# КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

# QUANTUM ENTANGLEMENT IN SECOND QUANTIZED FERMION SYSTEMS

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In this communication we consider the zero-temperature properties of entanglement in free and interacting fermion systems following Bogoliubov's excitation approach. We investigate spin biparticle entanglement in BCS superconductor ground state of electron gas and in EPS state of <sup>3</sup>He atoms. The relation between pair-distribution functions and biparticle quantum entanglement is discussed.

В работе рассматриваются свойства квантового перепутывания в системах многих фермионов при нулевой температуре с помощью метода квазичастиц Боголюбова. Исследуется двухчастичное спиновое перепутывание в основном состоянии сверхпроводящего электронного газа и в сверхтекучем состоянии атомов гелия-3. Обсуждается связь между квантовым перепутыванием и двухчастичными корреляционными функциями.

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# INTRODUCTION

Quantum entanglement is viewed as a precious resource in quantum information processing [1]. It is believed to be the main ingredient of the quantum speed-up in quantum computation and communication. A quantum computer is a many-body system where the Hamiltonian can be manipulated. And experience built up over the years in condensed matter is helping in finding new protocols for quantum computation and communication. At the same time, the study of the ground state of many-body systems with methods developed in quantum information may unveil new properties. Recently, considerable interest has been devoted to entanglement of two subsystems of a many-body system [2]: quantum spin systems [3,4], spins of noninteracting electron gas [5,6], entanglement in many-body systems [7,8].

In realistic systems containing a large number of particles the concept of a particle actually fades away and is replaced by a notion of excitation modes. Individual particles really become indistinguishable. In addition to that, the concept of fermion (versus boson) particle statistics then also becomes directly relevant and it is important to understand its relation to entanglement.

In many-body systems the correlation functions play a fundamental role in describing their physical phenomena. Thus, it is natural to explore the relation between entanglement

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and correlation functions. In this paper we find the two-spin state of a fermion system with pairing and discuss the relation between entanglement measure and pair distribution functions.

We consider many fermion systems. Let  $\hat{\Psi}$  be the field operator and obey the usual fermion anticommutation relations

$$\{\hat{\Psi}_{\sigma'}^{+}(\mathbf{r}'), \hat{\Psi}_{\sigma}(\mathbf{r})\} = \delta_{\sigma'\sigma}\delta(\mathbf{r}'-\mathbf{r}), \quad \{\hat{\Psi}_{\sigma'}(\mathbf{r}'), \hat{\Psi}_{\sigma}(\mathbf{r})\} = 0,$$

where **r** is the position vector and  $\sigma = +1/2, -1/2$  is the spin of the fermion.

The creation  $\hat{a}^+(\mathbf{f})$  and annihilation  $\hat{a}(\mathbf{f})$  fermion operators with momentum  $\hbar \mathbf{f}$  satisfy the relations

$$\{\hat{a}(\mathbf{f}), \hat{a}^{+}(\mathbf{f}')\} = \delta_{\mathbf{f},\mathbf{f}'},\\ \{\hat{a}(\mathbf{f}), \hat{a}(\mathbf{f}')\} = 0, \quad \mathbf{f} \equiv (\mathbf{f}, \sigma).$$

The Bogoliubov transformation from particle fermion operators  $\hat{a}^+(\mathbf{f}), \hat{a}(\mathbf{f})$  to quasiparticle fermion operators  $\hat{\alpha}^+_{\xi}, \hat{\alpha}_{\xi}$  has the form

$$\hat{a}(\mathbf{f}) = u_{\mathbf{f}\xi}\hat{\alpha}_{\xi} + v_{\mathbf{f}\xi}^*\hat{\alpha}_{\xi}^+,$$
$$\hat{a}^+(\mathbf{f}) = u_{\mathbf{f}\xi}^*\hat{\alpha}_{\xi}^+ + v_{\mathbf{f}\xi}\hat{\alpha}_{\xi}.$$

The functions  $u_{f\xi}$ ,  $v_{f\xi}$  satisfy orthonormal and completeness conditions. Anticommutation relations for quasiparticle operators are

$$\{\hat{\alpha}_{\xi}, \hat{\alpha}_{\xi'}^+\} = \delta_{\xi,\xi'}, \quad \{\hat{\alpha}_{\xi}, \hat{\alpha}_{\xi'}\} = 0.$$

The new «vacuum»  $|c\rangle$  is a ground state of the system. It is defined by condition

$$\hat{\alpha}_{\xi}|c\rangle = 0, \quad \forall \xi, \qquad \langle c|c\rangle = 1$$

#### 1. IDEAL FERMI GAS

We start with noninteracting nonrelativistic Fermi gas. The energy spectrum of particles is

$$E(f) = \frac{f^2\hbar^2}{2m} - \mu,$$

where  $\mu$  is the chemical potential for particle, and it is assumed that  $\mu > 0$ . There is a Fermi surface, which bounds the volume in momentum space where the energy is negative, E(f) < 0, and where the particle states are all occupied at T = 0. For an isotropic system the Fermi surface is a sphere of radius  $f_F = \sqrt{2m\epsilon_F/\hbar}$ ,  $\epsilon_F = \mu$ . Thus,

$$\hat{a}(\mathbf{f},\sigma) = \hat{\alpha}^{+}(\mathbf{f},\sigma) \quad (v_f = 1, u_f = 0), \quad \text{if} \quad f < f_F, \\ \hat{a}(\mathbf{f},\sigma) = \hat{\alpha}(\mathbf{f},\sigma) \quad (v_f = 0, u_f = 1), \quad \text{if} \quad f > f_F.$$

The density of number of fermions for each spin projection is

$$n_{\sigma} = \langle c | \hat{\Psi}_{\sigma}^{+}(\mathbf{r}) \hat{\Psi}_{\sigma}(\mathbf{r}) | c \rangle = \frac{1}{(2\pi)^{3}} \int d\mathbf{f} |v_{\mathbf{f}}|^{2}.$$
 (1)

For free fermions  $n_{\sigma} = \frac{1}{6\pi^2} f_F^3$ .

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Correlation functions are defined by relation

$$\mathcal{K}(\mathbf{r},\sigma,\sigma') = \langle c | \hat{\Psi}_{\sigma}^{+}(\mathbf{r}_{1}) \hat{\Psi}_{\sigma'}^{+}(\mathbf{r}_{2}) \hat{\Psi}_{\sigma'}(\mathbf{r}_{2}) \hat{\Psi}_{\sigma}(\mathbf{r}_{1}) | c \rangle,$$

where  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ . For two free fermions with parallel spins we get

$$\mathcal{K}(\mathbf{r},\sigma,\sigma) = n_{\sigma}^2 (1 - \phi^2(r)),$$

where

$$\phi(r) = \frac{1}{n_{\sigma}(2\pi)^3} \int d\mathbf{f} \,\mathrm{e}^{i\mathbf{f}\mathbf{r}} \,|v(\mathbf{f},\sigma)|^2. \tag{2}$$

For free fermions the function  $\phi(r) = 3(\sin (f_F r) - \cos (f_F r) f_F r)/(f_F r)^3$  satisfies relations  $0 \le \phi^2(r) \le 1, \phi^2(0) = 1, \phi^2(\infty) = 0.$ 

Therefore, fermions with parallel spin are negative correlated. The correlation radius is defined by radius  $f_F$  of Fermi sphere  $r_- \sim r_F \equiv 1/f_F$ .

For  $\sigma = \pm 1/2$  we get

$$\mathcal{K}(\mathbf{r},\sigma,-\sigma)=n_{\sigma}^2.$$

Free fermions with opposite spins are independently distributed.

For vacuum state  $|c\rangle$  two-spin reduced density matrix of two fermions at  $\mathbf{r}_1$  and  $\mathbf{r}_2$  positions equals

$$\hat{\rho}(\mathbf{r}) = \frac{1}{\gamma} \hat{R}(\mathbf{r}), \quad \gamma = \operatorname{Tr} \hat{R}(\mathbf{r}),$$

where

$$R(\sigma_1, \sigma_2; \sigma'_1, \sigma'_2, \mathbf{r}) = \langle c | \hat{\Psi}^+_{\sigma_1}(\mathbf{r}_1) \hat{\Psi}^+_{\sigma_2}(\mathbf{r}_2) \hat{\Psi}_{\sigma'_2}(\mathbf{r}_2) \hat{\Psi}_{\sigma'_1}(\mathbf{r}_1) | c \rangle$$

and r is a distance between fermions.

It is easy to calculate that

$$R(\sigma, -\sigma; \sigma, -\sigma; r) = -n_{\sigma}^2 \phi^2(r).$$

Thus,

$$\hat{\rho}(r) = \frac{1}{\gamma'} \begin{pmatrix} 1 - \phi^2(r) & 0 & 0 & 0\\ 0 & 1 & -\phi^2(r) & 0\\ 0 & -\phi^2(r) & 1 & 0\\ 0 & 0 & 0 & 1 - \phi^2(r) \end{pmatrix}$$

where

 $\gamma' = 2(2 - \phi^2(r)).$ 

According to Peres–Horodeski criterion [9] a condition of entanglement is a matrix  $\tilde{\rho}$ , obtained by partial transposition of  $\rho$ , i.e.,  $\tilde{\rho}_{\mu\nu;\mu'\nu'} = \rho_{\mu\nu';\mu'\nu}$ , has only non-negative eigenvalues. It gives  $\phi^2(r) > 1/2$ . This result for noninteracting electron gases was got in [5] in Green's functions approach.

This means that two free fermions are entangled if the relative distance between them is smaller than  $1.8r_F$  at T = 0. Two fermions are maximally entangled if they are at the same position.

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# 2. ELECTRONS IN BCS STATE

In superconductors the electrons with opposite momentums are pairing in s-state with zero spin of pair. One has

$$\hat{a}\left(\mathbf{f},\frac{1}{2}\right) = u_f \hat{\alpha}\left(\mathbf{f},\frac{1}{2}\right) + v_f \hat{\alpha}^+ \left(-\mathbf{f},-\frac{1}{2}\right),$$
$$\hat{a}\left(\mathbf{f},-\frac{1}{2}\right) = u_f \hat{\alpha}\left(\mathbf{f},-\frac{1}{2}\right) - v_f \hat{\alpha}^+ \left(-\mathbf{f},\frac{1}{2}\right),$$

where

$$u_f = \cos \frac{\theta_f}{2}, \quad v_f = \sin \frac{\theta_f}{2}, \quad \tan \theta_f = \frac{\Delta_f}{E(f)},$$

and  $\Delta_f$  is the energy gap. If  $\Delta_f = 0$ , then  $u_f v_f = 0$ .

Correlation function for two electrons with parallel spins equals

$$\mathcal{K}(\mathbf{r},\sigma,\sigma) = n_{\sigma}^2 (1 - \phi^2(r)),$$

(see (1), (2)). The electrons with parallel spins are negative correlated with correlation radius  $r_{-} \sim r_{F}$ .

For opposite spins we get

$$\mathcal{K}(\mathbf{r},\sigma,-\sigma) = n_{\sigma}^2 (1+|\phi_1(r)|^2),$$

where

$$\phi_1(r) = \frac{1}{n_\sigma (2\pi)^3} \int d\mathbf{f} \, \mathrm{e}^{i\mathbf{f}\mathbf{r}} \, v^*(\mathbf{f}) \, u(\mathbf{f}). \tag{3}$$

The electrons with opposite spins are positive correlated with correlation radius  $r_+$ . This radius is defined by the width of the layer in which  $v(\mathbf{f}) u(\mathbf{f})$  is much different from zero:

$$f_F - \frac{\Delta(f_F)m}{\hbar^2 f_F} < f < f_F + \frac{\Delta(f_F)m}{\hbar^2 f_F}.$$

The correlation radius  $r_+$  is a value of order

$$r_+ \sim \left(\frac{\Delta(f_F)}{\epsilon_F}\right)^{-1} r_-,$$

where  $\epsilon_F$  is Fermi energy. Since  $\Delta(f_F) \ll \epsilon_F$  in BCS state, it follows that  $r_+ \gg r_-$ .

Two-spin reduced density matrix equals

$$\hat{\rho}(r) = \frac{1}{\gamma'} \begin{pmatrix} 1 - \phi^2 & 0 & 0 & 0 \\ 0 & 1 + \phi_1^2 & -(\phi^2 + \phi_1^2) & 0 \\ 0 & -(\phi^2 + \phi_1^2) & 1 + \phi_1^2 & 0 \\ 0 & 0 & 0 & 1 - \phi^2 \end{pmatrix},$$

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where

$$\gamma' = 2(2 - \phi^2(r) + \phi_1^2(r)).$$

According to Peres–Horodeski criterion [9] two spins are entangled if  $(2\phi^2(r) - \phi_1^2(r)) > 1$ .

In BCS state when the energy gap  $\Delta_f$  is different from zero only in narrow spherical layer in the neighborhood of  $f_F$  we get  $\phi_1^2(r) \ll 1/2$  everywhere. This means that two-spins entanglement is similar to free electron case and two fermions are entangled if the relative distance between them is smaller than  $1.8r_F$ .

The matrix  $\rho(r)$  has the form

$$\hat{\rho}(r) = (1-p)\frac{\hat{I}}{4} + p|\Psi^{-}\rangle\langle\Psi^{-}|, \quad p = \frac{2(\phi^{2}(r) + \phi_{1}^{2}(r))}{\gamma'},$$

where  $|\Psi^-\rangle = 1/\sqrt{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$  is the maximally entangled spin singlet state of the pair. The range of entanglement is p > 1/3.

#### 3. EQUAL SPIN PAIRING

In superfluid state of <sup>3</sup>He [10] the fermion (s = 1/2) atoms with opposite momentums are pairing in *p*-state with spin of the pair equal unity. We consider one of the Equal Spin Pairing (ESP) state in which the pairing of atoms has the same spin projection, for example, *A*-phase. The quasiparticle operators are defined by transformation

$$\hat{a}\left(\mathbf{f},\frac{1}{2}\right) = u_{\mathbf{f}}\hat{\alpha}\left(\mathbf{f},\frac{1}{2}\right) + v_{\mathbf{f}}\hat{\alpha}^{+}\left(-\mathbf{f},\frac{1}{2}\right),$$
$$\hat{a}\left(\mathbf{f},-\frac{1}{2}\right) = u_{\mathbf{f}}\hat{\alpha}\left(\mathbf{f},-\frac{1}{2}\right) + v_{\mathbf{f}}\hat{\alpha}^{+}\left(-\mathbf{f},-\frac{1}{2}\right),$$

where

$$u_{\mathbf{f}} = u_{-\mathbf{f}}, \quad v_{\mathbf{f}} = -v_{-\mathbf{f}}, \quad u_{\mathbf{f}}^2 + v_{\mathbf{f}}^2 = 1.$$

Correlation function for two fermions with parallel spins equals

$$\mathcal{K}(\mathbf{r},\sigma,\sigma) = n_{\sigma}^{2}(1 - |\phi(r)|^{2} + |\phi_{1}(r)|^{2}),$$

(see (1)–(3)). The particles with parallel spins are correlated. The negative correlation radius is  $r_{-} \sim 1/f_F$ . If energy gap  $\Delta_f$  is essentially different from zero only in the narrow layer near  $f_F$ , then the positive correlation radius is  $r_{+} \sim \left(\frac{\Delta(f_F)}{\epsilon_F}\right)^{-1} r_{-}$  and  $r_{-} \ll r_{+}$ . The opposite spins are not correlated

$$\mathcal{K}(\mathbf{r},\sigma,-\sigma)=n_{\sigma}^2$$

We obtain

$$\hat{\rho}(\mathbf{r}) = \frac{1}{\gamma''} \begin{pmatrix} 1 - |\phi|^2 + |\phi_1|^2 & 0 & 0 & 0 \\ 0 & 1 & -|\phi|^2 & 0 \\ 0 & -|\phi|^2 & 1 & 0 \\ 0 & 0 & 0 & 1 - |\phi|^2 + |\phi_1|^2 \end{pmatrix}$$

where

$$\gamma'' = 2(2 - |\phi(\mathbf{r})|^2 + |\phi_1(\mathbf{r})|^2).$$

According to Peres-Horodeski criterion [9] the condition of entanglement is

$$(2|\phi(\mathbf{r})|^2 - |\phi_1(\mathbf{r})|^2) > 1.$$

In ESP state when the energy gap  $\Delta_f$  is different from zero only in narrow spherical layer in the neighborhood of  $f_F$  we get  $|\phi_1(r)|^2 \ll 1/2$  everywhere. This means that two-spins entanglement is similar to the free electron case.

### CONCLUSION

The two-particle density matrices of Fermi systems with coupling were obtained. We present the relation between the total correlation, the entanglement measure and the pair-distribution functions.

It is well known that the physical properties of the systems depend on the *s*- or *p*-pairing significantly. Nevertheless, in BCS approximation when energy gap is essentially different from zero only in the narrow layer near Fermi surface, the pairing changes two-spins entanglement slightly. Entanglement is essentially defined by Fermi statistics. The existence of Fermi pairs slightly reduced the entanglement measure.

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