Valence Bond Entanglement Entropy

Fabien Alet,[1,*] Sylvain Capponi,[1] Nicolas Laflorencie,[2,1] and Matthieu Mambrini[1]
[1]*Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, CNRS, 31062 Toulouse, France*
[2]*Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*

(Received 16 March 2007; published 12 September 2007)

We introduce for SU(2) quantum spin systems the valence bond entanglement entropy as a counting of valence bond spin singlets shared by two subsystems. For a large class of antiferromagnetic systems, it can be calculated in all dimensions with quantum Monte Carlo simulations in the valence bond basis. We show numerically that this quantity displays all features of the von Neumann entanglement entropy for several one-dimensional systems. For two-dimensional Heisenberg models, we find a strict area law for a valence bond solid state and multiplicative logarithmic corrections for the Néel phase.

DOI: 10.1103/PhysRevLett.99.117204 PACS numbers: 75.10.Jm, 03.67.Mn, 05.30.−d

Entanglement is probably the most prominent feature that allows us to distinguish quantum from classical systems. While being an inherent ingredient of quantum information processing, the study of entanglement properties of quantum many-body states has recently shed new light on our understanding of condensed matter systems at zero temperature [1]. Over the past few years, various measures of entanglement have been used to investigate quantum phase transitions and states of matter [1–4]. Among them, the von Neumann entanglement entropy (EE) quantifies the bipartite entanglement between two parts of a quantum system [5]. The EE of a quantum state $|\Psi\rangle$ between a part Ω and the rest of a system is

$$S_\Omega = -\mathrm{Tr}\rho_\Omega \ln\rho_\Omega,$$

where $\rho_\Omega = \mathrm{Tr}_{\bar\Omega}|\Psi\rangle\langle\Psi|$ is the reduced density matrix of Ω obtained by tracing out the rest of the system $\bar\Omega$. An important property of EE is that $S_\Omega = S_{\bar\Omega}$, and it appears naturally that S_Ω is only related to the common property of Ω and $\bar\Omega$, their boundary: general arguments indeed indicate that S_Ω typically scales with the size of the boundary (area law) [6]. For critical systems, however, logarithmic corrections can be present. If the critical system is conformal invariant, the amplitude of the logarithmic corrections is related to the central charge of the corresponding conformal field theory (CFT). This has been shown in one dimension (1D) [3,7] and more recently for some CFT in two dimensions (2D) [8], in which case the coefficient also depends on the geometry of Ω. For systems possessing topological order, other subleading corrections also depend on the topology of Ω [9]. The scaling of the EE with the size of Ω therefore contains precious information on the state of the physical system and can be used, e.g., to detect criticality. This has been successfully demonstrated in quantum spin systems [2–4,7,10,11], which are natural candidates for such studies as they are both of theoretical and experimental relevance in condensed matter.

While many interesting properties of EE have been derived exactly for integrable models or systems with exactly known ground states (GS), the calculation of EE for general interacting quantum systems is an exacting task. On the practical side, even numerical simulations are difficult. Exact diagonalization, limited to small systems, cannot precisely verify scaling properties and EE is not accessible to quantum Monte Carlo (QMC) methods. In 1D, EE can be calculated within the Density Matrix Renormalization Group method [12] but this technique is no longer available in higher dimensions. In this Letter, we introduce another measure of entanglement, called valence bond entanglement entropy (denoted hereafter S^{VB}), which is defined for quantum spin systems with SU(2) symmetry. It can be measured efficiently in all dimensions for nonfrustrated antiferromagnetic (AF) spin systems via QMC simulations in the valence bond (VB) basis [13]. We show that S^{VB}, albeit different, captures all features of the von Neumann EE. In particular, it obeys the same scaling properties: for 1D quantum spin systems, we recover CFT predictions. We also investigate the properties of S^{VB} for a 2D Heisenberg model possessing Néel and valence bond solid phases. Our numerical results show that S^{VB} obeys an area law for both phases, with the presence of logarithmic corrections for the Néel phase.

We focus on the AF spin-1/2 Heisenberg Hamiltonian

$$H = \sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j,$$

which conserves the total spin S_T of the system. AF interactions $J_{ij} > 0$ favor a singlet $S_T = 0$ ground state.

Definition.—It is well known that any singlet state can be expressed in the VB basis, where spins couple pairwise in singlets $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. The VB basis is overcomplete (there are more VB coverings than the total number of singlets). Another basis is the *bipartite* VB basis [14], where the system is decomposed into two sets (for instance different sublattices for a bipartite lattice) such that two spins forming a singlet necessarily belong to different sets. This basis is smaller, but still overcomplete. In a given bipartition of sites and bipartite VB state $|\Psi\rangle$ such as the

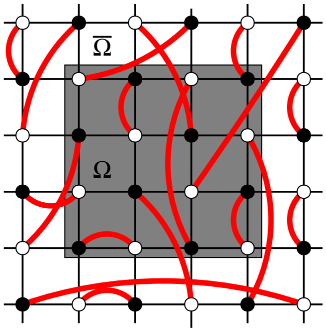

FIG. 1 (color online). A bipartite valence bond state. The valence bond entanglement entropy of the area Ω (shaded square) is equal to the number of singlets shared between Ω and the rest of the system $\bar{\Omega}$ (here 8), times ln(2).

ones in Fig. 1, consider a subsystem Ω (shaded area in the figure). We define the valence bond entanglement entropy of this state as

$$S^{\rm VB}_{\Omega}(|\Psi\rangle) = \ln(2).n^{c}_{\Omega}(|\Psi\rangle),$$

where $n^{c}_{\Omega}(|\Psi\rangle)$ is the number of singlets that cross the boundary of Ω (i.e., singlets with one and only one constituting spin within Ω). The constant ln(2) is used to match the EE for a unique singlet. In general, the GS of the Hamiltonian H is not a single VB state. For a linear combination $|\Phi\rangle = \sum_i a_i|\Psi_i\rangle$ with $|\Psi_i\rangle$ bipartite VB states, we define $S^{\rm VB}_{\Omega}(|\Phi\rangle) = \sum_i a_i S^{\rm VB}_{\Omega}(|\Psi_i\rangle)/\sum_i a_i$. An estimate of $S^{\rm VB}$ for the GS of H can then be obtained by using the projector QMC method recently proposed by Sandvik [13], which precisely works in a bipartite VB basis (as soon as H is not frustrated). In this method, the GS is sampled by applying H^n stochastically (with n sufficiently large) to an initial VB state $|\Psi_0\rangle$ in order to obtain a projected state $|\Psi_n\rangle$. In this process, $|\Psi_n\rangle$ appears a number of times proportional to its coefficient in the GS wave function. The GS estimate of $S^{\rm VB}$ is obtained by Monte Carlo averaging $S^{\rm VB}(|\Psi_n\rangle)$ over the projected states obtained in all Monte Carlo steps.

Bipartite basis and overcompleteness.—At first glance, $S^{\rm VB}$ seems ill defined as the bipartite VB basis is overcomplete. $|\Phi\rangle$ can indeed be rewritten as a linear combination of other states for which $S^{\rm VB}$ could be different. However, $S^{\rm VB}$ turns out to be *conserved* in any linear combination between the bipartite VB states. Via an algebraic representation of the singlet wave function, it can be indeed shown that for any linear relation $\sum_i c_i|\Psi_i\rangle = 0$ between the bipartite VB states $|\Psi_i\rangle$, we have $\sum_i c_i S^{\rm VB}_{\Omega}(|\Psi_i\rangle) = 0$ for all Ω [15]. Another issue is the choice of the bipartite basis: in the general case, $S^{\rm VB}$ *does* depend on the precise choice of bipartition. However, if $|\Phi\rangle$ satisfies a Marshall sign criterion [16], a genuine bipartition where all $a_i > 0$ exists and should be taken. Not all singlet states satisfy this, but this is the case for, e.g., the GS of H on bipartite lattices [16]. In practice, the QMC method is efficient only for bipartite H (when all $a_i > 0$) and the Marshall condition is not a restriction. This implies that $S^{\rm VB}$ is a well-defined quantity for any singlet wave function satisfying the Marshall criterion and that it can easily be measured (e.g., graphically as in Fig. 1) for any bipartite VB state.

Entanglement properties.—$S^{\rm VB}$ is in general different from EE (this can be seen by computing exactly both quantities on a small system). However, $S^{\rm VB}$ share many properties with EE: (i) $S^{\rm VB}$ is a subadditive quantity: $S^{\rm VB}_{\Omega_1\cup\Omega_2} \leq S^{\rm VB}_{\Omega_1} + S^{\rm VB}_{\Omega_2}$, (ii) $S^{\rm VB}_{\Omega} = S^{\rm VB}_{\bar{\Omega}}$ as any singlet crossing the boundary belongs to both subsystems, (iii) $S^{\rm VB}_{\Omega} = S_{\Omega}$ if Ω contains a single site, (iv) $S^{\rm VB}_{\Omega} = S_{\Omega}$ for all Ω when the GS is a single VB state: this is the case in the thermodynamic limit for the Majumdar-Ghosh spin chain [17] or for the Random Singlet phase [18] of disordered spin chains where one VB state essentially dominates [4]. Finally, we note that $S^{\rm VB}$ offers a simple geometrical interpretation of entanglement properties of a quantum spin state: Ω is entangled with the rest of the system $\bar{\Omega}$ iff there are singlets in between these two parts.

In the rest of this Letter, we will show that $S^{\rm VB}$ captures both qualitative and quantitative features of the EE. $S^{\rm VB}$ can be calculated for all systems that can be simulated with the VB QMC method, in particular, all spin-1/2 AF Heisenberg-like models on bipartite lattices in all dimensions, including models with multiple-spin interactions [19]. We first start with 1D models, where all the characteristics of the EE are recovered with high precision. We then present results on entanglement properties of 2D AF Heisenberg models.

1D systems.—We first consider 1D uniform AF Heisenberg chains where the GS is known to be critical, with algebraic decay of spin correlations. For systems of finite size L with periodic boundary conditions (PBC), CFT predicts that the EE of a block of spins of size x scales (for large x) as $S(x) = c/3\ln(x') + S_0$, where $x' = L/\pi \sin(\pi x/L)$ is the conformal distance, the central charge $c = 1$, and S_0 is a nonuniversal constant [3]. Figure 2(a) displays $S^{\rm VB}(x')$ for a 1D uniform chain of size $L = 128$ and the resulting curve is well fitted by the form $S^{\rm VB}(x') = c_{\rm eff}/3\ln(x') + S_0$ with $c_{\rm eff} = 1$, in full agreement with CFT predictions for EE.

Now we turn to uniform AF Heisenberg chains with open boundary conditions (OBC). For a segment of size x starting at the open boundary, the CFT prediction for EE is $S(x) = c/6\ln(x') + S_1$ with $c = 1$ and S_1 another constant related to S_0 [3]. Our results [see Fig. 2(b)] for $S^{\rm VB}(x)$ for an $L = 128$ open chain also clearly follow this scaling form. We also recover the alternating term found for the EE of open Heisenberg chains [11], as can be seen from the two distinct odd-even sets of points in Fig. 2(b).

We next consider an alternating Heisenberg spin chain, where the coupling is $1 + \delta$ (respectively, $1 - \delta$) for all

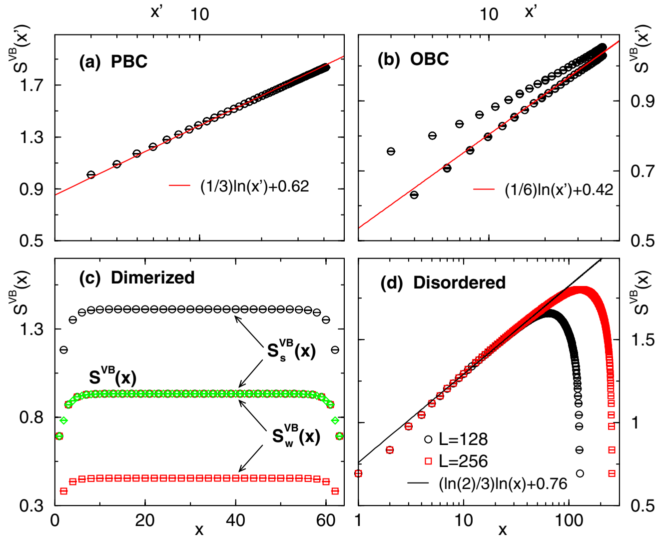

FIG. 2 (color online). S^{VB} versus distance for 1D AF Heisenberg quantum spin systems: (a) chain with PBC, (b) chain with OBC, (c) alternating chain ($\delta = 1/3$) with PBC, (d) random AF chain with PBC. In (a), (b), and (d), scale is log-linear. For (a) and (b), $x' = L/\pi \sin(\pi x/L)$ is the conformal distance. Solid lines are scaling forms for EE predicted by CFT [(a) and (b)] and RSRG [(d)]. Simulation parameters are the following: (a) $n = 70L$, (b) $n = 60L$, (c) $n = 30L$, (d) $n = 10L$ and 500 disorder samples.

even (respectively, odd) bonds. This system is noncritical with a finite correlation length for all $\delta \neq 0$ and the EE $S(x)$ of a segment of size x saturates to a finite value for large enough x [2,3]. We calculate $S_{\mathrm{VB}}(x)$ for $\delta = 1/3$ and a system of size $L = 64$ [see Fig. 2(c)]. There are two types of inequivalent blocks x depending on whether the block starts with a strong bond $1 + \delta$ or a weak one $1 - \delta$. We denote the corresponding entropies by $S_s^{\mathrm{VB}}(x)$ and $S_w^{\mathrm{VB}}(x)$ and by symmetry $S_s^{\mathrm{VB}}(x) = S_w^{\mathrm{VB}}(x)$ for all odd x. Both entropies show an alternating pattern, a consequence of the explicit dimerization. This is in contrast with the average entropy $S^{\mathrm{VB}}(x) = 1/2[S_s^{\mathrm{VB}}(x) + S_w^{\mathrm{VB}}(x)]$ which is a smooth function of x. All entropies clearly display a saturation at large x. These features also appear in the study of EE for the same model.

We conclude this section by showing results on the disordered AF Heisenberg chain. Here all couplings are random variables uniformly distributed in [0, 1]. This system is in the random singlet phase [18], a gapless critical phase where spins are coupled pairwise in singlets at all length scales. As understood from a real space renormalization group (RSRG) procedure [20], the physics is dominated by a single VB covering in the thermodynamic limit [18]. Calculating the disorder average EE $\overline{S(x)}$ with RSRG, Refael and Moore [4] obtained the scaling form $\overline{S(x)} = \gamma/3 \ln(x) + S_2$ with $\gamma = \ln(2)$, a result confirmed by numerical simulations of random spin chains [21]. We simulated disordered chains of sizes up to $L = 256$ starting from an initial VB state $|\Psi_0\rangle$ obtained applying the RSRG decimation scheme, which ensured a faster convergence with the projection index n. Figure 2(d) presents our numerical results for $\overline{S^{\mathrm{VB}}(x)}$, and the data (for $10 \leq x \leq L/2$) are well fitted by the previous functional form with a prefactor $\gamma_{\mathrm{eff}} = 0.6(1)$, in agreement with the RSRG prediction for the average EE. Actually, as the average in the thermodynamic limit is dominated by a single VB state, we expect $\overline{S^{\mathrm{VB}}}$ and $\bar{S}$ to coincide. This is, however, difficult to check numerically because of the finite L and the small number of random samples used in the simulations. This also accounts for the small discrepancy in our numerical estimate of γ_{eff} with respect to the RSRG prediction [note that a fit forcing $\gamma_{\mathrm{eff}} = \ln(2)$ is also of good quality as seen in Fig. 2(d)].

2D systems.—The previous section showed the precise agreement between the VB entanglement entropy S^{VB} and the true EE S in both quantitative and qualitative respects for 1D systems. This gives us confidence that S^{VB} is a good observable to quantify entanglement also in larger dimensions d. This is an important point as the VB QMC simulations (and therefore the calculation of S^{VB}) can easily be extended to higher d. Note at this stage that only a few results are available on entanglement properties in high d: exact results have been derived for free fermions [22,23], bosons [6,23,24], and some exactly solvable spin models [25], but EE has never been calculated numerically for large $d > 1$ systems to the best of our knowledge [26]. At the present time, the connection between the area law and the precise nature of the ground state (range of correlations, presence of a gap) is not fully understood for $d > 1$ (see discussions in Ref. [24]).

We now investigate 2D Heisenberg systems and calculate S^{VB} for a square subsystem Ω of linear size x (such as the one in Fig. 1), for $L \times L$ samples with PBC up to $L = 64$. In particular, we consider a model of coupled dimers in two dimensions depicted in the inset of Fig. 3, where dimers (with intradimer exchange $J = 1$) are coupled with an interdimer exchange λ. The physics of this model is well understood [27]: at low λ, the system is in a dimerized valence bond solid (VBS) phase, whereas the case $\lambda = 1$ corresponds to the Néel phase of the isotropic 2D Heisenberg model. The system undergoes a quantum phase transition between these two states at $\lambda_c = 0.52337(3)$ [27]. Figure 3(a) displays the average valence bond entanglement entropy divided by the linear size $S^{\mathrm{VB}}(x)/x$ for the point $\lambda = 0.2$ located in the VBS phase. All the curves for different L saturate for large enough x, indicating that the valence bond entanglement entropy obeys an area law $S^{\mathrm{VB}}(x) \propto x$, as expected for a gapped phase. For the isotropic case $\lambda = 1$ located in the Néel phase, $S^{\mathrm{VB}}(x)/x$ does not saturate, and the curve is actually well fitted by a log form, as exemplified by the log-linear scale of Fig. 3(b). Our numerical results therefore indicate that the valence bond entanglement entropy scales as

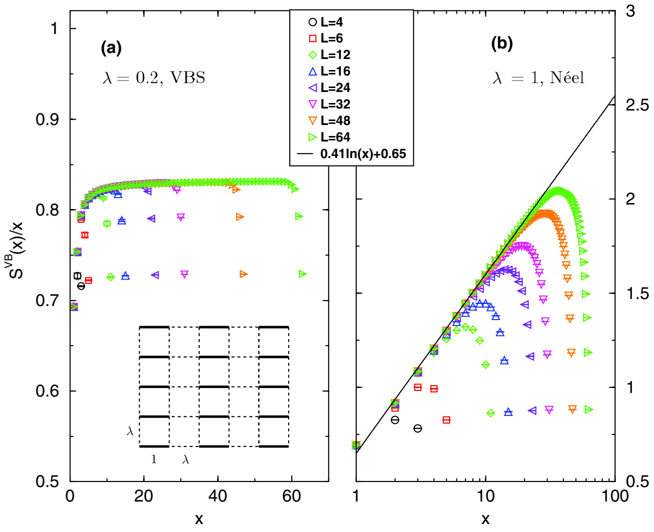

FIG. 3 (color online). S^{VB}/x versus distance x for 2D quantum spin systems: (a) 2D AF dimerized Heisenberg model ($\lambda = 0.2$), (b) 2D AF Heisenberg model ($\lambda = 1$) (log-linear scale). Solid line is a fit to a logarithmic divergence form. Inset: Illustration of the coupled-dimer model. Simulation parameters are $n = 30L^2$ for $L \leq 32$, $n = 20L^2$ for $L > 32$.

$S^{\mathrm{VB}}(x) \propto x \ln(x)$ in the Néel phase. Multiplicative logarithmic corrections have also been found for the EE of fermions [22,23]. They are tentatively attributed here to the Goldstone modes present in the Néel phase, which also make for the algebraic transverse spin correlations. Scaling of S^{VB} at the critical point λ_c is currently under investigation.

To summarize, we have proposed the valence bond entanglement entropy as a new measure of entanglement for SU(2) quantum spin systems. S^{VB} offers a powerful tool to quantitatively investigate the deep connection between VB physics and the amount of entanglement present in spin systems, although its precise connection to EE needs further studies. Several questions then arise, pointing, for instance, towards $d \geq 2$ exotic phases (such as resonating valence bond spin liquids) and quantum critical points (as in Ref. [19]), which should hopefully exhibit striking valence bond entanglement features. Finally, in the absence of a Marshall sign rule (as for some frustrated systems) where S^{VB} depends on the choice of a bipartite basis, the usefulness of S^{VB} has to be clarified.

We thank O. Giraud and G. Misguich for fruitful discussions. Calculations were performed using the ALPS libraries [28]. We thank IDRIS and CALMIP for allocation of CPU time. Support from the French ANR program (F. A., S. C., and M. M.), the Swiss National Fund and MaNEP (N. L.) is acknowledged.

*alet@irsamc.ups-tlse.fr

[1] A. Osterloh *et al.*, Nature (London) **416**, 608 (2002); T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002); F. Verstraete, M. Popp, and J. I. Cirac, Phys. Rev. Lett. **92**, 027901 (2004); for a recent review, see L. Amico *et al.*, arXiv:quant-ph/0703044.
[2] G. Vidal *et al.*, Phys. Rev. Lett. **90**, 227902 (2003); J. I. Latorre, E. Rico, and G. Vidal, Quantum Inf. Comput. **4**, 48 (2004).
[3] P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.
[4] G. Refael and J. E. Moore, Phys. Rev. Lett. **93**, 260602 (2004).
[5] C. H. Bennett *et al.*, Phys. Rev. A **53**, 2046 (1996).
[6] M. Srednicki, Phys. Rev. Lett. **71**, 666 (1993).
[7] V. E. Korepin, Phys. Rev. Lett. **92**, 096402 (2004).
[8] E. Fradkin and J. E. Moore, Phys. Rev. Lett. **97**, 050404 (2006).
[9] A. Kitaev and J. Preskill, Phys. Rev. Lett. **96**, 110404 (2006); M. Levin and X.-G. Wen, *ibid.* **96**, 110405 (2006).
[10] B.-Q. Jin and V. E. Korepin, J. Stat. Phys. **116**, 79 (2004).
[11] N. Laflorencie *et al.*, Phys. Rev. Lett. **96**, 100603 (2006).
[12] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[13] A. W. Sandvik, Phys. Rev. Lett. **95**, 207203 (2005).
[14] K. S. D. Beach and A. W. Sandvik, Nucl. Phys. **B750**, 142 (2006).
[15] M. Mambrini, arXiv:0706.2508.
[16] W. Marshall, Proc. R. Soc. A **232**, 48 (1955); E. H. Lieb and D. C. Mattis, J. Math. Phys. (N.Y.) **3**, 749 (1962).
[17] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. (N.Y.) **10**, 1388 (1969); **10**, 1399 (1969).
[18] D. S. Fisher, Phys. Rev. B **50**, 3799 (1994).
[19] A. W. Sandvik, Phys. Rev. Lett. **98**, 227202 (2007); K. S. D. Beach and A. W. Sandvik, *ibid.* **99**, 047202 (2007).
[20] S. K. Ma, C. Dasgupta, and C. K. Hu, Phys. Rev. Lett. **43**, 1434 (1979); C. Dasgupta and S. K. Ma, Phys. Rev. B **22**, 1305 (1980).
[21] N. Laflorencie, Phys. Rev. B **72**, 140408(R) (2005); G. De Chiara *et al.*, J. Stat. Mech. (2006) P03001.
[22] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006); D. Gioev and I. Klich, *ibid.* **96**, 100503 (2006); W. Li *et al.*, Phys. Rev. B **74**, 073103 (2006).
[23] M. Cramer, J. Eisert, and M. B. Plenio, Phys. Rev. Lett. **98**, 220603 (2007).
[24] M. Cramer *et al.*, Phys. Rev. A **73**, 012309 (2006); T. Barthel, M.-C. Chung, and U. Schollwöck, *ibid.* **74**, 022329 (2006).
[25] A. Hamma, R. Ionicioiu, and P. Zanardi, Phys. Rev. A **71**, 022315 (2005).
[26] For the most recent calculations of EE in 2D, see S. Furukawa and G. Misguich, Phys. Rev. B **75**, 214407 (2007).
[27] M. Matsumoto *et al.*, Phys. Rev. B **65**, 014407 (2001).
[28] F. Alet *et al.*, J. Phys. Soc. Jpn. Suppl. **74**, 30 (2005); M. Troyer, B. Ammon, and E. Heeb, Lect. Notes Comput. Sci. **1505**, 191 (1998); see http://alps.comp-phys.org.