The transition from an ordered antiferromagnet to a quantum disordered spin liquid in a solvable bilayer model

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We present a spin-1/2 bilayer model for the quantum order-disorder transition which (i) can be solved by mean-field theory for bulk quantities, (ii) becomes critical at the transition, and (iii) allows to include intralayer frustration. We present numerical data (for systems with up to 240 sites) and analytical results for the critical coupling strength, ground-state energy, order parameter and for the gap. We show that the critical coupling decreases linearly with frustration.

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The model of two coupled antiferromagnetic layers, the ‘bilayer model’, has attracted much attention in the last years [1,2]. The physics of this model is dominated by the competition between the in-plane coupling $J_1$ and the inter-plane coupling $J_{12}$. A transition occurs from an ordered antiferromagnetic state to a spin-liquid state with a gap at a certain critical ratio $J_{12}/J_1$, Millis and Monien [3] proposed that certain anomalies in the magnetic response of $YBa_2Cu_3O_6+x$, interpreted commonly as evidence for a spin gap might be explained within the bilayer model.

Solvable model Hamiltonians play an important role in condensed matter theory, as they provide new insights and because they can be used as references for approximate theories. Here we propose a non-trivial ‘long-range’ bilayer model.

We define the ‘long-range’ bilayer Hamiltonian as

$$H_{LR} = \sum_{\gamma} H_1 + H_{12},$$

and $J_1, J_2, J_{12} > 0$. Here $S_{i,\gamma}$ are the spin-1/2 operators of the first ($\gamma = 1$) and of the second ($\gamma = 2$) layer respectively and $S_{A\gamma} = \sum_{i \in A} S_{i,\gamma}$, $S_{B\gamma} = \sum_{i \in B} S_{i,\gamma}$ are the total-spin operators of the A/B sublattice in the respective layers. Each sublattice contains $N$ spins, the total number of sites is $N_s = 4N$.

The first term of the intra-layer interaction ($J_1$), favours an anti-alignment of the sublattice spins, i.e. an antiferromagnetically ordered state. The second, frustrating, intra-layer interaction ($J_2$) favours minimal sublattice magnetisation and therefore tends to suppress the antiferromagnetic order. The local inter-plane coupling term $H_{12}$ favours the formation of local singlets. As a result, this model contains the relevant interactions to exhibit a quantum order-disorder transition as the relative strength of intra- and inter-layer interactions are varied. For small values of the interlayer coupling $J_{12}$ the ground-state is characterized by long-range antiferromagnetic order and gapless magnetic excitations. The spin-liquid state, realized for large $J_{12}$, is characterized by a finite spin gap and the absence of antiferromagnetic order.

The long-range bilayer Hamiltonian $H_{LR}$ has a close relation to its ‘short-range’ counter-part, $H_{SR} = \sum_{\gamma} H_{12}$, with

$$H_{12} = \sum_{\gamma}^2 \sum_{i,l} S_{i,\gamma} \cdot S_{i,l} + J_{12} \sum_{i,l} S_{i,\gamma} \cdot S_{l,\gamma} \quad (2)$$

where the symbols $< i, j >$ and $[i, l]$ denote pairs of n.n. and n.n.n sites on a square lattice respectively and where the terms $\sim J_{11}$ and $\sim J_{12}^\prime$ correspond to the term $\sim J_1$ and $\sim J_2$ in (1) respectively. In order to make connection between $H_{LR}$ and $H_{SR}$ we compare the energies of the respective couplings. In $H_{SR}$ the order-disorder transition occurs at $J_{12}/J_11 = 2.51$ [4]. We expect the true
critical interlayer coupling for $H_{LR}$ to be somewhat larger than the value $J_1/2J_s \approx 2.51/4 \approx 0.628$ suggested by this naive rescaling, since intra-plane quantum fluctuations are suppressed by the long-range nature of $J_1$.

**Results:** In the limit of decoupled layers $J_{12} = 0$ the expectation value of the energy per layer is

$$E_1 = \frac{J_1}{2N} S_1(S_1 + 1) + \frac{2J_2 - J_1}{2N} [S_{A1}(S_{A1} + 1) + S_{B1}(S_{B1} + 1)].$$

where $S_{A1}, S_{B1}$ are the eigenvalues of $S_{A1}, S_{B1}$ and of the total-spin operator $S_{A1} + S_{B1}$ respectively [10]. For $J_2 < J_1/2$ the ground state is a singlet with $S_1 = 0$ and maximal sublattice magnetization, $S_{A1} = S_{B1} = N/2$. In the thermodynamic limit the ground-state energy per site is then $(2J_2 - J_1)/8$. In the opposite limit $J_{12} = \infty$ the ground state is a product of interlayer singlet pairs with energy $-3/8J_2$ per site and a gap of order $J_{12}$ to the lowest excited state, a spin triplet.

**Variational Analysis:** In the presence of a finite interlayer coupling a natural ansatz for a variational wavefunction interpolates between the two extremal regimes:

$$\Psi(\alpha) = \prod_i^N (1 - \alpha[S_{i1}^2 + S_{i2}^2]) |AF>, \quad (3)$$

where $|AF>$ is the Néel state [4]. A straightforward minimization of the energy yields the critical coupling constant $J_c = J_1 - 2J_2$. The optimal value for the variational parameter is found to be $\alpha = 1$, for $J_{12} > J_c$, and to be $\alpha = J_c/J_{12} - \sqrt{(J_c/J_{12})^2 - 1}$ for $J_{12} < J_c$.

Of interest are the expectation values of the ground-state energy per site:

$$e_N = \langle H \rangle_0/(4N) + 3/8J_{12}, \quad (4)$$

where we have subtracted the energy of the product state realized for $J_{12} \rightarrow \infty$, and for the in-plane staggered order parameter,

$$o_N = \sqrt{\langle S_{A1} \cdot S_{B1} + S_{A2} \cdot S_{B2} \rangle}/(4N). \quad (5)$$

The variational ground-state energy per site [4] and the order parameter [1] are then computed to be

$$e_0 = -J_c \frac{1 - J_{12}/J_c}{8} \quad (6)$$

$$o_0 = \frac{1}{\sqrt{32}} \sqrt{1 - (J_{12}/J_c)^2} \quad (7)$$

for $J_{12} < J_c$. For $J_{12} > J_c$ both $e_0$ and $o_0$ are zero. For $J_{12} > J_c$ the ground state is a product of inter-layer spin singlets, for $J_{12} < J_c$ an ordered antiferromagnet.

The quality of a trial wavefunction $|\Psi>$ is measured by its variance,

$$\sigma = \frac{\langle (H - \langle H \rangle)^2 \rangle}{\langle \Psi | \Psi \rangle}$$

which is zero for an exact eigenstate of $H$. In general, variational wavefunctions which are not exact eigenstates lead to an extensive variance, $\sigma \sim O(N)$ [13]. For the wavefunction given by [4], however, we find an intensive variance, $\sigma(\alpha) \sim O(N^0)$, which indicates that the expressions for the variational ground-state energy $e_0$, Eq. [4] and order parameter, Eq. [1], are exact in the thermodynamic limit. However, since the energy is known only up intensive correction, the gap cannot be determined in this framework.

**Numerical Analysis:** The Hamiltonian [4] is separately invariant under any permutation within the A-sublattice and within the B-sublattice. The ground-state singlet and the lowest excited triplet state belong to the symmetric subspace of the permutation symmetry, as we found by diagonalizing small clusters with $N_s = 4 - 20$ spins within the full Hilbert space. We conjecture that the symmetry of the lowest singlet state and of the lowest triplet state does not change for $N_s > 20$. Within the symmetric representation the size of the Hilbert space grows only $\sim N_s^4$, i.e. algebraically. We have numerically diagonalized systems with up to $N_s = 4N = 240$ sites, using a specially adapted exact diagonalization technique [4]. The results for the ground-state energy per site, are presented in Fig. 2 for $J_{2}/J_1 = 0, 0.2$. The width of the transition from the ordered state at small $J_{12}/J_1$ to the quantum disordered spin liquid at large $J_{12}/J_1$ is attributable to finite size effects [4,10].

Using finite-size scaling we have estimated the critical exponents of the finite-size corrections to the data for the order parameter presented in Fig. 4. We found the finite-size corrections to scale like $N^{-1}, N^{-1/3}$ and $N^{-1/2}$ for $J_{12} < J_1$, $J_{12} > J_1$ and $J_{12} > J_1$ (with $J_2 = 0$) respectively. A similar behaviour has been found for the long range Ising model in a transversal field [10].

We have extrapolated the numerical data obtained from clusters with up to 240 sites to the thermodynamic limit via the formula $\lim_{N \rightarrow \infty} e_N = e_\infty + B/N + C/N^2 + \ldots$, where we have used the $1/N$ finite size scaling of the Lieb-Mattis antiferromagnet as the leading term [4,11]. The $1/N$ scaling for the finite-size corrections of the ground-state energy is also found in a least square fit to the numerical data presented in Fig. 1. For all parameter values considered, i.e for $J_{12}/J_1 = 0, 0.1, \ldots, 1.0$ and for $J_2/J_1 = 0, 0.125, \ldots, 0.5$, we found agreement to at least six digits between the such obtained $e_\infty$ and the analytical formula for $e_0$ [4]. This very good agreement between the numerical and analytical results gives us confidence that the gap, which is accessible only to numerical calculation can be determined with similar precision.

In Fig. 2 we present the numerical results of the gap, $\Delta_N$, for clusters with up to $N_s = 240$ sites and $J_2 = 0$ together with the mean-field prediction for the gap,

$$\Delta_{MF} = \frac{J_c + J_{12}}{2} \theta(J_c - J_{12}) + J_{12} \theta(J_{12} - J_c). \quad (9)$$

Due to the spin-rotational invariance of [4] the gap $\Delta_N$ differs non-trivially from the mean-field result. Note, that this is possible only because the variance [4] of the mean-field solution [3] is intensive and not zero. Fig. 2
also contains a conjecture for the gap in the thermodynamic limit,

$$\Delta_0 = J_{12} \sqrt{1 - J_c / J_{12}},$$

(10)

for $J_{12} > J_c = J_1 - 2J_2$. In the inset of Fig. 2 we have plotted $\log(\Delta_N - \Delta_o)$ versus $\log(1/N)$. We note that the data fall on a straight line with slope one for all $J_{12} > J_c$, suggesting that (11) is indeed the correct expression for the gap in the thermodynamic limit. At the critical point, $J_{12} = J_1 - 2J_2$, the finite-size corrections scale like $(1/N)^\nu$. We estimate numerically $\nu = 0.3$, a value which deviates from mean-field predictions and for which we do not have an explanation at present.

**Discussion:** In (3) we defined the order parameter $\sigma_N$ of the bilayer system. It is of interest to examine with $\sigma_N = \sqrt{\langle S_{A1} \cdot S_{B2} + S_{B1} \cdot S_{A2} \rangle} / (4N)$ the relative ordering of the two layers. An inspection of the variational wavefunction (3) shows that $\sigma_N$ and $\sigma_{\bar{N}}$ are directly proportional in the thermodynamic limit. A similar result has been found in a numerical study of the short range model [1]. The equivalence of $\sigma_N$ and $\sigma_{\bar{N}}$ implies that the magnetic order parameters of the two layers are aligned for any $0 < J_{12} < J_c$. This type of magnetic correlation has been found in neutron scattering experiments on YBaCuO system [7]. Physically we understand that any $J_{12} > 0$ lifts the degeneracy of the two intra-layer Néel states and correlates the two layers magnetically.

In the long range bilayer model the order-disorder transition is second order with mean-field exponents for ground-state properties [18]. The gap opens continuously on the disordered side, with an exponent for the finite-size correction which deviates from the predictions of mean-field theory. While the in-plane quantum fluctuations are too weak to influence bulk properties like the ground-state energy, they are important for the gap between the exact ground-state, which is an overall spin singlet, and the lowest excited triplet state. In the asymptotic limit $J_{12}/J_1 \to \infty$ the gap (11) is $J_{12}$ but for any $J_{12}/J_1 < \infty$ the gap is reduced by the in-plane quantum fluctuations and is strictly smaller than $J_{12}$.

Our rigorous result that the critical coupling strength depends linearly on the frustration is consistent with a recent effective-action mean-field approach 13 to the frustrated bilayer model 14. Furthermore this results does support, to some extent, the possible explanation of the observed spin-gap in the YBaCuO System, in view of the recent estimate of $J_{12}/J_1 \approx 0.55$ by infrared absorption 15, by a doping-frustrated bilayer system 16. Let us also note in this context that the linear reduction of the sublattice magnetization by the inter-layer coupling 17 is due to quantum fluctuations only and that the order-disorder transition found in $H_{LR}$ has no classical analogon. Eq. (6) represents therefore the first rigorous result for the reduction of a classical order parameter by quantum fluctuations in dimensions greater than one.

In summary we have presented a novel, solvable model for the quantum order-disorder transition. The quantity of interest, the spin gap, is critical at the transition while the bulk properties of this model can be determined analytically. The intra-layer quantum fluctuations are only intensive, which allows a complete characterization of the quantum order-disorder transition. The inter-layer quantum fluctuations remain extensive, introducing the criticality neccessary for the transition.

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1. A.W. Sandvik and D.J. Scalapino, Phys. Rev. Lett. 72, 2777 (1994).
2. T. Matsuda and K. Hida, J. Phys. Soc. Jpn. 59, 2223 (1990); K. Hida, J. Phys. Soc. Jpn. 61, 1013 (1992).
3. N. Elstner, G.L. Glenister, R.R.P. Singh and A. Sokol, Phys. Rev. B 51, 8984 (1995).
4. A.J. Millis and H. Monien, Phys. Rev. Lett. 70, 2810 (1993); for a recent discussion see B.L. Altshuler, L.B. Ioffe and A.J. Millis, sissa preprint.
5. A Schwinger boson calculation finds a quadratic dependence of the critical coupling, H. Monien, private communication.
6. Note, that it has been suggested that a substantial effective frustration could be induced by doping, see M. Inui, S. Doniach and M. Gabay, Phys. Rev. B 38, 6631 (1988).
7. Grüninger et al., Sissa preprint # 9501065.
8. F. Barriquand and G. A. Sawatzky, Phys. Rev. B 50, 16649 (1994).
9. Note, however, that a recent analysis of NMR experiments by A.J. Millis and H.Monien, Sissa preprint # cond-mat/9506088 finds a small ratio of $J_{12}/J_1$.
10. E. Lieb and D.C. Mattis, J. Math. Phys. 3, 749 (1962).
11. J. Richter, Phys. Rev. B 47, 5794 (1993); J. Richter, S.E. Krüger, A. Voigt and C. Gros, Europhys. Lett. 28, 363 (1994).
12. Let $i \in A$ and $j \in B$. The Néel state is then defined by $S_{i,1}^z |AF >= +1/2 |AF >$ and $S_{i,2}^z |AF >= -1/2 |AF >$ for the first layer and by $S_{i,3}^z |AF >= -1/2 |AF >$ and $S_{j,2}^z |AF >= +1/2 |AF >$ for the second layer.
13. C. Gros, Phys. Rev. B 42, 6835 (1990).
14. W. Wenzel and K.G. Wilson, Phys. Rev. Lett. 69, 800 (1992).
15. C. Kittel and H. Shore, Phys. Rev. 138, A 1165 (1965).
16. R. Botet, R. Jullien and P. Pfeuty, Phys. Rev. Lett. 49, 478 (1982).
17. J.Rossat-Mignod et al., Physica 180-181, 383 (1992); J.M. Tranquada et al., Phys. Rev. B 46, 5561 (1992); H.A. Mook et al., Phys. Rev. Lett. 70, 3490 (1993); R. Stern et al., Phys. Rev. B 50, 426 (1994).
18. We find a close correspondence between these results and the appropriately scaled results, which A.V. Chubukov
and D.K. Morr, (ssisa preprint) obtained for an interacting Bose-gas approach to $H_{SR}$.

[19] A.V. Dotsenko, sissa preprint.

FIG. 1. For $N = 10, 20, 30, 40, 50, 60$ and a) $J_2/J_1 = 0$ and b) $J_2/J_1 = 0.2$ the numerical results for the order parameter (open squares, smallest $N$ at the top) and for the ground-state energy per site (open circles, smallest $N$ at the bottom). The dashed lines are the analytic expressions corresponding to Eq. (6) and Eq. (7).

FIG. 2. For $N = 10, 20, 30, 40, 50, 60$ and $J_2/J_1 = 0$ the numerical results for the gap $\Delta N$ (open circles, smallest $N$ at the top). The dashed line is the analytic expression corresponding to Eq. (10), the dotted line is the mean-field prediction, Eq. (9). Insert: A log-log of the data for $J_{12}/J_1 = 1.0, 1.2, 1.6, 2.0$. 