Entanglement of Hard-Core Bosons in Bipartite Lattices

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The entanglement of hard-core bosons in square and honeycomb lattices with nearest-neighbor interactions is estimated by means of quantum Monte Carlo simulations and spin-wave analysis. The particular $U(1)$-invariant form of the concurrence is used to establish a connection with observables such as density and superfluid density. For specific regimes the concurrence is expressed as a combination of boson density and superfluid density.

1 Introduction

The past few years have seen a large explosion of interest in the studies of the interfaces between quantum information and many body systems. Among the subjects of interest can be cited quantum information processing in ultracold atomic gases [1]. This subject was initiated by the first proposal of using ultracold atoms on optical lattices for quantum information [2]. The physics of quantum ultracold gases in optical lattices has rapidly grown in interest [3]. Recent theoretical developments suggest that ultracold gases may be used for the experimental realization of the phenomenon of a supersolid [4,5,6,7,8,9,10,11].

In another register, entanglement is an important element in quantum information. It is used in quantum computation [12] and is also a valuable resource in quantum thermodynamics [13,14]. Meanwhile it can characterize quantum phase transitions (QPTs) [15,16,17,18,19,20,21,22,23]. QPTs occur when the ground state of a many-body system at absolute zero temperature undergoes a qualitative change by variation of a coupling and/or an external parameter [15]. The detailed analysis of QPTs is a very rich field and has the potential to uncover interesting physics and unexpected phase diagrams in a variety of many-body quantum systems, such as models with spins, bosons, or fermions on frustrated lattices [10,23,24,25,26,27], quasi one-dimensional (1D) ladders [28,29] and chains [10,17,18,30], and unfrustrated geometries in 2D or higher dimensions [9,19,20,31,32,33]. In this paper we will take a closer look at the signatures of QPT’s in the pairwise entanglement between two sites for the example of hard-core bosons on the square lattice and the honeycomb lattice. Entanglement is maximal close to the critical points and its derivatives can signal more precisely the presence of a quantum phase transition at the critical points [16,17,18,19,20,21,22,23].

Among the various quantities that can extract information on entanglement can be mentioned the concurrence [34,35], the quantum discord [36,37], the entropy of entanglement [38] and the negativity [39] for the most renowned. Concurrence and quantum discord are pairwise measures of entanglement while entropy of entanglement and negativity are bipartite measures. Bipartite measures of entanglement are by construction isotropic measures. Pairwise measures of entanglement can be anisotropic for the same system under considerations. The last point strongly motivates us to use concurrence to describe entanglement in hard-core bosonic models. Here we focus our attention to entanglement between hard-core bosons on square and honeycomb lattices with nearest-neighbor interactions.

For particular cases the hard-core boson model with nearest-neighbor interactions in two spatial dimensions can be mapped onto a two dimensional spin-1/2 XXZ model [40]. By means of quantum Monte Carlo simulations (QMC) and spin-wave analysis (SW), we estimate the entanglement by using concurrence. The particular $U(1)$-invariant form of the concurrence takes a very simple form [41]. This particular $U(1)$-invariant form is used to establish a connection with observables such as boson density and superfluid density of the hard-core boson system.
Concurrence can henceforth be expressed as a combination of boson density and superfluid density.

The outline of the paper is as follows. In section 2 we present the hard-core boson model and its mapping onto the XXZ spin model. In section 3 we recall the elements of information theory which leads to the U(1)-invariant form of the concurrence. In section 4 the quantum Monte Carlo and spin-wave approaches used to derive the quantum correlations are presented. In section 5 we provide the results of QMC simulations and SW analysis. In section 6 the connection between concurrence and observables is established. In section 7 we conclude and discuss on potential outlooks.

2 The model We will consider a two dimensional system of hardcore bosons on the square lattice and the honeycomb lattice. The Hamiltonian is given by

\[ H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i \hat{n}_i + V \sum_i \hat{n}_i \hat{n}_j, \tag{1} \]

where \( \langle ij \rangle \) denotes nearest neighbor bonds, \( a_i \) (\( a_i^\dagger \)) destroys (creates) a hard-core boson on site \( i \), and \( \mu \) is the chemical potential. The hopping parameter is denoted by \( t \) and the interaction between nearest neighbors is introduced by \( V \).

To enforce the hard-core constraint in a simple way, the Hamiltonian (1) is mapped onto the two dimensional XXZ model with external magnetic field. The exact mapping is performed by \( a_i^\dagger \leftrightarrow S_i^+, a_i \leftrightarrow S_i^-, \) and \( \hat{n}_i \leftrightarrow S_i^z + 1/2 \) \[40, 42\]. For the particular case with \( V/2t = \Delta \) and \( \mu = \lambda V \), where \( \lambda \) is half the coordination number \( (z = 3 \text{ for a honeycomb lattice and } z = 4 \text{ for a square lattice}) \), and in units of \( t/2 \) the Hamiltonian reduces to the familiar XXZ spin model

\[ H_{XXZ} = \sum_{\langle ij \rangle} \left[ -\frac{1}{4} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \Delta \sigma_i^z \sigma_j^z \right] + \kappa_\Delta, \tag{2} \]

where the sum is taken over nearest neighbor sites on a lattice which is bipartite. The operators \( \sigma^\alpha \) with \( \alpha = x, y, z \) are Pauli matrices and \( \sigma^0 \) is the unit matrix. The constant \( \kappa_\Delta \) is equal to \(-\Delta z N/8 \) and simply arises from the mapping between the spins and bosons operators. \( N \) is the number of sublattice spins of the bipartite honeycomb lattice. We keep explicitly the constant \( \kappa_\Delta \) present in the Hamiltonian (2) because it will be important for the computation of spin-spin correlations functions. The Hamiltonian is real and invariant under U(1) rotation about the spin \( z \) axis. This continuous symmetry can only be spontaneously broken in dimensions higher than one and for \( |\Delta| < 1 \). A global Z2 symmetry about the spin \( x \) (or \( y \)) is also present.

At the critical point \( \Delta_c = 1 \) the XXZ spin lattice undergoes a quantum phase transition between an XY phase for \(-1 < \Delta < 1 \) and an Ising antiferromagnetic phase for \( \Delta > 1 \). For \( \Delta < -1 \) the XXZ system is in a ferromagnetic phase.

In order to extract information about entanglement in the system by means of concurrence, we need to build the joint state of two spin sites. The two-site density matrix provides such requirement.

3 Concurrence The information on the joint state is contained in the two-site density matrix \( \rho_{ij} \) which is derived from the following operator expansion \[21\]

\[ \rho_{ij} = \text{Tr}_{ij} | \rho \rangle = \frac{1}{4} \sum_{\alpha, \beta = 0}^3 \Theta_{\alpha \beta} \sigma_i^\alpha \otimes \sigma_j^\beta, \tag{3} \]

where the trace is taken over the whole system excluding the sites \( i \) and \( j \). The coefficients \( \Theta_{\alpha \beta} \) of the expansion are related to the spin-spin correlation functions through the relation

\[ \Theta_{\alpha \beta} = \text{Tr} \left[ \sigma_i^\alpha \sigma_j^\beta \rho_{ij} \right] = \langle \sigma_i^\alpha \sigma_j^\beta \rangle. \tag{4} \]

Owing to the symmetry of the Hamiltonian most of the coefficients \( \Theta_{\alpha \beta} \) are equal to zero. Translation invariance requires that the density matrix \( \rho_{ij} \) is only a function of distance \( r = i - j \) independent of the position \( i \). The reflection symmetry leads to \( \rho_{ij} = \rho_{ji} \), the Hamiltonian being real the density matrix verifies \( \rho_{ij}^* = \rho_{ij} \). Combining all symmetry constraints the density matrix expressed in the natural basis \( \{|\downarrow \downarrow \rangle, |\downarrow \uparrow \rangle, |\uparrow \downarrow \rangle, |\uparrow \uparrow \rangle \} \) reduces to

\[ \rho_{ij} = \begin{pmatrix} u & g & w & x \\ g & w & x & g \\ y & g & y & u \\ y & g & y & u \end{pmatrix}, \tag{5} \]

where the matrix elements are given by \( u = \frac{1}{4} + \frac{\langle \sigma_i^x \sigma_j^x \rangle}{4}, \) \( w = \frac{1}{4} - \frac{\langle \sigma_i^y \sigma_j^y \rangle}{4} \), \( x = \frac{\langle \sigma_i^x \sigma_j^y + \sigma_i^y \sigma_j^x \rangle}{4}, \) \( g = \frac{\langle \sigma_i^z \sigma_j^z \rangle}{4}, \) and \( y = \frac{\langle \sigma_i^x \sigma_j^x - \sigma_i^y \sigma_j^y \rangle}{4} \). Therefore, information on entanglement of the system can be extracted easily from the two-point correlators.

As mentioned before, a good indicator of entanglement is provided by the concurrence \( C \). The concurrence of two spins may be computed from the joint state \( \rho_{ij} \) through the formula \( C = \max \{0, \gamma_1 - \gamma_2 - \gamma_3 - \gamma_4 \} \) where the \( \gamma_i \) are the eigenvalues in decreasing order of the matrix \( \Gamma = \rho_{ij} \rho_{ji} \) \[34, 35\]. The square root of the eigenvalues of the matrix \( \Gamma \) are given by

\[ \Gamma_{\pm} = \frac{1}{4} \sqrt{\left(1 + \langle \sigma_i^x \sigma_j^x \rangle \right)^2 - 4 \langle \sigma_i^x \sigma_j^x \rangle \pm \left| \langle \sigma_i^y \sigma_j^y \rangle - \langle \sigma_i^z \sigma_j^z \rangle \right|}, \]

\[ \Theta_{\pm} = \frac{1}{4} \left|1 - \langle \sigma_i^x \sigma_j^x \rangle \pm \left( \langle \sigma_i^y \sigma_j^y \rangle + \langle \sigma_i^z \sigma_j^z \rangle \right) \right|. \tag{6} \]

For two-space dimensions and for \( |\Delta| < 1 \) the average \( \langle \sigma^x \rangle \) takes spontaneous non-zero values, the \( U(1) \) symmetry of the XXZ model is spontaneously broken. According to SyljuÅsen \[41\] the concurrence in the symmetry-broken state \[5\] can take the invariant \( U(1) \) form

\[ C = \frac{1}{2} \left( \langle \sigma_i^x \sigma_j^x \rangle + \langle \sigma_i^y \sigma_j^y \rangle - \langle \sigma_i^z \sigma_j^z \rangle - 1 \right) \tag{7} \]
if and only if the spin-spin correlation functions verify
\( \langle \sigma_i^x \sigma_j^y \rangle + \langle \sigma_i^y \sigma_j^x \rangle > \langle \sigma_i^z \sigma_j^z \rangle - 1 \) and \( \langle \sigma_i^x \sigma_j^x \rangle > \langle \sigma_i^z \sigma_j^z \rangle \).

The \( U(1) \)-invariant form of the concurrence is of particular importance for two reasons. The first reason is that it allows computation of concurrence by means of quantum Monte Carlo simulations. The second reason is that it helps to establish a connection between entanglement and observables such as boson density and superfluid density. As will be shown later the concurrence can be expressed as a linear combination of boson density and superfluid density.

To work out the correlation functions we will apply both an analytical approach using spin-wave theory and a numerical approach with quantum Monte Carlo methods.

4 Spin-wave analysis and Quantum Monte Carlo simulations
Spin-wave analysis provides a good analytical approach as was shown for the hardcore bosons problem on the square lattice \([40]\) and the effective honeycomb lattice \([8]\). A spin-wave analysis can be performed in the regime \(-1 < \Delta < 1\) for which the ground state corresponds to spins aligned in any direction within the XY plane. In order to grab fully the particular symmetry of the XY interactions a Haldane mapping is performed \([43]\) and a semi-classical approach can be applied \([44]\) to compute the spin-spin correlation function.

We first recall the transformations applied to the Hamiltonian \([2]\) that lead to a diagonalized Hamiltonian as demonstrated in Ref. \([44]\). The following demonstration is in some steps very similar to the derivation of the non-linear sigma model \([43]\). We are going to work out the spin-spin correlations by means of a semi-classical version of the Hamiltonian \([2]\).

First the spin operators are expressed by means of the Haldane mapping. In terms of the in-plane angular coordinate \( \phi \) and the spin projection \( \sigma_i^z \) in the direction \( Oz \), the spin operators read
\[
\sigma_i = \left( \sqrt{1 - \sigma_i^z^2} \cos \phi_i, \sqrt{1 - \sigma_i^z^2} \sin \phi_i, \sigma_i^z \right). \tag{8}
\]

With this mapping the Hamiltonian \([2]\) becomes
\[
H = \sum_{\langle i,j \rangle} \left( - \sqrt{1 - \sigma_i^z^2} \sqrt{1 - \sigma_j^z^2} \cos (\phi_i - \phi_j) \right.
\]
\[
+ \Delta \sigma_i^z \sigma_j^z \left) + \kappa_\Delta. \tag{9}
\]

At zero temperature we can assume a dilute spin-wave boson gas. In this case, the Hamiltonian can reasonably be expanded for small \( \sigma^z \) and \( \phi \). The expansion of the Hamiltonian up to quadratic terms and to second order in \( \sigma^z \) and \( \phi \) reads
\[
\begin{align*}
H^{(2)} & = \sum_{\langle i,j \rangle} \left( - 1 + \frac{1}{2} (\sigma_i^z^2 + \sigma_j^z^2) + \frac{1}{2} (\phi_i - \phi_j)^2 \\
& + \Delta \sigma_i^z \sigma_j^z \right) + \kappa_\Delta. \tag{10}
\end{align*}
\]

Higher orders of the expansion are not explicitly considered. Later in the derivation of the spin-spin correlation functions we introduce corrections arising from those neglected higher order terms. After Fourier transformation the Hamiltonian \( H^{(2)} \) becomes
\[
H^{(2)} = \sum_k \left( (1 - |\gamma_k| \cos \varphi_k) \phi_k \phi_{-k} \right.
\]
\[
+ (1 + \Delta |\gamma_k| \cos \varphi_k) \sigma_k^z \sigma_{-k}^z \right) + \kappa_\Delta + \kappa_0, \tag{11}
\]

where \( \kappa_0 = -z N \) collects the constant parts of \( H^{(2)} \). We also introduced the structure factor \( \gamma_k = \frac{1}{2} \sum_e e^{i \mathbf{k} \cdot \mathbf{r}_e} = |\gamma_k| e^{i \varphi_k} \) which is a complex number for the honeycomb lattice and where the sum runs over nearest neighbors sites. The amplitude of the structure factor for the honeycomb lattice reads
\[
|\gamma_k| = \frac{1}{3} \left[ 3 + 4 \cos \frac{3k_x}{2} \cos \frac{\sqrt{3}k_y}{2} + 2 \cos \left( \sqrt{3}k_y \right) \right]^{1/2}. \tag{12}
\]

For square lattices the phase \( \varphi_k \) equals zero and the structure factor is given by \( \gamma_k = (\cos k_x + \cos k_y) / 2 \). We then use the canonical transformation \( \phi_k = \alpha_k (b_k^\dagger + b_{-k}) \) and \( \sigma_k^z = i \beta_k (b_k^\dagger - b_{-k}) \) where \( b_k \)'s are bosons and
\[
\alpha_k = \frac{1 + \Delta |\gamma_k| \cos \varphi_k}{1 - |\gamma_k| \cos \varphi_k}^{1/4}, \tag{13}
\]
\[
\beta_k = \frac{1 - |\gamma_k| \cos \varphi_k}{1 + \Delta |\gamma_k| \cos \varphi_k}^{1/4}.
\]

Finally, the Hamiltonian takes the diagonalized form
\[
H^{(2)} = \kappa_0 + \kappa_\Delta + \sum_k \omega_k \left( b_k^\dagger b_k + \frac{1}{2} \right), \tag{14}
\]

where \( \omega_k = 4 z \left[ (1 - |\gamma_k| \cos \varphi_k) (1 + \Delta |\gamma_k| \cos \varphi_k) \right]^{1/2} \).

In order to compute the spin-spin correlations functions we can employ the Hellmann-Feynman theorem which relates the correlations functions to the bond-energy of the system \([45, 46]\). The bond-energy \( e(\Delta) \) is defined as the average of the Hamiltonian \( H \) divided by the number of bonds, \( e(\Delta) = \langle H \rangle / z N \). The spin-spin correlations functions are easily given by \( \langle \sigma_i^x \sigma_j^x \rangle = \frac{\partial e(\Delta)}{\partial \Delta} \) and \( \langle \sigma_i^y \sigma_j^y \rangle = - e(\Delta) + \Delta \frac{\partial e(\Delta)}{\partial \Delta} \). Taking the average of the sec-ond order Hamiltonian \( H^{(2)} \) over the ground state leads to the approximated ground state energy \( e^{(2)} = \langle H^{(2)} \rangle / z N \). The spin-spin correlations functions can then be expressed in terms of the approximated bond energies
\[
\langle \sigma_i^x \sigma_j^x \rangle \approx \frac{\partial e^{(2)}(\Delta)}{\partial \Delta} + \kappa_{zz}, \tag{15}
\]
\[
\langle \sigma_i^y \sigma_j^y \rangle \approx - e^{(2)}(\Delta) + \Delta \frac{\partial e^{(2)}(\Delta)}{\partial \Delta} + \kappa_{xy}. \tag{16}
\]

Non-negligible corrections to the spin-spin correlations functions \([15, 16]\) may be taken into account from
higher order terms of the expansion of the Hamiltonian (9). These corrections, κ_{zz} and κ_{zy}, are functions of the anisotropic parameter ∆. In the region −1 < ∆ < 0, we approximate κ_{zz} and κ_{zy} by constants. For the honeycomb lattice we find κ_{zz} ≈ 0.15 and κ_{zy} ≈ 1.65, while for the square lattice we obtain κ_{zz} ≈ 0.5 and κ_{zy} ≈ 2 from fits to the Monte Carlo simulation results at ∆ = −1. Despite the aggressive approximations we have applied here we will see that a reasonable description of the system is obtained.

The QMC simulations used in the present work are based on the stochastic series expansion algorithm [47,48,49]. The numerical results are obtained for lattices of size $L \times L$ ($L = 12, 18$ and $24$ for honeycomb lattices, and $L = 16, 20$ and $24$ for square lattices) with periodic boundary conditions and a finite inverse temperature of $\beta t = 50$.

5 Results Figures [1a] and [1b] provide a comparison between the spin-spin correlation functions derived from quantum Monte Carlo simulations and the spin-wave approach on the honeycomb lattice. For the region $\Delta < 0$ spin-wave theory provides a good approximation of the corrections, for larger anisotropic parameter $\Delta$ the deviations increase slowly. As the interaction between spin waves become more and more relevant. Note that the correlation function $\langle \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \rangle$ is larger than one for $\Delta > -1$. This may surprise at a first glance however considering the two inequalities $-1 \leq \langle \sigma_i^z \sigma_j^z \rangle \leq 1$ and $-1 \leq \langle \sigma_i^y \sigma_j^y \rangle \leq 1$ we expect that $\langle \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \rangle$ belongs to the range $[−2, 2]$. In particular, for the spin singlet and triplet $T_{1/2} = (|↑↓\rangle ± |↓↑\rangle)/\sqrt{2}$ the XY-correlation function reads $\langle T_{1/2} | \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y | T_{1/2} \rangle = \pm 2$. This supports the fact that the absolute value of the XY-correlation function can take values larger than one.

Figure [2] depicts the concurrence obtained from quantum Monte Carlo on honeycomb lattices. For $\Delta < -1$ the spin systems is in a ferromagnetic phase. The state of the system can be expressed as a product of separate states, the concurrence is equal to zero and the system is separable. For $\Delta > 0$, the system is in an antiferromagnetic phase. For $\Delta = 1$ the concurrence is maximal and the system is maximally entangled. Increasing the parameter $\Delta$ from the ferromagnetic to the antiferromagnetic phase increases the entanglement of the spin system (or equivalently the hard-core boson system).

The concurrence obtained from spin-wave approach on honeycomb lattices (dashed line in Figure [2]) agree with QMC predictions close to the ferromagnetic phase transition, for $\Delta \rightarrow -1$. For larger values of $\Delta$ the boson gas of spin-wave excitations becomes denser. Hence the approximation of a dilute gas no longer holds and our present spin-wave is no longer valid.

Similar results are obtained for hard-core bosons on square lattices as depicted in figures [3] and [4].

6 Concurrence, boson density and superfluidity

According to the mapping relating the hard-core bosons and spins, the $U(1)$-invariant form of the concurrence can be expressed in terms of the boson density and superfluid density of the hard-core boson system.

Indeed the spin-spin correlation function in the $z$ direction can be easily expressed in terms of the boson density by making use of the exact mapping $\hat{n}_i \leftrightarrow S_i^z + 1/2$ which leads to $\langle S_i^+ S_j^- \rangle = 1/4 - \langle \hat{n}_i \rangle + \langle \hat{n}_i \hat{n}_j \rangle$.

The superfluid density is related to the energy cost to introduce a twist $\nu$ between pairs of nearest neighbor spins. The superfluid density is given by the second derivative of the energy of the spin system with respect to the twist $\nu$, $\rho_s = d^2 U(\nu)/d\nu^2$ [50,51]. The Hamiltonian $H(\nu)$ is derived from the XXZ model by application of a local rotation at site $i$ by an angle $\nu_i$ around the $z$ axis, $S_i^z \rightarrow S_i^z e^{i\nu_i}$, $S_i^+ \rightarrow S_i^+ e^{-i\nu_i}$ and $S_i^- \rightarrow S_i^- e^{-i\nu_i}$.
to \( C \approx \) linear expressions with respect to the boson density and \( U \) lattice and the square lattice. By means of the particular glement in a hard-core boson model on the honeycomb bical as well as numerical approach to estimate the entan-
glement in hard-core boson system. Moreover, we also show the existence of generic and may be easily applied to different lattice sym-
metrics. The \( U(1) \)-form of the concurrence is sensitive to the lattice symmetry only through the spin-spin correlation functions. The linear relation of the concurrence with ob-
servables should also remain valid.

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