + 4\lambda)$, the ground state is of the form $(\pi, 0, 0)$.

Proof. Since $Q > 16$, the $(q,0,0)$ states need not be considered because there is no solution to Eq. (4.2) for q. Similarly, for the mode $(\pi, q, 0)$, the defining equation reads $(1 + 4V_q)^2 = Q/(1 + 4\lambda)$ (where here, and in what is to follow, we use the notation $V_q \equiv V(q)$). Hence this mode is forbidden if $Q < 16(1 + 4\lambda)$. In the same region, for the same reason, the mode (π, q, q) is disallowed and similarly, the mode (π, π, q) is forbidden for $Q < 64(1 + 8\lambda)$. Now the "energy" for the current state, $\mathcal{J}(\pi, 0, 0)$, is simply $4 + Q/4$. In the stated region, this is a whole lot less than $8 + Q/8 + 16\lambda$ and $12 + Q/12 + 48\lambda$ which eliminates $(\pi, \pi, 0)$ and (π, π, π) from consideration. This leaves as contenders only the modes (q, q, q) and $(q, q, 0)$. The energy for $(q, q, 0)$ is given by

$$\mathcal{J}(q,q,0) \equiv \mathcal{E}_{q,q,0} = 2V_q + Q/2V_q + \lambda V_q^2. \tag{4.24}$$

Now in general, the energy of any state increases with λ however $\mathcal{E}_{\pi,0,0}$ is independent of λ. It is therefore sufficient to establish $\mathcal{E}_{q,q,0} > \mathcal{E}_{\pi,0,0}$ at the lower-right boundary of the region under consideration. To this end, we write

$$\mathcal{E}_{q,q,0} = 2V_q + Q/2V_q + 4\lambda[2V_q] - 16\lambda + \lambda(4 - V_q)^2. \tag{4.25}$$

Neglecting the quadratic term and minimizing at $Q = 16(1 + 4\lambda)$, this is maximized when $2V_q = 4$ and weighs in at exactly $4 + Q/4$. Using the fact that we are interested in Q's that are *strictly* less than $16(1 + 4\lambda)$ and, the fact that $\mathcal{E}_{q,q,0}$ is a strictly increasing function of λ we find $\mathcal{E}_{q,q,0} > \mathcal{E}_{\pi,0,0}$. The mode (q,q,q) has energy $3V_q + Q/3V_q + 3\lambda V_q^2$ which (when regarded as a function of $3V_q$) is manifestly larger than $\mathcal{E}_{q,q,0}$.

Proposition 4.4.2. In the region $\lambda > 0$, $16(1 + 4\lambda) < Q < 64(1 + 4\lambda)$, the ground state is of the form $(\pi, q, 0)$.

Proof. Notice that this is exactly the region where Eq. (4.2) has a solution for the mode $(\pi, q, 0)$. The mode (π, π, q) has no solution in this region (and nor does $(q, 0, 0)$). We write

$$\mathcal{E}_{\pi,q,0} = \min_{\omega}(\omega + Q/\omega + 4\lambda\omega - 16\lambda) \tag{4.26}$$

[with $\omega \equiv 4 + V_q$; note that the minimizing ω equals $\sqrt{Q/(1 + 4\lambda)}$]. On comparison to $\mathcal{E}_{q,q,0}$ as expressed in Eq.(4.25), it is clear that $\mathcal{E}_{\pi,q,0}$ is lower. This also eliminates (q,q,q) on the basis of the final argument in Proposition 3.4.1. Next we have $\mathcal{E}_{\pi,\pi,0} = 8 + Q/8 + 16\lambda$ and plugging $\omega = 8$ into the expression on the right-hand side of Eq. (4.26), this is exactly what we get. The minimizing ω will do better.

Thus we may turn our attention to the mode at (π, q, q) – the ones at $(\pi, 0, 0)$ and (π, π, π) then follow immediately. The energy, $\mathcal{E}_{\pi,q,q}$ admits the expression

$$\mathcal{E}_{\pi,q,q} = 4 + 2V_q + Q/(4 + 2V_q) + 4\lambda(4 + 2V_q) - 16\lambda + 8\lambda V_q^2. \tag{4.27}$$

Regarding this as a function of $4 + 2V_q$, and comparing to Eq. (4.26), this energy is clearly larger than $\mathcal{E}_{\pi,q,0}$ whenever we are in a region where a minimizing ω for Eq. (4.26) exists.

Proposition 4.4.3. In the region $\lambda > 0$, $(1 + 4\lambda) < Q/64 < 64(1 + 8\lambda)$, the ground state is of the form $(\pi, \pi, 0)$.

Proof. The modes $(q, 0, 0)$ and $(\pi, q, 0)$ are eliminated from consideration. Similarly, V_q for $(q, q, 0)$ must satisfy

$$4V_q^2 = Q/(1 + \lambda V_q), \tag{4.28}$$

but

$$Q/(1 + \lambda V_q) \geq Q/(1 + 4\lambda) > 64, \tag{4.29}$$

so for $(q, q, 0)$, V_q cannot get big enough.

For the mode at hand, the energy $\mathcal{E}_{\pi,\pi,0}$ is given by the simple formula

$$\mathcal{E}_{\pi,\pi,0} = 8 + Q/8 + 16\lambda. \tag{4.30}$$

Subtracting this from various expressions for the energy of various other modes, we see $\mathcal{E}_{\pi,0,0} - \mathcal{E}_{\pi,\pi,0} \propto Q - 16(1+4\lambda) > 0$, $\mathcal{E}_{\pi,\pi,\pi} - \mathcal{E}_{\pi,\pi,0} = 4(1+8\lambda) - Q/24 > 0$ and similarly, $\mathcal{E}_{\pi,\pi,q} - \mathcal{E}_{\pi,\pi,0} = V_q(1+8\lambda - Q/(8)(8+V_q)) > 0$. Notwithstanding the losing status of the state (π,π,q), for the benefit of the final two states on the list, let us write its energy:

$$\mathcal{E}_{\pi,\pi,q} = 8 + V_q + Q/(8+V_q) + \lambda(16+8V_q) = \eta + \frac{Q}{\eta} + 8\lambda\eta - 48\lambda, \tag{4.31}$$

where $\eta \equiv 8 + V_q$. Similarly, $\mathcal{E}_{q,q,q}$ may be written

$$\mathcal{E}_{q,q,q} = \sigma + Q/\sigma + 8\lambda\sigma - 48\lambda + \lambda(\tfrac{1}{3}\sigma^2 + 48 - 8\sigma), \tag{4.32}$$

with $\sigma = 3V_q$. (Of course the q's referred to in Eqs. (4.31) and (4.32) pertain to different solutions of Eq. (4.2) and are not to be identified with one another.) It is easily checked that $\frac{1}{3}\sigma^2 + 48 - 8\sigma > 0$ for $\sigma < 12$ and hence it is seen that $\mathcal{E}_{q,q,q} > \mathcal{E}_{\pi,\pi,q}$.

Similarly, we write

$$\begin{aligned}\mathcal{E}_{\pi,q,q} &= 4 + 2V_q + Q/(4+2V_q) + \lambda(8V_q + V_q^2)\\ &= \zeta + Q/\zeta + 8\lambda\zeta - 48\lambda + \lambda(\tfrac{1}{4}\zeta^2 - 6\zeta + 36),\end{aligned} \tag{4.33}$$

and again the term in square brackets is positive if $\zeta < 12$.

Proposition 4.4.4. In the region $\lambda > 0$ and $64 < Q/(1+8\lambda) < 144$, the ground state is of the form (π,π,q).

Proof. The modes $(q,0,0)$, $(\pi,q,0)$ and $(q,q,0)$ are already out of the loop. In Proposition 4.4.3, we have (just) shown $\mathcal{E}_{q,q,q} > \mathcal{E}_{\pi,\pi,q}$ and $\mathcal{E}_{\pi,q,q} > \mathcal{E}_{\pi,\pi,q}$ so these are out. Now at the minimum, V_q satisfies $(8+V_q)^2 = Q/(1+8\lambda)$. In the specified region, this is not solved by $V_q = 0$ or $V_q = \pi$ so evidently $\mathcal{E}_{\pi,\pi,\pi} > \mathcal{E}_{\pi,\pi,q}$ and $\mathcal{E}_{\pi,\pi,0} > \mathcal{E}_{\pi,\pi,q}$. Finally, we dispense with $(\pi,0,0)$ by noting that in this region, $\mathcal{E}_{\pi,\pi,0} < \mathcal{E}_{\pi,0,0}$.

Proposition 4.4.5. In the region $\lambda > 0$, $Q > 144(1+8\lambda)$ the ground state is of the form (π,π,π).

Proof. Examining Eq. (4.2) for V_{q_1} in the state (q_1,q_2,q_3), we have

$$1 + \lambda(V_{q_2} + V_{q_3}) = Q/(V_{q_1} + V_{q_2} + V_{q_3})^2. \tag{4.34}$$

The right hand side is larger than $Q/144$ and the left hand side is smaller than $(1+8\lambda)$. Thus there are no solutions with any component not equal to 0 or π. It follows from earlier results (or it can be easily checked) that in this region, $\mathcal{E}_{\pi,\pi,\pi} < \mathcal{E}_{\pi,\pi,0} < \mathcal{E}_{\pi,0,0}$. □

Corollary. Along the line $Q/(1+4\lambda) = 36$, the ground state is $(\pi, \frac{1}{2}\pi, 0)$ and along the line $Q(1+8\lambda) = 100$, the ground state is $(\pi,\pi,\frac{1}{2}\pi)$.

Proof. This follows from setting $V_q = 2$ in the appropriate region and solving Eq. (4.2) for $Q(\lambda)$. □

Remark. The case $\lambda < 0$ is far easier to analyze. Indeed, writing $\mathcal{J}(\boldsymbol{k}) = \Delta(\boldsymbol{k}) + \frac{1}{2}|\lambda|[\Delta(\boldsymbol{k})] + Q/\Delta(\boldsymbol{k}) - \frac{1}{2}|\lambda|\sum_a V(k_a)^2$, let $\boldsymbol{k}$ denote any wave vector, and let $\tilde{q}$ satisfy $dV(\tilde{q}) = \Delta(\boldsymbol{k})$. It is clear that $\mathcal{J}(\tilde{q},\ldots,\tilde{q}) < \mathcal{J}(\boldsymbol{k})$ unless $\boldsymbol{k} = ((\tilde{q},\ldots,\tilde{q}))$. Indeed, this amounts to showing that $\sum_a V^2(k_a) \geq (1/d)[\Delta(\boldsymbol{k})]^2$ and the latter is just (the discrete form of) Hölder's inequality which holds as an equality if and only if the $V(k_a)$ are independent of a. Evidently the minimizer is "diagonal" fr om which it is easy to see that (in three dimensions) the Néel ground state dominates in the region $Q \leq 144 - 1152|\lambda|$ for $\lambda < 0$.

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[10] The one dimensional hard-core bose gas on the lattice is easily mapped onto a spin 1/2 XXZ spin-chain problem, in which the XY part of the Hamiltonian is ferromagnetic (reflecting the nodelessness of a boson ground-state) with a magnitude J_{xy} given by the boson kinetic energy and the Ising part J_z reflects a nearest- neighbor interaction between bosons and can be ferromagnetic (attractive) or antiferromagnetic (repulsive); one can also include a chemical potential, which translates into a magnetic field in the z direction. At zero temperature and zero magnetic field this has an XY (superconducting) phase with power-law order for $J_{xy} > |J_z|$, a period-two Néel (charge-density wave) phase for $J_z > J_{xy}$ and is

ferromagnetic (phase separates) for $J_z < -J_{xy}$. At finite temperature, of course, there are no ordered phases. The quantum spherical model defined as in the present paper has precisely these phases, in addition to a zero-temperature quantum disordered phase.

[11] It is easy to see that as long as α_x and α_p are both positive and non-zero, we can rescale the spins and momenta, with a suitable rescaling of physical parameters (including $\hbar$) to write the model in a form with $\alpha_x = \alpha_p = 1$.

[12] Th.M. Nieuwenhuizen, Phys. Rev. Lett. 74 (1995) 4293. In this paper, the classical spherical model is quantized by first defining a second flavor of spin variables, with the same classical Hamiltonian and then writing a path integral expression for the square of the partition function in terms of a Euclidean path integral, in which both flavors of spin are required to satisfy the same global constraint and which quantum dynamics are introduced into the model through a term in the Euclidean action which is linear in time derivatives and off diagonal in the flavor index. This model can be transformed into a model of the sort considered in the present paper by first integrating out the second flavor of spins to obtain an effective action in terms of the original spin variables alone and then transforming from Lagrangian to Hamiltonian form. The result is a model of the same general form as the present model but with the substitution $W\Delta(k) \to \mathcal{J}(k) + \mu_2$ where μ_2 is the Lagrange multiplier for the second spin flavor. The constraint equation is unaffected by these transformations, and so remains a constraint expressed in terms of the spin variables alone. However, since the symmetry between the two spin flavors is unbroken, the constraint equation must be solved subject to the condition $\mu = \mu_2$, where $\mu \equiv \mu_1$ is the Lagrange multiplier for the first spin-flavor. At the end of the day, this makes the model of Nieuwenhuizen equivalent to the special, degenerate case of our model in which the classical and quantum pieces of the Hamiltonian in Eq. (1.8) are equal and hence the only possible ordered phase is the supersolid phase.

[13] J.W. Hartman and P.B. Weichman, Phys. Rev. Lett. 74 (1995) 4584. This paper deals with a large n generalization of a model of rigid rotors. In the usual language of superconductivity, the angular momentum of the rotor is identified with the local particle density, so the kinetic energy is the (short-ranged) Coulomb interaction between particles, while ordering of the rotor coordinate is identified with superconducting order. For this reason, in making comparison with the model in the present paper, we have performed a canonical transformation interchanging the momenta and coordinates of Hartman and Weichman. Since in the original language, the constraint equation involved the spin coordinates alone, after this transformation it involves the momenta only.
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[14] Note that for $\mu \neq 0$, $\omega_k \sim \sqrt{\mu Q}/k$ as $k \to 0$, which is unphysical; this mode would be expected to approach the plasma freqency as $k \to 0$ in the absence of any addition degrees of freedom which might screen the Coulomb interactions. However, this unphysical aspect of the model does not appear to have much effect on the central physical results. For instance, if we imagine that the Coulomb interactions were screened at long distances, this would remove this unphysical divergence without affecting the physics of the model at finite Q; effects of $1/n$ corrections typically produce such screening and so might be expected to remove this unphysical aspect of the model, as well. In the superconducting state, this mode approaches a finite freqency, $\omega_k \to \sqrt{WQ}$ as $k \to 0$, which has a natural interpretation as the plasma mode.

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