Bond and Néel order and fractionalization in ground states of easy-plane antiferromagnets in two dimensions

Kwon Park and Subir Sachdev

Department of Physics, Yale University, P.O. Box 208120, New Haven CT 06520-8120

(Dated: December 2, 2001)

We describe the zero temperature phases and phase boundaries of an effective lattice model for frustrated, easy-plane, spin $S = 1/2$ quantum antiferromagnets. The model contains states with Néel and bond-centered charge order and fractionalization in different limiting regimes, and we describe how these orders compete at intermediate coupling. The complex Berry phase terms render this model unsuitable for direct simulation; however, a duality mapping leads to a model of interacting current loops with positive weights, which is then studied by Monte Carlo simulations.

Understanding the zero temperature phase diagram of frustrated, spin $S = 1/2$, quantum antiferromagnets in two dimensions [1] is one of the central problems in the theory of correlated electron systems. Such an understanding is expected to prove valuable in a description of the cuprate superconductors. Moreover, a number of frustrated two-dimensional antiferromagnets with a non-magnetic ground state have been discovered[2, 3]: these could possibly be doped with charge carriers in the future, leading to exciting possibilities for new physics.

Some understanding of the different classes of possible ground states of insulating antiferromagnets has emerged in recent years. States can be classified by their possession of one or more distinct types of 'order'[4]: magnetic order involving breaking of spin-rotation invariance (as in a Néel state), bond order arising from a spontaneous modulation in the magnitude of the exchange energy which breaks lattice symmetries (as in spin-Peierls or 'plaquette' states), or 'fractionalization' leading to excitations characteristic of the deconfined phase of a Z_2 gauge theory [4, 5, 6, 7, 8, 9]. However, general principles which place constraints on the possible co-existence of such orders, on phases which can be separated by a continuous quantum phase transition, and on the topology of the phase diagram have so far not been delineated. Some issues along these lines have been addressed in recent studies[10, 11], where the problems have typically been related to strongly-coupled field theories whose properties are not reliably understood.

It is clear that large scale numerical studies will be required to address these subtle questions, but these have not been possible so far, because Monte Carlo simulations are impeded by the complex weights of the quantum spins. Exact diagonalization and series expansion studies yield only limited information which cannot easily describe the vicinity of phase boundaries. One strategy to overcome these obstacles is to abandon study of the quantum spin model itself, and to focus instead on effective lattice models which can more easily explore the different limiting regimes of the phase diagram[12]. We will follow such an approach here. We will consider only quantum antiferromagnets with an easy-plane plane U(1)

symmetry, as that makes them amenable to duality mappings: the dual representation of our lattice model has only positive weights, allowing Monte Carlo exploration of the phase diagram on reasonably large lattices. This will allow us to present the first results on the phase diagram of a model containing states whose orders extend over all those noted above.

We will study an effective lattice model defined on a 3-dimensional cubic lattice of sites, j, representing a discretized spacetime with the three directions x, y, τ, the last being imaginary time. Each site has an angular degree of freedom, θ_j, with $(-1)^{j_x + j_y} e^{i\theta_j} \sim \hat{S}_{+j}$, the $S = 1/2$ spin raising operator on site j; the prefactor of $e^{i\theta_j}$ is the sublattice staggering associated with the easy-plane Néel ordering. In addition, there is a Z_2 gauge field, $s_{j,j+\hat{\mu}} = \pm 1$ residing on the links of the cubic lattice, where $\mu = x, y, \tau$; this is an auxilliary field which arises in a number of distinct derivations of the effective model from the underlying quantum spin model[4, 6, 10, 13], and including it allows for an especially simply description of phases with fractionalization. The partition function controlling these degrees of freedom is

$$\mathcal{Z} = \sum_{\{s_{j,j+\hat{\mu}}=\pm 1\}} \int \prod_j d\theta_j \exp\left(K \sum_\square \prod_\square s_{j,j+\hat{\mu}} \right.$$
$$\left. + \frac{4}{g} \sum_{j,\hat{\mu}} s_{j,j+\hat{\mu}} \cos\left(\frac{\Delta_\mu \theta_j}{2}\right) - i\frac{\pi}{2} \sum_j (1 - s_{j,j+\hat{\tau}}) \right), \quad (1)$$

where Δ_μ is a discrete lattice derivative ($\Delta_\mu f_j \equiv f_{j+\hat{\mu}} - f_j$ for any f_j), and $\square$ indicates all the elementary square plaquettes of the cubic lattice. A fundamental property of $\mathcal{Z}$ is its invariance under the Z_2 gauge transformation $s_{j,j+\hat{\mu}} \to \eta_j s_{j,j+\hat{\mu}} \eta_{j+\hat{\mu}}$, $\theta_j \to \theta_j + \pi(1 - \eta_j)$, where $\eta_j = \pm 1$ is an arbitrary field (we assume periodic boundary conditions along the τ direction). The model is characterized by two dimensionless coupling constants, g, and K, and we will explore its phase diagram in the g, K plane. The coupling g controls the propensity to Néel order in the easy-plane, with the small g region having magnetic order with $\langle e^{i\theta_j} \rangle \neq 0$. The value of K is controlled most easily by ring-exchange terms in the underlying quantum spin system[13, 14, 15]. At $K = 0$, we

can independently sum over $s_{j,j+\hat\mu}$ on each link, leading to weights dependent only on $\cos(\Delta_\mu\theta_j)$, which describes bosonic, $S_z = 1$ quanta of $e^{i\theta_j}$ hopping in spacetime; conversely at large K (strong ring exchange), the Z_2 flux of the gauge field $s_{j,j+\hat\mu}$ is suppressed, and the $1/g$ term in (1) describes the propagation of $S_z = 1/2$ quanta, $e^{i\theta_j/2}$ ('spinons'), allowing the possibility of fractionalized phases. The last term in (1) is the crucial remnant of the Berry phases of the $S = 1/2$ spins of the quantum antiferromagnet: it imposes quantization of half-integral spin on each lattice site. Notice that this term can make the weights in (1) negative: this is the central reason for the novelty and difficulty of the theory of two-dimensional quantum antiferromagnets. The theory $\mathcal{Z}$ was proposed as an effective model for $S = 1/2$ quantum antiferromagnets in Ref. 13; it was also obtained[10] by taking the easy-plane limit of the effective lattice models of quantum antiferromagnets with SU(2) symmetry proposed some time ago [12]. Upon identifying the spin raising operator with a hard-core boson $\hat{S}_{+j} \sim b_j^\dagger$, we can also consider $\mathcal{Z}$ as a model of a boson system with off-site interactions and plaquette exchange terms, at a mean density per site which is half-integral[16].

Sedgewick et al.[17] have recently studied the properties of $\mathcal{Z}$ but without the Berry phase term: their physical motivation was slightly different (the $e^{i\theta_j}$ represented Cooper pair quanta in a superconductor), for which this neglect could be justified under suitable conditions. For our purposes of using $\mathcal{Z}$ as a model of quantum antiferromagnets, it is essential to include the Berry phase, and a description of its consequences is one of the purposes of this paper. However, because of the non-positive-definite weights, we cannot perform a direct Monte Carlo sampling over θ_j and $s_{j,j+\hat\mu}$ configurations, which was the method used by Sedgewick et al.[17]. Instead, we will now present a dual representation of $\mathcal{Z}$ which does have positive-definite weights.

The duality mapping[10] proceeds by first replacing each cosine term in $\mathcal{Z}$ by a periodic Gaussian:

$$W(\theta) = \sum_{\{m_{j\mu}\}}{}' \exp\left(-\frac{1}{2g}\sum_{j,\hat\mu}(\Delta_\mu\theta_j - 2\pi m_{j\mu})^2\right), \quad (2)$$

where the $m_{j\mu}$ are integers on the links of the direct lattice, and the prime indicates the constraint $m_{j,\mu}$ is even (odd) for $s_{j,j+\hat\mu} = +1(-1)$. In this form $\mathcal{Z}$ can be subjected to a series of mappings which are described in Ref. 10: these are standard in the theory of duality of models with Z_2 and U(1) symmetry and will not be reproduced here. The end result is the partition function

$$\mathcal{Z}_d = \sum_{\{\ell_{\bar{j}\mu}\}} \exp\left(K_d\sum_{\bar{j}}\varepsilon_{\bar{j},\bar{j}+\hat\mu}\sigma_{\bar{j},\bar{j}+\hat\mu} - \frac{g}{8}\sum_{\square}(\epsilon_{\mu\nu\lambda}\Delta_\nu\ell_{\bar{j}\lambda})^2\right)$$
$$(3)$$

in which θ_j and $s_{j,j+\mu}$ have been integrated out, and

the degrees of freedom are integers $\ell_{\bar{j}\mu}$ on the sites, $\bar{j}$, of the dual cubic lattice; $\tanh K_d \equiv e^{-2K}$ is the coupling dual to K, the second sum on $\square$ is over plaquettes on the dual lattice, and $\epsilon_{\mu\nu\lambda}$ is the antisymmetric tensor. The fields $\varepsilon_{\bar{j},\bar{j}+\hat\mu}$, $\sigma_{\bar{j},\bar{j}+\hat\mu}$ are Ising variables on the links of the dual lattice: $\varepsilon_{\bar{j},\bar{j}+\hat\mu}$ takes a set of fixed values such that $\prod_\square \varepsilon_{\bar{j},\bar{j}+\hat\mu}$ is -1 on every spatial plaquette and +1 on all other plaquettes (these values are linked to the Berry phase in (1)), while $\sigma_{\bar{j},\bar{j}+\hat\mu}$ measures the parity of $\ell_{\bar{j}\mu}$:

$$\sigma_{\bar{j},\bar{j}+\hat\mu} \equiv 1 - 2(\ell_{\bar{j}\mu} \bmod 2). \quad (4)$$

The physical meaning of the fields in (3) becomes clear upon relating them to observable properties of the antiferromagnet. The quantity $(1/2)\epsilon_{\mu\nu\lambda}\Delta_\nu\ell_{\bar{j}\lambda}$ is associated with links of the direct lattice, and is the conserved 3-current of the spin-flip bosons $b_j^\dagger$ introduced earlier: notice that this current can take half-integral values, representing the transfer of $S_z = 1/2$ spinons in a singlet background. Also, the $\mu = \tau$ component measures the boson density, or $\hat{S}_{zj}$. The first term in (3) lies on the links of the dual lattice, each of which can be associated with a plaquette of the direct lattice; for $\mu = x, y$, each such plaquette is associated with a single bond of the antiferromagnet. In this manner we conclude that $\varepsilon_{\bar{j},\bar{j}+\hat\mu}\sigma_{\bar{j},\bar{j}+\hat\mu}$ for $\mu = x, y$ is a measure of the exchange energy of the antiferromagnet on corresponding bonds in the y, x directions.

We begin our study of $\mathcal{Z}_d$ by considering various limiting regimes where it reduces to models studied earlier. (i) $\underline{K_d = \infty\ (K = 0)}$: In this case $\sigma_{\bar{j},\bar{j}+\hat\mu} = \varepsilon_{\bar{j},\bar{j}+\hat\mu}$ and (3) becomes exactly equivalent to a dual current loop model of the Hubbard model of the $b_j^\dagger$ bosons at half-integral filling considered by Otterlo et al. [18]. This also in keeping with the our earlier discussion that this limit of (1) describes the facile motion of $e^{i\theta_j}$ quanta. From the earlier work [18] we know that the boson ground state is superfluid (i.e. the spin system has easy-plane Néel order) for all g in such a model with only on-site interactions. (ii) $\underline{K_d = 0\ (K = \infty)}$: The term involving $\sigma_{\bar{j},\bar{j}+\hat\mu}$ disappears, and (3) becomes a model of half-boson current loops with on-site interactions. This is dual [18] to the quantum XY model of half-angles, $\theta_j/2$, obtained in (1) in this limit. This model has a superfluid phase at small g, and a fractionalized phase with freely propagating and gapped $S_z = 1/2$ spinons at large g. (iii) $\underline{g = 0}$: Both (1) and (3) become trivial, and the ground state has superfluid (easy-plane Néel order). (iv) $\underline{g = \infty}$: The action (1) is that of a pure Z_2 gauge theory with a Berry phase term. In (3), this limit implies that $\sigma_{\bar{j},\bar{j}+\hat\mu} = \varsigma_{\bar{j}}\varsigma_{\bar{j}+\hat\mu}$ with $\varsigma_j = \pm 1$ an Ising spin on the sites of the dual lattice; then (3) becomes an 2+1 dimensional Ising model with every spatial plaquette frustrated, introduced in Ref. 6 as a model for the non-magnetic states of frustrated quantum antiferromagnets. The ς_j quanta are the 'visons' of Ref. 4. This model has a fractionalized phase at small K_d
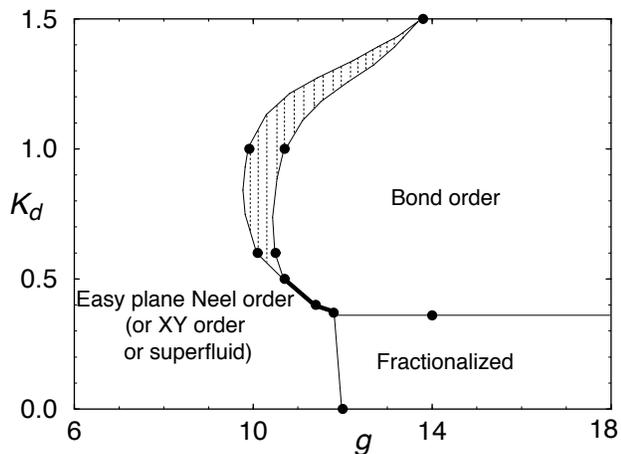
FIG. 1: Monte Carlo results for the phase diagram of $\mathcal{Z}_d$ as function of g and K_d. Thin lines represent second order transitions, while the thick line appears to be first order. We present evidence below that the hatched region has co-existing Néel and bond order. As $K_d \to \infty$, the region with superfluid order broadens and eventually extends to all g at $K_d = \infty$.

(visons gapped), and a confining, bond-ordered phase at large K_d (visons condensed).

Combining all the limiting cases above, and with information gained from Monte Carlo simulations on (3) to be described below, we obtain the phase diagram shown in Fig 1. The simulations were performed by the Metropolis algorithm on cubic systems of size $L \times L \times L$, with periodic boundary conditions.

Let us consider first the behavior as a function of K_d for large g. At $g = \infty$, as mentioned above, there is a second order transition[6] from a fractionalized phase at small K_d to bond-ordered phase at large K_d. Our simulations show that this transition persists into the region with g large but finite. As before[6], we define a complex bond-order parameter $\Psi_B = \sum_{\bar{j}} [(-1)^{\bar{j}_x} \varepsilon_{\bar{j},\bar{j}+\hat{x}} \sigma_{\bar{j},\bar{j}+\hat{x}} + i(-1)^{\bar{j}_y} \varepsilon_{\bar{j},\bar{j}+\hat{y}} \sigma_{\bar{j},\bar{j}+\hat{y}}]$; this order parameter is non-zero for both columnar and plaquette orderings of the bonds, which are distinguished[10] by distinct values of $\arg(\langle \Psi_B \rangle)$. We merely tested for non-zero values $\langle \Psi_B \rangle$ and did not perform the more subtle tests required to determine $\arg(\langle \Psi_B \rangle)$; this we did by computing the Binder cummulant $r_B = \langle |\Psi_B|^4 \rangle / \langle |\Psi_B|^2 \rangle^2$. The results are shown in Fig 2, and lead to the roughly horizontal phase boundary between the bond-ordered and fractionalized phases in Fig 1.

Next we looked at the boundary between the Néel and bond-ordered phases as a function of g for different values of K_d. The simplest mean-field theory of $\mathcal{Z}_d$ predicted[10] that this should be a direct second-order transitions. Typical sets of our numerical results are shown in Figs 3 and 4. Apart from r_B, we measured two additional physical quantities. The quantity C_V is the root-mean-square fluctuation in the action per unit
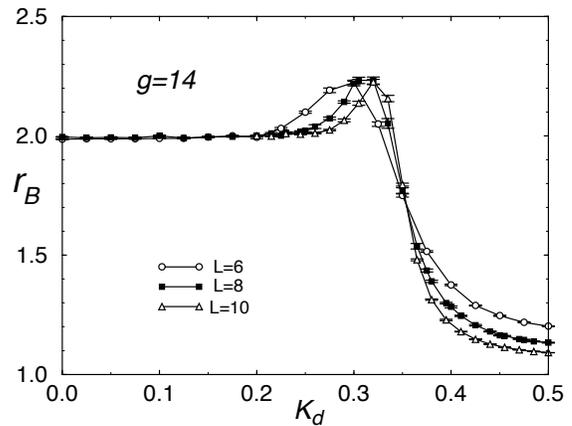

FIG. 2: Monte Carlo results for the Binder cumulant, r_B, of the bond order parameter Ψ_B at $g = 14$. The results indicate a second order transition from a phase with $\langle \Psi_B \rangle = 0$ at small K_d (where the value of r_B is that associated with a Gaussian random field Ψ_B with zero mean), to a phase with $\langle \Psi_B \rangle \neq 0$ at larger K_d (where $r_B = 1$, the value expected by Ψ_B condenses). The crossing points indicate that this transition occurs at $K_d \approx 0.35$.
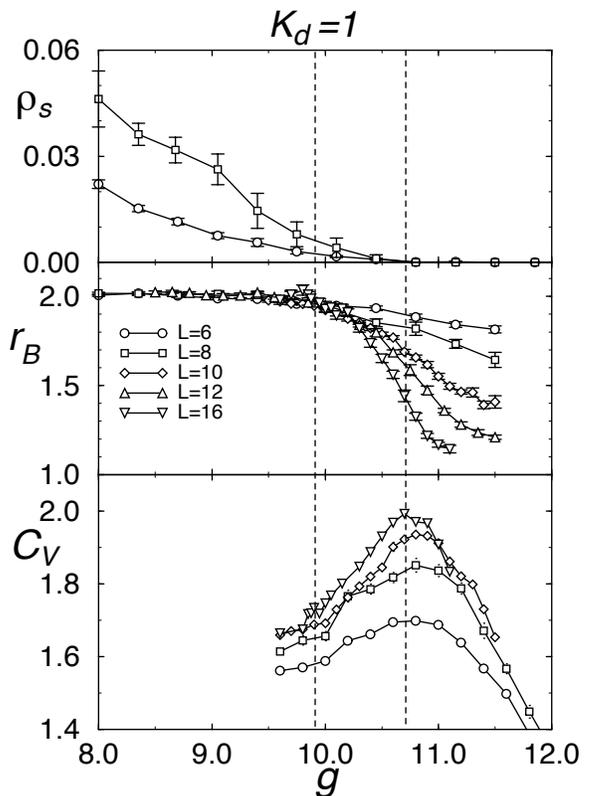

FIG. 3: Monte Carlo results for $K_d = 1.0$ as a function of g. The dashed lines indicate positions of proposed phase transitions. Notice that there is a small peak in C_V for the largest system sizes at the transition at the smaller value of g. Data for ρ_s are not available for the largest system sizes because of long equilibration times in the winding number sector.
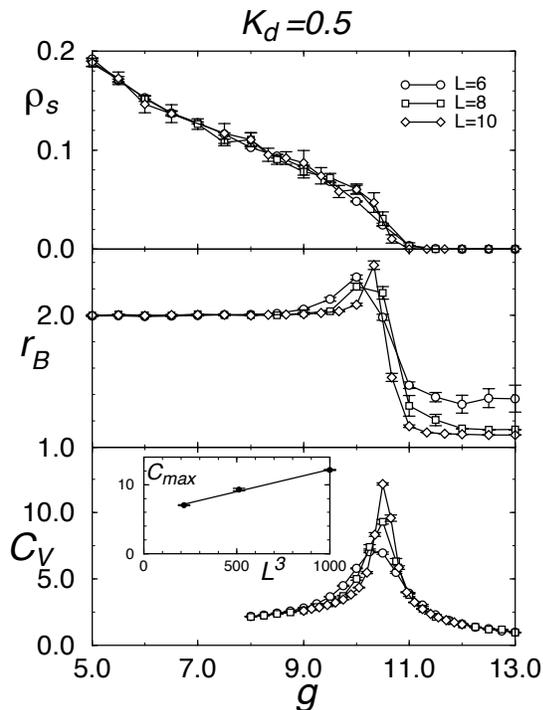
FIG. 4: As in Fig 3 but for $K_d = 0.5$. The inset shows the system volume dependence of maximum value of C_V at the peak as a function of g. The proportionality is suggestive of a first order transition. Notice that the L dependence of the peak in C_V is much stronger than that in Fig 3.

volume: if we interpret $\mathcal{Z}_d$ in (3) as a classical statistical mechanical model in 3 dimensions, then C_V would be its specific heat (note, however, that C_V is not the specific heat of the quantum antiferromagnet). It is an unbiased measure of the location of phase transitions and of their order. In addition we measured the stiffness, ρ_s of the Néel (or superfluid) order: this was done, as in Ref. 18, by generalizing the current loop model to its non-zero 'winding number' sector, and measuring the fluctuations in winding number.

The weight of the evidence in Fig 3 for $K_d = 1.0$ favors two second order transitions as a function of g, which are denoted by the dashed lines. At small g we are clearly in the superfluid phase with a non-zero ρ_s, and no bond order. Conversely at large g, bond order is present, but there is no superfluidity as ρ_s is vanishingly small. However the onset of superfluid order (as measured by ρ_s) clearly occurs at a point distinct from the onset of bond order (as measured by r_B): there is an intermediate range where superfluid and bond order are both present. This is also supported by the measurements of C_V, which show peaks at both transitions.

The nature of the data in Fig 4 at $K_d = 0.5$ is quite distinct. Now the crossovers in ρ_s and r_B happen at roughly the same value of g. Moreover there is only a single peak in the specific heat, whose maximum value is

proportional to the system volume: this latter observation suggests a first-order transition.

This paper has described the phase diagram of a 2+1 dimensional XY model coupled to a Z_2 gauge field with a Berry phase term. We reviewed arguments [4, 10, 12, 13, 15] asserting that this is an effective model for frustrated, easy-plane, $S = 1/2$, two-dimensional quantum antiferromagnets. We believe this is the first study of quantum phase transitions in the presence of Berry phase terms (which completely accounts for fluctuations of gauge fields), and which allows for the various orders that may be present in the ground state: magnetic, bond, and fractionalization. We found that fluctuations induced an intermediate regime with co-existence of magnetic and bond orders in our U(1) symmetric model; a similar co-existence has also been argued recently for frustrated $S = 1/2$ models with SU(2) symmetry [10, 19].

[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] H. Kageyama *et al.*, Phys. Rev. Lett. **82**, 3168 (1999).
[3] R. Coldea, D. A. Tennant, A. M. Tsvelik, and Z. Tylczynski, Phys. Rev. Lett. **86**, 1335 (2001); R. Coldea *et al.*, cond-mat/0111079.
[4] T. Senthil and M. P. A. Fisher, Phys. Rev. B **62**, 7850 (2000).
[5] N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991).
[6] R. Jalabert and S. Sachdev, Phys. Rev. B **44**, 686 (1991).
[7] X.-G. Wen, Phys. Rev. B **44**, 2664 (1991).
[8] C. Mudry and E. Fradkin, Phys. Rev. B **49**, 5200 (1994).
[9] R. Moessner, S. L. Sondhi, and E. Fradkin, cond-mat/0103396.
[10] S. Sachdev and K. Park, cond-mat/0108214.
[11] C. Lannert, M. P. A. Fisher, and T. Senthil, Phys. Rev. B **63**, 134510 (2001).
[12] S. Sachdev and R. Jalabert, Mod. Phys. Lett. B **4**, 1043 (1990).
[13] E. Demler, C. Nayak, H.-Y. Kee, Y. B. Kim, and T. Senthil, cond-mat/0105446.
[14] L. Balents, M. P. A. Fisher, and S. M. Girvin, cond-mat/0110005.
[15] Using (2), we can also write $\mathcal{Z}$ as [10] $\mathcal{Z} = \int \prod_j d\theta_j W(\theta) e^{-S_B - E_v(n_{\bar{j}\mu})}$ where S_B contains the Berry phases of the underlying spins, the sum over $m_{j\mu}$ is unconstrained (unlike in (2)), $n_{\bar{j}\mu} = \epsilon_{\mu\nu\lambda}\Delta_\nu m_{j\lambda}$ is the current of the vortices in the b_j bosons, and E_v depends only on n_v(mod 2), with E_v(even) $- E_v$(odd) $= -2K$. So K lowers the core energy of *double* vortices, as discussed in [14].
[16] F. Hebert, G. G. Batrouni, R. T. Scalettar, G. Schmid, M. Troyer, and A. Dorneich, cond-mat/0105450.
[17] R. D. Sedgewick, D. J. Scalapino, and R. L. Sugar, cond-mat/0012028.
[18] A. van Otterlo, K.-H. Wagenblast, R. Baltin, C. Bruder, R. Fazio, and G. Schön, Phys. Rev. B **52**, 16176 (1995).
[19] O. P. Sushkov, J. Oitmaa, and Zheng Weihong, Phys. Rev. B **63**, 104420 (2001).