Entanglement of electron spins in many-body systems

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Abstract. We study entanglement of electron spins in many-body systems based on the Green's function approach. We obtain the two-particle density matrix of a non-interacting electron gas and examine entanglement between two-electron spins at zero and finite temperatures. If the off-diagonal matrix elements of the space density matrix decay to zero, the two-particle density matrix becomes Vedral's result[quant-ph/0302040].

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Entanglement is considered to be essential in quantum information processing. Much attention has been paid to quantify degrees of entanglement, to generate entangled states, and to apply entangled states to quantum communication and quantum teleportation [1]. Recently there have been considerable works on entanglement properties of many-body systems [2, 3, 4]. In this paper we study these based on the Green's function approach.

Consider a system of N identical particles described by a symmetric or antisymmetric state $|\Psi\rangle$. The density operator of the system $\rho^{(N)} = |\Psi\rangle\langle\Psi|$ is written in the coordinate representation as $\rho^{(N)}(x_1,\ldots,x_N;x'_1,\ldots,x'_N) \equiv (x_1,\ldots,x_N|\rho^{(N)}|x'_1,\ldots,x'_N)$, where $|x_1,\ldots,x_N) \equiv |\mathbf{r}_1\sigma_1\rangle\otimes\cdots\otimes|\mathbf{r}_N\sigma_N\rangle$ and $x\equiv(\mathbf{r},\sigma)$ denotes the position and spin quantum number of a particle. From $\rho^{(N)}$, the one-particle reduced density matrix $\rho^{(1)}$ can be calculated [5]

$$\rho^{(1)}(x_1;x'_1) = N\,\mathrm{Tr}_{x_2,\cdots,x_N}\{\rho^{(N)}\}\,. \tag{1}$$

Note that $\rho^{(1)}$ is normalized to the number of particles, $\mathrm{Tr}\,\{\rho^{(1)}\} = N$. Similarly p-particle reduced density matrices are defined by

$$\rho^{(p)}(x_1,\cdots,x_p;x'_1,\cdots,x'_p) = {}_N\mathrm{C}_p\,\mathrm{Tr}_{x_{p+1},\cdots,x_N}\{\rho^{(N)}\}\,,$$

where ${}_N\mathrm{C}_p = N!/(N-p)!p!$. Notice that $\mathrm{Tr}\{\rho^{(2)}\} = N(N-1)/2$, the number of pairs. If a state of a many-body system is given, then it is possible to calculate a two-particle reduced density matrix directly and to study the entanglement properties between two particles. However, it is impossible to obtain exact many-body states except for very simple systems. Usually one works with the Green's functions to obtain useful physical quantities of many-body systems. We also introduce the Green's function to study entanglement properties of many-body systems.

Let us consider a system of N non-interacting electrons in a box with volume V following Vedral's work [4]. The ground state of the system is given by

$$|\Psi_0\rangle = \prod_{|\mathbf{k}|\le k_F} c^\dagger_{\mathbf{k}\sigma}|0\rangle\,, \tag{2}$$

where $k_F = (3\pi^2 N/V)^{1/3}$ is the Fermi momentum. From the density matrix $\rho^{(N)} = |\Psi_0\rangle\langle\Psi_0|$ of the system, it is straightforward to obtain the two-particle reduced density matrix [6]

$$\rho^{(2)}(x_1,x_2;x'_1,x'_2) = \frac{1}{2}\begin{vmatrix} \rho^{(1)}(x_1;x'_1) & \rho^{(1)}(x_1;x'_2) \\ \rho^{(1)}(x_2;x'_1) & \rho^{(1)}(x_2;x'_2) \end{vmatrix}\,, \tag{3}$$

where the single-particle reduced density matrix $\rho^{(1)}$ can be written by

$$\rho^{(1)}(x;x') = \sum_{k=1}^{N}\phi^*_k(x)\phi_k(x')\,,\quad \phi_k(x) = \frac{1}{\sqrt{V}}e^{\mathbf{k}\cdot\mathbf{r}}\chi_\sigma\,.$$

Using Eq. (3), one can examine entanglement of two-electron spins in free-electron gas.

Now let us obtain Eq. (3) based on the Green's function approach. The one-particle space-spin density matrix in the second quantization is given by [5, 7]

$$\rho^{(1)}(x;x') = \langle\Psi_0|\hat\rho^{(1)}|\Psi_0\rangle = \langle\Psi_0|\hat\psi^\dagger(x')\hat\psi(x)|\Psi_0\rangle\,,$$

where $\hat\rho^{(1)}(x,x') \equiv \hat\psi^\dagger(x_1)\hat\psi(x'_1)$ and $|\Psi_0\rangle$ is the Heisenberg ground state of a system. At zero temperature the single-particle Green's function is defined by

$$iG_{\sigma\sigma'}(\mathbf{r}t,\mathbf{r}'t') = \langle\Psi_0|T[\hat\psi_{H\sigma}(\mathbf{r}t)\hat\psi^\dagger_{H\sigma'}(\mathbf{r}'t')]|\Psi_0\rangle\,, \tag{4}$$

where $\hat\psi_{H\sigma}(\mathbf{r}t)$ is a Heisenberg operator and T is a time ordering operator. Here $\langle\Psi_0|\Psi_0\rangle = 1$ is assumed. One can easily express the single-particle density matrix in terms of the single-particle Green's function

$$\rho^{(1)}(x;x') = -iG_{\sigma,\sigma'}(\mathbf{r}t,\mathbf{r}'t^+)\,, \tag{5}$$

where t' denotes a time infinitesimally later than t. Similarly the two-particle density matrix in the second quantization is written by

$$\rho^{(2)}(x_1,x_2;x'_1x'_2) = \frac{1}{2}\langle\Psi_0|\hat\psi^\dagger(x'_2)\hat\psi^\dagger(x'_1)\hat\psi(x_1)\hat\psi(x_2)|\Psi_0\rangle\,. \tag{6}$$

The two-particle Green's function is defined by

$$\begin{aligned}&G_{\sigma_1\sigma_2;\sigma'_1\sigma'_2}(1,2;1',2')\\ &= (-i)^2\langle\Psi_0|T[\hat\psi_{H\sigma_1}(1)\hat\psi_{H\sigma_2}(2)\hat\psi^\dagger_{H\sigma'_2}(2')\hat\psi^\dagger_{H\sigma'_1}(1')]|\Psi_0\rangle\,,\end{aligned}$$

where the number 1 denotes the variable $(\mathbf{r}_1,t_1)$. For $t'_2 > t'_1 > t_1 > t_2$ and all t's go to zero, the two-particle density

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matrix is related to the two-particle Green's function

$$\rho^{(2)}(x_1,x_2;x_1',x_2') = -\frac{1}{2}G_{\sigma_1\sigma_2;\sigma_1'\sigma_2'}(\mathbf{r}_1 0,\mathbf{r}_2 0;\mathbf{r}_1' 0^+,\mathbf{r}_2' 0^+)\,. \tag{7}$$

Using Wick's theorem, the interacting two-particle Green's function can be written approximately in terms of the single-particle Green's function

$$\begin{aligned} &G_{\sigma_1\sigma_2;\sigma_1'\sigma_2'}(1,2;1',2') \\ &= G_{\sigma_1\sigma_1'}(1,1')G_{\sigma_2\sigma_2'}(2,2') - G_{\sigma_1\sigma_2'}(1,2')G_{\sigma_2\sigma_1'}(2,1')\,. \end{aligned} \tag{8}$$

With Eqs. (8) and (7), we have the same form of Eq. (3). In Eq. (3), the one-particle density matrix is connected with the non-interacting single-particle Green's function

$$\begin{aligned} \rho^{(1)}(x;x') &= -iG^0_{\sigma\sigma'}(\mathbf{r}0,\mathbf{r}'0^+) \\ &= \frac{\delta_{\sigma\sigma'}}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\theta(k_F-k)\,. \end{aligned} \tag{9}$$

Therefore one can obtain the explicit form of the two-particle space-spin density matrix [5, 4]

$$\begin{aligned} \rho^{(2)}_{\sigma_1\sigma_2;\sigma_1'\sigma_2'}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2') &= g(\mathbf{r}_1-\mathbf{r}_1')g(\mathbf{r}_2-\mathbf{r}_2')\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'} \\ &\quad - g(\mathbf{r}_1-\mathbf{r}_2')g(\mathbf{r}_2-\mathbf{r}_1')\delta_{\sigma_1\sigma_2'}\delta_{\sigma_1'\sigma_2}\,, \end{aligned}$$

where the space density matrix $g(\mathbf{r}-\mathbf{r}') = \langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ is given by

$$g(\mathbf{r}) \equiv \frac{1}{V}\sum_{\mathbf{k}}^{k_F} e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{(2\pi)^3}\int_0^{k_F} e^{i\mathbf{k}\cdot\mathbf{r}}dk^3\,. \tag{10}$$

Depending on the space density matrix, the spins are entangled. One obtains Vedral's result [4] only if $\mathbf{r}_1 = \mathbf{r}_1'$ and $\mathbf{r}_2 = \mathbf{r}_2'$. This means the classical limit; only diagonal elements of a space density matrix are considered. In this case one can expect the entanglement of two spins within the Fermi wave length $1/k_F$. In usual metals, the Fermi wave length is order of Å. However we would like to point out that the Fermi wave length of a 2D electron gas is about hundreds Å. Thus it may be possible to extract entangled spins out of a 2D electron gas.

For finite temperature, $T \neq 0$, the two-particle density matrix is defined by

$$\rho^{(2)}(x_1x_2;x_1'x_2') = \frac{1}{2}\mathrm{Tr}\{\rho_G\,\hat\psi^\dagger(x_2')\hat\psi^\dagger(x_1')\hat\psi(x_1)\hat\psi(x_2)\}\,. \tag{11}$$

The two-particle temperature Green's function is defined as

$$\begin{aligned} &\mathcal{G}_{\sigma_1\sigma_2;\sigma_1'\sigma_2'}(1,2;1',2') \\ &\equiv \mathrm{Tr}\{\hat\rho_G\,T_\tau[\hat\psi_{K\sigma_1}(1)\hat\psi_{K\sigma_2}(2)\hat\psi^\dagger_{K\sigma_2'}(2')\hat\psi^\dagger_{K\sigma_1}(1')]\}\,, \end{aligned} \tag{12}$$

where the number 1 denotes the variable $(\mathbf{r}_1,\tau_1)$, $\tau = it$, and

$$\hat\rho_G = \frac{e^{-\beta(\hat H-\mu\hat N)}}{Z_G}\,. \tag{13}$$

A generalized Wick's theorem makes it possible to factor the two-particle temperature Green's function into the single-particle Green's function

$$\begin{aligned} &\mathcal{G}_{\sigma_1\sigma_2;\sigma_1'\sigma_2'}(1,2;1'2') \\ &= \mathcal{G}_{\sigma_1\sigma_1'}(1,1')\mathcal{G}_{\sigma_2\sigma_2'}(2,2') - \mathcal{G}_{\sigma_1\sigma_2'}(1,2')\mathcal{G}_{\sigma_2\sigma_1'}(2,1'), \end{aligned} \tag{14}$$

The single-particle temperature Green's function for a noninteracting system can be easily computed

$$\mathcal{G}^0_{\sigma\sigma'}(\mathbf{r}0;\mathbf{r}'0^+) = -\frac{\delta_{\sigma\sigma'}}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\,n^0_{\mathbf{k}}\,, \tag{15}$$

where $n^0_{\mathbf{k}} = \{\exp[\beta(\epsilon^0_{\mathbf{k}}-\mu)]+1\}^{-1}$ is the mean occupation number in state $\mathbf{k}$. Thus we have the single-particle space density matrix at finite temperatures as follows

$$g(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}}^{k_F} e^{i\mathbf{k}\cdot\mathbf{r}}n^0_{\mathbf{k}}\,. \tag{16}$$

As the temperature goes to high, $g(\mathbf{r}_1-\mathbf{r}_2)$ goes to zero even if $|\mathbf{r}_1-\mathbf{r}_2|$ is less than the Fermi wave length $1/k_F$. Thus one cannot expect the entanglement between two spins at high temperature.

In summary, we examine entanglement of spins in a many-body system based on the Green's function method. For the simple system, the non-interacting electron gas, the exact ground state is well known and one can find the two-particle density matrix directly. However for interacting systems, it is preferable to use the Green's function. It may be interesting to investigate how the entanglement of electron spins could be modified by the interaction between them. Finally we would like to notice that the BCS ground state has the similar form of Eq. (2) and that two electrons of a Cooper pair are naturally entangled [8].

References

[1] V. Vedral. The role of relative entropy in quantum information theory. *Rev. Mod. Phys.*, 74:197–234, 2002.

[2] Y. Omar, N. Paunković, S. Bose, and V. Vedral. Spin-space entanglement transfer and quantum statistics. *Phys. Rev. A*, 65:062305, 2002.

[3] J. R. Gittings and A. J. Fisher. Describing mixed spin-space entanglement of pure states of indistinguishable particles using an occupation-number basis. *Phys. Rev. A*, 66:032305, 2002.

[4] V. Vedral. Entanglement in the second quantization formalism. quant-ph/0302040, 2003.

[5] C. N. Yang. Concept of off-diagonal long-range order and the quantum phases of liquid He and of superconductors. *Rev. Mod. Phys.*, 34:694–704, 1962.

[6] P.-O. Löwdin. Quantum theory of many-particle systems. II. Study of the ordinary Hartree-Fock approximation. *Phys. Rev.*, 97:1490–1508, 1955.

[7] A. L. Fetter and J. D. Waleka. *Quantum Theory of Many-Particle Systems.* McGraw-Hill, 1971.

[8] P. Fulde. *Electron Correlations in Molecules and Solids.* Springer-Verlag, 1991.