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# Quantum information aspects on bulk and nano interacting Fermi system: A spin-space density matrix approach

R. Afzali [a,*], N. Ebrahimian [b], B. Eghbalifar [c]

[a] Department of Physics, K. N. Toosi University of Technology, Tehran, 15418, Iran
[b] Department of Physics, Faculty of Basic Sciences, Shahed University, Tehran, 18155-159, Iran
[c] Department of Agricultural Management, Marvdasht Branch, Azad University, Marvdasht, Iran

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ABSTRACT

By approximating the energy gap, entering nano-size effect via gap fluctuation and calculating the Green's functions and the space-spin density matrix, the dependence of quantum correlation (entanglement, discord and tripartite entanglement) on the relative distance of two electron spins forming Cooper pairs, the energy gap and the length of bulk and nano interacting Fermi system (a nodal d-wave superconductor) is determined. In contrast to a s-wave superconductor, quantum correlation of the system is sensitive to the change of the gap magnitude and strongly depends on the length of the grain. Also, quantum discord oscillates. Furthermore, the entanglement length and the correlation length are investigated. Discord becomes zero at a characteristic length of the d-wave superconductor.



## 1. Introduction

Entanglement and quantum discord (QD) are the key resources in quantum communication, quantum teleportation and quantum computation. Quantum entanglement (QE) is a physical resource, like energy, associated with quantum correlations that are possible between separated quantum systems [1–10]. One of the measures of quantum entanglement namely concurrence can be used for the determination of correlation of systems [11–14]. A study of QD and QE in many-body systems is very important to give new insights on physical properties via correlations, however, QD and QE have many applications to quantum information processing and to protocols such as quantum teleportation and quantum algorithm. On the other hand, QD and QE can be used to determine quantum phase transitions [15–18]. QD is defined as the difference between quantum mutual information and classical correlation in a bipartite system. In general, quantum discord may be nonzero even for certain separable states namely when entanglement of system is zero. QD can be considered as resource for remote state preparation [19]. QD specifies the interferometric power of quantum states [20].

Entanglement in many-body systems was studied [21–32]. The history of the investigation of entanglement of spins returns to Ref. [16] where the properties of entangled systems in the second quantization formalism were studied. In Ref. [33], the entanglement of electron spins of noninteracting electron gases based on the Green's function approach was discussed. By considering the screened Coulomb interaction between electrons, the entanglement between two electrons in a degenerate electron gas was studied [34,35]. Bipartite entanglement (BE) in the s-wave superconductor was also studied [36]. Also, in momentum space, the expression of the spin entanglement of electrons in the Cooper pairs was derived [37] and the brief discussion of BE on Fulde–Ferrell–Larkin–Ovchinnikov superconductor was already done [38]. Furthermore, for finite superconductor, using the average local concurrence, entanglement of the full system was discussed [39]. Quantum tripartite entanglement and multipartite entanglement in terms of the fermions separation were investigated in a noninteracting fermion gas, using the density matrix [40]. Dependence of tripartite entanglement (TE) of electron spins of a noninteracting Fermi gases with respect to the temperature and the relative distance between the three spins was determined [41,42]. QD was defined as a measure of the quantumness of correlations [43]. Necessary and sufficient condition for nonzero quantum discord was derived [44]. Review of quantum discord in bipartite and multipartite systems was done [45]. Quantum discord for two-qubit systems was derived [35,36] and for two-qubit X-states was calculated [48,49].

* Corresponding author.
*E-mail addresses:* afzali@kntu.ac.ir (R. Afzali), n.ebrahimian@shahed.ac.ir (N. Ebrahimian), b.eghbali2011@yahoo.com (B. Eghbalifar).

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In condensed matter physics, it was known that the d-wave symmetry of superconductor is more important than the s-wave symmetry (in this symmetry, it is supposed that the energy gap is constant). d-wave superconductors are considered as unconventional superconductors. Usually high temperature superconductors (HTSC) have the gap with d-wave symmetry (of course HTSC usually are with strong coupling regime). It is important that one gets the knowledge of a superconductor with momentum-dependence gap. Therefore, we pay attention to the d-wave case. The energy gap depends on the angle between the electron momentum and the nodal axis; and at zero temperature we use an approximation in which the energy gap is considered as the linear function of the angle. For obtaining the concurrence and bipartite entanglement of electron spins, we must calculate the two-electron space-spin density matrix (which has a X-state form) with the aid of two-particle and single-particle Green's function. Meanwhile, for some purposes we calculate an analytic form of dominated Green's function, but for studying effect of length of the d-wave nano-superconductor grain or when concentrating on the gap change, the numerical calculation of Green's function is used. Then, the two-electron space-spin density matrix can be written in terms of normal and anomalous single-particle Green's functions. In this paper, at zero temperature, the dependence of quantum correlation (via quantum entanglement of two electron spins forming Cooper pairs (Werner state), tripartite entanglement and quantum discord) of system to the relative distance of electrons spins of the Cooper pair and the energy gap is investigated. Of course, tripartite entanglement of system is genuine; that will be discussed in detail. For investigating TE of the electron spins of the Cooper pair of the d-wave superconductor as an interacting system, new parameters for a three-spin reduced density matrix are calculated. Robustness of TE, which is defined in Refs. [42,50,51], is obtained. Lower bound of robustness of TE, $E_{R,\min}(\rho_3)$, is determined and the role of interaction that is principally revealed via the gap, whether in the d-wave or in the s-wave, is identified. Then, quantum discord is presented. Then, we consider the three-dimensional rectangular nano-superconducting grain in the weak coupling frame. Finally, we suppose that the single particle level spacing of the system is much smaller than the energy gap and this assumption guarantees to satisfy Bardeen–Cooper–Schrieffer (BCS) model [52]. It is seen that, in general, the nano-size effect, which is entered via gap fluctuation (thereby there is the change in the interaction), influences deeply and widely quantum correlations. Therefore, the nano-size effect is more efficient on properties of system via the change of quantum correlation. Dependence of correlation to the electrons distance and the length of the superconductor in spin space is determined. Moreover, we show that quantum correlation of the d-wave nano-size superconducting grain strongly depends on the length of grain (in contrast to the s-wave case). In general, it is found that if the length of grain is lower, the effect of nano-size on quantum correlation is higher. Quantum tripartite entanglement for the nano-scale d-wave superconductor is better than for the bulk d-wave superconductor. However, we find both bulk and nano-size s-wave superconductors have the same tripartite entanglement. Furthermore, the entanglement length and the quantum correlation length are investigated and it is shown that there is a length of superconductor in which discord becomes zero. Also, for a given fixed length of superconductor, both a peak in discord and a peak in concurrence occur simultaneously.

Paper will be organized as follows. In section 2, after writing the Hamiltonian of the d-wave superconductor and the energy gap function, we obtain Green's functions and thereby we get the density matrix of the system. We calculate the concurrence, the three-spin reduced density matrix accompanied with the identification of TE and $E_{R,\min}$, and quantum discord of the system. In section 3, the nano-size effect on quantum correlation is determined and discussed in detail. In section 4, some remarks and conclusions are given.

## 2. Quantum correlation of the bulk case

### 2.1. Green's function of system

First, we proceed to obtain quantum bipartite entanglement of the system. For this purpose, we calculate concurrence of the system. We start to obtain the density matrix of the system by using Green's function of the d-wave superconductor. Hamiltonian of the d-wave superconductor is given by [53]

$$H = \sum_{ks} \varepsilon_k c^\dagger_{ks} c_{ks} + \sum_{k,k'} V_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \quad (1)$$

where $\varepsilon_k$, $c^\dagger_{ks}$ and $c_{ks}$ are the excitation energy with respect to chemical potential, the creation operator and the annihilation operator, respectively. The interaction potential of the d-wave superconductor, $V_{k,k'}$, is given by [54,55]

$$V_{kk'}(\vec{v}_F, \vec{v}'_F) = V_d \cos 2(\theta_k - \chi) \cos 2(\theta'_k - \chi) \quad (2)$$

where $\vec{v}_F$, $\chi$ are the Fermi velocity, and the angle between the crystallographic a-direction and the x-axis, respectively. Also, $\theta_k$ (and $\theta'_k$) is the direction of $\vec{v}_F(\vec{v}'_F)$ in the ab-plane. Also, $V_d$ is defined by the dimensionless BCS constant of interaction $\lambda_d$ given by $\lambda_d = V_d N(0)/2$, wherein $N(0)$ is the density of states. On the contrary, Hamiltonian can be written in terms of gap energy using mean field approximation as follows

$$H = \sum_{ks} \varepsilon_k c^\dagger_{ks} c_{ks} + \sum_{k,k'} \Delta_{k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \sum_{k,k'} \Delta^*_k c_{-k'\downarrow} c_{k'\uparrow} \quad (3)$$

where indices $k$ and $s$ denote the wave vector and spin component, respectively.

Next, we explain mean field approximation used here. It should be noted that the description of properties of superconductors based on the BCS theory has been widely successful when mean field approximation is used. This approximation is very useful. In mean field approximation, Hamiltonian is written as an effective one-electron Hamiltonian and the interaction term that contains 4 operators is converted to terms that contain two operators each. Then, the total free energy of the system is minimized, and expectation values such as $\langle \sum_{k'} V_{k,k'} c_{-k'\downarrow} c_{k'\uparrow} \rangle (\equiv \Delta_k)$ are obtained. The key feature of this approximation is that the expectation values of these spin-paired operators exist and are nonzero [53]. However, caution must be exercised while using this approximation because of limitations in its application [40,56]. The mean field approximation can influence the amount of correlations and entanglement [56]; an upper bound for these amounts was determined in interacting systems. The amount of entanglement affects physical quantities; this amount especially (and its accuracy) directly affects the susceptibility (and the true value) of many body system [56]. Also, mean field approximation for obtaining the true amount of entanglement is accurate when the fluctuation due to all interactions is not large, and we consider establishing this condition in our system under investigation.

For a d-wave case with $d_{x^2-y^2}$ symmetry, we have $\Delta_k = \Delta(\hat{k}^2_x - \hat{k}^2_y) = \Delta\cos(2\theta_k)$ where $\theta_k$ is the angle between the electron momentum and the gap axis and $\Delta$ is the magnitude of the gap. The d-wave gap becomes zero on the Fermi surface at 4 nodes, where low-energy excitations are possible. The order parameter with d-wave symmetry has 4 nodal points, $\vec{k}_i = (\pm k_F/\sqrt{2}, \pm k_F/\sqrt{2})$, where the Fermi surface crosses the nodal directions $k_x = \pm k_y$. At these points, $\Delta_k$ becomes zero. Furthermore, we can approximate the energy gap at low temperatures [57]. For this limit, and for