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Entanglement and off-diagonal long-range order of an η-pairing state

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Abstract

Off-diagonal long-range order (ODLRO) which is believed to be one characteristic of superconductivity is a quantum phenomenon not describable in classical mechanical terms. The quantum state constructed by η-pairing demonstrates ODLRO. Entanglement is a key concept of the quantum information processing and has no classical counterpart. We study the entanglement property of the η-pairing quantum state by concurrence and entropy which are two measures of the entanglement. We show that the concurrence of entanglement between one-site and the rest sites is exactly the correlation function of the ODLRO for the η-pairing state in the thermodynamic limit. So, when the η-pairing state is entangled, it demonstrates ODLRO and is thus in the superconducting phase, if it is a separable state, there is no ODLRO. In the thermodynamical limit, the entanglement between the M-site and other sites of the η-pairing state does not vanish. Other types of ODLRO of the η-pairing state are presented. We show that the behaviour of the ODLRO correlation functions is equivalent to that of the entanglement of the η-pairing state. The scaling of the entropy of the entanglement for the η-pairing state is studied.

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1. Introduction

Quantum entanglement plays a central role in quantum information and quantum computation [1–9]. On the other hand, quantum entanglement may also be regarded as an important parameter in quantum phase transitions [10, 11]. It is also pointed out that entanglement of the ground state of XXZ and XY spin chains at a critical point is closely related with the

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conformal field theories [12]. Some related works were also performed for various models [13–17]. Recent experiments have shown that entanglement can contribute significantly to the bulk susceptibility [18].

Off-diagonal long-range order (ODLRO) is an important concept in condensed matter physics [19, 20]. It is proved that ODLRO implies both the Meissner effect and the quantization of magnetic flux, which are the basic characteristic properties of superconducting states [19, 21]. It is argued that since off-diagonal elements have no classical analogue, the off-diagonal long-range order is a quantum phenomenon not describable in classical mechanical terms [19]. From quantum information theory, it is presently obvious that quantum entanglement is quantum mechanical and has no classical counterpart. And also the entangled state may be shared by spatially separated parties and thus can have long-range correlation. Consequently, superconductors may also be characterized by the existence of quantum entanglement, and the property of quantum entanglement could be the hidden reason that ODLRO can characterize the superconductivity. We may also argue that entanglement may be one basic quantity which could closely relate with different physical phenomena. So, it is necessary to explore the property of entanglement for various quantum systems.

2. η-pairing state with ODLRO

The entanglement of ground states for various one-dimensional spin models is well studied. The case of a higher-dimensional system, for example the Hubbard model, is comparatively complicated. However, in three dimensions (also in one and two dimensions), it is well known that the Hubbard model has an eigenstate with η-pairing [20]. It is argued that this state is metastable. We know that this eigenstate with η-pairing possesses ODLRO. And since this state is symmetric and relatively simple, its entanglement can be analysed explicitly. In this paper, we will study the entanglement of the η-pairing quantum state.

The Hamiltonian of the Hubbard model is as follows:

$$H = -\sum_{\sigma,\langle j,k\rangle}\left(c^{\dagger}_{j,\sigma}c_{k,\sigma} + c^{\dagger}_{k,\sigma}c_{j,\sigma}\right) + U\sum_{j=1}^{L}\left(n_{j\uparrow} - \frac{1}{2}\right)\left(n_{j,\downarrow} - \frac{1}{2}\right),$$

where $\sigma = \uparrow, \downarrow$, and j, k are nearest-neighbouring sites, $n_{j,\sigma} = c^{\dagger}_{j,\sigma}c_{j,\sigma}$ are number operators. $c^{\dagger}_{j,\sigma}$ are standard fermion operators with anticommutation relations given by $\left\{c^{\dagger}_{j,\sigma}, c_{k,\sigma'}\right\} = \delta_{j,k}\delta_{\sigma,\sigma'}$. We assume the lattice under consideration is three dimensional, and the total number of lattice sites is L. The η-pairing operators at lattice site j are defined as $\eta_j = c_{j,\uparrow}c_{j,\downarrow}, \eta^{\dagger}_j = c^{\dagger}_{j,\downarrow}c^{\dagger}_{j,\uparrow}, \eta^z_j = -\frac{1}{2}n_j + \frac{1}{2}$. These operators form a $SU(2)$ algebra as shown by the relations $\left[\eta_j, \eta^{\dagger}_j\right] = 2\eta^z_j, \left[\eta^{\dagger}_j, \eta^z_j\right] = \eta^{\dagger}_j, \left[\eta_j, \eta^z_j\right] = -\eta_j$. The η operators are defined as $\eta = \sum_{j=1}^{L}\eta_j, \eta^{\dagger} = \sum_{j=1}^{L}\eta^{\dagger}_j$. Yang pointed out that the following quantum state is an eigenstate of the Hubbard model [20]:

$$|\Psi\rangle = (\eta^{\dagger})^N|\mathrm{vac}\rangle. \tag{1}$$

This quantum state is not only an eigenstate of the Hubbard model, but also an eigenstate of other models which are exactly solvable by the Bethe ansatz method in one dimension [22, 23]. In particular, it is the ground state for the model in [22] for a special case. We should also point out that the quantum state (1) actually is not tied to any specific model, and it can be in any dimensions and with any lattice configurations. The ODLRO of this quantum state is shown as [20, 22],

$$C_1 = \frac{\langle\Psi|\eta^{\dagger}_k\eta_l|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{N(L-N)}{L(L-1)}, \quad k \neq l. \tag{2}$$

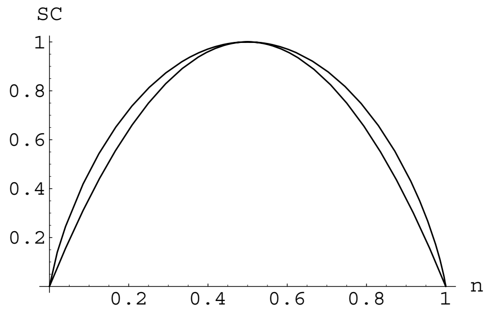

Figure 1. The outside curve is S_1, the inside curve is C_1 normalized by factor 4. For the η-pair half filled case $n = 1/2$, S_1 and C_1 achieve the maximal point.

We can find the off-diagonal element is constant for large distances $|k - l|$. In the thermodynamic limit, $N, L \to \infty$ where $N/L = n$, the off-diagonal correlation is $n(1 - n)$ which generally does not vanish except for $n = 0, 1$. For the η-pairing half-filled case $n = 1/2$, this correlation achieves the maximum.

3. Entanglement of the η-pairing state

It is of interest to study the entanglement of the η-pairing state. Zanardi *etal* [26] were the first to study the pair-wise entanglement of this quantum state (1). In the thermodynamic limit, it was shown that the pair-wise entanglement vanishes. This coincides with the entanglement sharing case [27]. Besides pair-wise entanglement, other entanglement properties of this quantum state in the thermodynamic limit should also be studied, as already done for various spin chains. We will consider the entanglement between M sites and the rest of the sites. For this case, the entanglement can be perfectly quantified by the von Neumann entropy of the reduced density operators of M sites since the quantum state (1) is a pure state. Some related works include [32, 34].

First, let us consider the entanglement between one site with the remaining $L - 1$ sites of the quantum state (1), $S_1 = -\mathrm{Tr}\rho_1 \log_2 \rho_1$, S_1 is the von Neumann entropy of the one-site reduced density operator of the quantum state (1). One finds that the one-site reduced density operator takes the form $\rho_1 = \left(1 - \frac{N}{L}\right)|0\rangle\langle 0| + \frac{N}{L}|1\rangle\langle 1|$, where $|0\rangle$ is the hole state, $|1\rangle$ is the η-pair filled state. As previously, we denote $n = N/L$. The one-site entanglement is

$$S_1 = -(1 - n)\log_2(1 - n) - n\log_2 n. \qquad (3)$$

So, in the thermodynamic limit, the entanglement between one site and other sites does not vanish. Interestingly, for the η-pair half filled case $n = 1/2$, the entanglement S_1 achieves the maximum. This is the same as the correlation function of ODLRO. We may also identify that the correlation of ODLRO in equation (2) has the hole-η-pair symmetry, i.e., changing N to $L - N$, this correlation is invariant. This symmetry also appears in the one-site entanglement as shown in equation (3). In the thermodynamic limit, we can find that the correlation function of the ODLRO and the one-site entanglement have the same monotonicity with respect to the density of the η-pair n; this is shown in figure 1.

This result draws our attention to the question of whether it is possible to quantify the entanglement by the correlation function of ODLRO. This means that correlation function of ODLRO can be identified as the entanglement measure of the quantum state (1). We know that the widely accepted measure of entanglement of a pure state is the von Neumann entropy

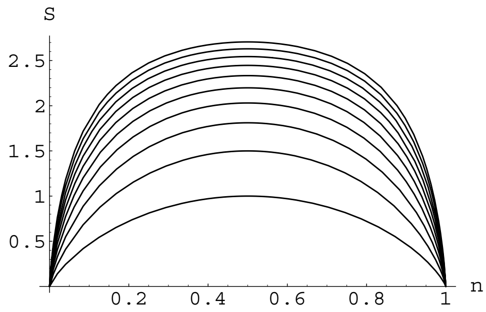

Figure 2. The functions of entanglement entropy S_M, taking $M = 1, 2, \ldots, 10$.

of the reduced density operator. However, indeed, we may quantify the entanglement by other measures, for example, the concurrence defined by Wootters is also a widely accepted measure of entanglement [28]. In the thermodynamic limit, the concurrence of one-site entanglement corresponding to S_1 in (3) is $n(1-n)$ which is exactly the correlation of the ODLRO (2). Thus the correlation of ODLRO C_1 is actually the concurrence of the quantum state (1) between one site and $L-1$ sites. So, we may say the appearance of one-site entanglement S_1 is the hidden reason that the off-diagonal elements have long-range correlation in the state (1). If the correlation function of ODLRO is zero, (1) is a separable state; if it is not zero, (1) is an entangled state.

We know that the pair-wise entanglement of quantum state (1) vanishes in the thermodynamic limit [26]. So, the ODLRO does not necessarily correspond to the pair-wise entanglement. However, we find that the correlation function of ODLRO is the concurrence of the one-site entanglement of the quantum state (1). The correlation function of ODLRO shown in equation (2) is in terms of the pair-wise form, i.e., the correlation function is concerned with two different sites, while the one-site entanglement is in the form: one site with the other $L-1$ sites. Here we argue that though the ODLRO is in terms of the pair-wise form, since this correlation is the same for all pairs, it can also be roughly understood as the correlation of one site with the other $L-1$ sites.

For multipartite state, we may not only consider the one-site entanglement. The M-site entanglement is also the basic property of the entanglement. Next, we consider the entanglement of M sites with the rest $L-M$ sites of the state (1) denoted as $S_M = -\mathrm{Tr}\rho_M \log_2 \rho_M$, where ρ_M is the reduced density operator of M sites of the quantum state (1). For convenience, we consider the thermodynamic limit, and assume M is finite. By some calculations, we find that the reduced density operator of M sites can be represented as $\rho_M = \sum_{i=0}^{M} |\bar{i}\rangle\langle\bar{i}| f_M(n,i)$, where we define $f_M(n,i) = n^i(1-n)^{M-i}\frac{M!}{i!(M-i)!}$, the quantum state $|\bar{i}\rangle$ is a symmetric state with i η-pairs filled in M sites. So, we know the von Neumann entropy of ρ_M takes the form

$$S_M = -\sum_{i=0}^{M} f_M(n,i) \log_2 f_M(n,i). \tag{4}$$

Here we remark that the M-site entanglement still has the hole-η-pair symmetry since mapping $|\bar{i}\rangle$ to $|\overline{L-i}\rangle$ does not change the von Neumann entropy of ρ_M. As an example, we recover equation (3) for $M = 1$. The behaviour of S_M is almost the same for all M. S_M achieves the maximum when $n = 1/2$ corresponding to η-pair half filled case. See figures 2 and 3 for the details.

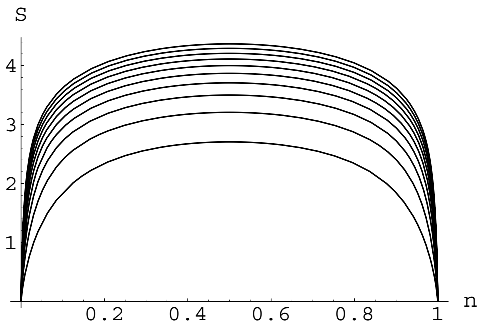

Figure 3. The functions of entanglement entropy S_M, and we take $M = 10, 20, \ldots, 100$.

We may note that the quantum state (1) is just a symmetric spin state. So, the entanglement of this quantum state is similar to the symmetric bosonic state in a lattice. The entanglement of a set of spatial bosonic modes localized on a graph has been studied in [29]. In this paper, we are mainly concerned with the relationship between the entanglement of quantum state (1) with the correlation function of the ODLRO.

4. The general ODLRO for the η-pairing state

Our results showed that the ODLRO in condensed matter physics may be related with the entanglement. However, we not only intend to just give an interpretation of ODLRO by the concurrence; we would also like to know whether quantum information theory can tell us more about the phenomenon of ODLRO. To study the entanglement property of a multipartite system, it is natural to consider not only the one-site entanglement S_1, but also the M-site entanglement S_M. Conversely, we may wonder whether there exist other types of ODLRO in η-pairing state. For example, we are interested to know whether the off-diagonal elements of $\langle\Psi|\big(\eta_{k_1}^\dagger\eta_{k_2}^\dagger\big)\big(\eta_{l_1}\eta_{l_2}\big)|\Psi\rangle/\langle\Psi|\Psi\rangle$ still have long-range correlation. This is a natural question if we relate ODLRO with entanglement. Of course, the pair-wise correlation as presented in equation (2) is enough to show that the quantum state (1) possesses ODLRO. However, other types of ODLRO may also be interesting properties of the quantum system. Since the entanglement S_M does not vanish in the thermodynamic limit, we expect that the general ODLRO also exist for η-pairing state. Next, we consider the general off-diagonal elements of $\langle\Psi|\big(\eta_{k_1}^\dagger,\ldots,\eta_{k_M}^\dagger\big)\big(\eta_{l_1},\ldots,\eta_{l_M}\big)|\Psi\rangle$ normalized by $\langle\Psi|\Psi\rangle$. Here, for convenience, we still assume M is finite and L, N are large enough to take the thermodynamic limit. We also assume that all l_i and k_j are different.

It can be checked that we have the relation $\langle\Psi|\Psi\rangle = N!L(L-1)\ldots(L-N+1)$. By some calculations, we can also find that

$$\langle\Psi|\big(\eta_{k_1}^\dagger,\ldots,\eta_{k_M}^\dagger\big)\big(\eta_{l_1},\ldots,\eta_{l_M}\big)|\Psi\rangle = N^2\langle\tilde{\Psi}|\big(\eta_{k_2}^\dagger,\ldots,\eta_{k_M}^\dagger\big)\big(\eta_{l_2},\ldots,\eta_{l_M}\big)|\tilde{\Psi}\rangle,$$

where state $|\tilde{\Psi}\rangle = \big(\sum_{j\neq l_1,k_1}\eta_j^\dagger\big)^{N-1}|vac\rangle$. With these results, we can readily show that

$$\begin{aligned} C_M &= \frac{\langle\Psi|\big(\eta_{k_1}^\dagger,\ldots,\eta_{k_M}^\dagger\big)\big(\eta_{l_1},\ldots,\eta_{l_M}\big)|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\ &= \frac{N\ldots(N-M+1)(L-N)\ldots(L-N-M+1)}{L\ldots(L-2M+1)}. \end{aligned}$$

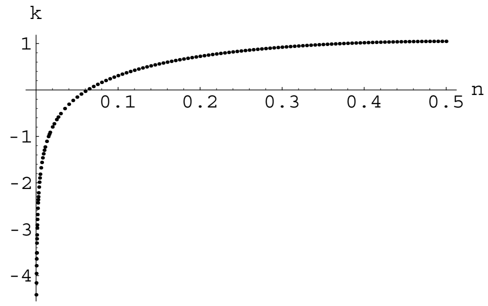

Figure 4. The dependence of $k(n)$ on n, the values of $k(n)$ are optimized for $M = 800$ to satisfy the scaling relation (5). Since S_M has η-pair-hole symmetry, i.e., S_M is invariant for map $n \to 1 - n$, we just need to let n range from 0 to 0.5.

The correlation function C_M does not depend on the distances of $|k_i - l_j|, i, j = 1, \ldots, M$. In fact, we can find other types of ODLRO for the state (1). We can still observe the hole-η-pair symmetry since the correlation function is invariant if we change N to $L - N$. In the thermodynamic limit, this correlation becomes $[n(1-n)]^M$ which is the M power of the original pair-wise ODLRO. In this sense, these ODLROs are also related with the concurrence of the one-site entanglement.

The concurrence of entanglement is well defined for 2-level quantum systems [28]. However, there is no consensus definition of concurrence for higher-level quantum systems even for pure states. Nevertheless, we remark that the concurrence hierarchy which includes several quantities is a much more general definition for the concurrence [30]. Considering the M-site reduced density operator ρ_M, we would like to point out that the quantity $\prod_{i=0}^{M} f_M(n, i)$ which is equal to $[n(1-n)]^{M(M+1)/2}$ up to a constant factor is one generalized concurrence. Recall that the general correlation function of ODLRO is $[n(1-n)]^M$, this provides more evidence that ODLRO is closely related with the entanglement for the η-pairing state (1).

The entanglement of S_M concerns about the correlation of M sites with the rest $L - M$ sites. Comparatively, it is meaningless to consider the correlation of the form $\langle\Psi|\big(\prod_{i=1}^{M} \eta_{k_i}^{\dagger}\big)\big(\prod_{j=1}^{M'} \eta_{l_j}\big)|\Psi\rangle$, $M \neq M'$ which is actually zero. So, the definitions of ODLRO and quantum entanglement cannot be completely identified. However, as we already showed, they are closely related. If ODLRO cannot be identified with entanglement in some other systems different from the η-pairing state, it is possible that ODLRO and quantum entanglement describe different aspects of the quantum systems.

5. Scaling behaviour for the entropy, and summary

It is shown that the entropy of entanglement of the ground states of gapless models demonstrates universal scaling behaviour which is related with the universal properties of the quantum phase transition [10–13]. We next show numerically that S_M also obeys universal scaling laws. Since the η-pairing state is simple, it is straightforward to check numerically the scaling of S_M up to, say, $M = 10^4$ sites in a desktop computer. We obtain the scaling form of S_M as

$$S_M \approx \tfrac{1}{2}\log_2(M) + k(n), \tag{5}$$

where $k(n)$ depends only on the η-pair density n. The correspondence between $k(n)$ and n is presented in figure 4; the exact data are also available. The factor $1/2$ in (5) could be related with the central charge of the conformal field theory [31] as for XY model and other models

[12, 13]. For cases $n = 0$ and $n = 1$, we have $S_M = 0$, thus the scaling relation (5) does not hold. We checked numerically that near $n = 0$, say, around $n = 0.001$, the scaling relation (5) is still correct with high precision. Even near $n = 10^{-4}$, the scaling relation is roughly correct. We remark that with $n \neq 0, 1$, the quantum state (1) is entangled with ODLRO and is thus in the superconducting phase. There will be a phase transition near $n = 0, 1$. Our results show that the scaling relation (5) for η-pairing state is generally correct except for $n = 0, 1$. Finally, we remark that our result of S_M in (4) is rigorous and exact.

We summarize that quantum entanglement plays an important role in the ODLRO of the quantum state (1) which is not tied to any specific model. Thus entanglement could also be regarded as one characteristic of superconductivity at least for the η-pairing quantum state. Though further research about the relationship between entanglement and ODLRO is necessary, we have already shown that for the well-known η-pairing state, the ODLRO and the entanglement (C_1 and S_1), two important concepts in condensed matter physics and quantum information processing, can be identified. Further, from quantum information theory, we expected from the fact that S_M in general does not vanish that other types of ODLROs exist in the thermodynamic limit. As presented in this paper the non-zero quantities C_M do exist in the thermodynamic limit.

Acknowledgments

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Note added. After we finished this paper, some closely related works appeared on the quant-ph archive [33–35].

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