From ODLRO to the Meissner Effect and Flux Quantization

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Abstract

It has been shown that the electron system with ODLRO in the reduced density matrix \( \rho_2 \) can not support a uniform magnetic field, i.e., ODLRO in \( \rho_2 \) implies the Meissner effect \(^2\), furthermore, the magnetic field trapped in the system is quantized \(^3\). This note extends above results in two cases. We show that (1) the system with ODLRO in \( \rho_2 \) can not support a non uniform, cylindrically symmetric magnetic field; (2) the system with ODLRO in \( \rho_2 \) can not support a magnetic field slowly varying in space, and the magnetic flux trapped in it is quantized.

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Introduction

In 1962 C. N. Yang proposed that the superconductivity is characterized by the existence of off-diagonal long-range order (ODLRO) in the two-particle reduced density matrix $\rho_2$ for a fermion system\[1\]. However, there was no clear-cut proof to show directly that ODLRO in $\rho_2$ leads to superconductivity for a long time. In recent works \[2\][3], it has been proved that ODLRO in $\rho_2$ implies that a non vanishing uniform magnetic field $B$ can not exist in an electron system, i.e., there is the Meissner effect. Furthermore, it has been shown that the magnetic flux trapped in the system is quantized\[3\]. However, the question of whether a non uniform magnetic field can be expelled from the system with ODLRO in $\rho_2$ is still open. The present work extends \[2\] and \[3\] in two cases. We show that 1. the system with ODLRO in $\rho_2$ can not support a non uniform, cylindrically symmetric magnetic field; 2. the system with ODLRO in $\rho_2$ can not support a non uniform magnetic field, which is slowly varying in space, and the magnetic flux trapped in the system is quantized.

System with Cylindric Symmetry

Consider the case that $N$ electrons are in a circular cylinder. We chose a cylindric coordinates with z-axis along the central line of the cylinder. In which $\mathbf{r} = (R, \theta, z)$, and $\hat{R}, \hat{\theta}$ and $\hat{z}$ are unit vectors along the $R, \theta$ and $z$ direction, respectively. Suppose that the magnetic field is cylindrically...
symmetric, and the gauge to be

\[ \mathbf{A}(\mathbf{r}) = -\theta \mathbf{B}(R) \hat{\mathbf{R}}, \]

where \( \mathbf{B}(R) \) is a continuous function. From (1), we have \( \mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) = \mathbf{B}(R) \hat{z} \). Suppose that the system undergoes an infinitesimal rotation \( \hat{z} \delta \theta \),

\[ \mathbf{A}(\mathbf{r}) \rightarrow -(\theta - \delta \theta) \mathbf{B}(R) \hat{\mathbf{R}} = \mathbf{A}(\mathbf{r}) + \nabla \chi_{\delta \theta}(\mathbf{r}), \]

\[ \chi_{\delta \theta}(\mathbf{r}) = \delta \theta \int_{R_0}^{R} R' \mathbf{B}(R') dR', \]

where \( R_0 \) is a constant. Eq.(2) shows that the rotation induces a gauge transformation. We shall see that it enable us to show that \( \mathbf{B}(\mathbf{r}) = 0 \) as the system has ODLRO in the two particle reduced density matrix \( \rho_2 \).

The Schrödinger equation of the electrons is

\[ \frac{1}{2m} \sum_{j} \left[ \frac{\hbar}{i} \nabla_j + e \mathbf{A}(\mathbf{r}_j) \right]^2 \psi_n(\mathbf{r}_1, ..., \mathbf{r}_N) + U(\mathbf{r}_1, ..., \mathbf{r}_N) \psi_n(\mathbf{r}_1, ..., \mathbf{r}_N) = E_n \psi_n(\mathbf{r}_1, ..., \mathbf{r}_N). \]

We assume that the potential \( U(\mathbf{r}_1, ..., \mathbf{r}_N) \) depends only on the distances between electrons. Under the rotation, (3) becomes

\[ \frac{1}{2m} \sum_{j} \left[ \frac{\hbar}{i} \nabla_j + e \mathbf{A}(\mathbf{r}_j) \right]^2 \psi'_n(\mathbf{r}_1, ..., \mathbf{r}_N) + U(\mathbf{r}_1, ..., \mathbf{r}_N) \psi'_n(\mathbf{r}_1, ..., \mathbf{r}_N) = E_n \psi'_n(\mathbf{r}_1, ..., \mathbf{r}_N), \]

where

\[ \psi'_n(\mathbf{r}_1, ..., \mathbf{r}_N) = \psi_n(\mathbf{r}_1 - \delta \mathbf{r}_1, ..., \mathbf{r}_N - \delta \mathbf{r}_N) \exp\left[ \frac{ie}{\hbar} \sum_j \chi_{\delta \theta}(\mathbf{r}_j) \right], \]

\[ \delta \mathbf{r}_i = \hat{\theta}_i R_i \delta \theta. \]

Both \( \{ \psi_n \} \) and \( \{ \psi'_n \} \) are complete sets of orthonormal eigenfunctions of the Hamiltonian, which are single-valued in \( \mathbf{r}_i \).
The element of the reduced density matrix for two particles can be expressed as

\[
\rho_2(r'_1, r'_2; r_1, r_2) = \int \cdots \int \frac{d\mathbf{r}_3 \cdots d\mathbf{r}_N}{(N-2)!} \frac{1}{Z} \sum_n \exp(-E_n/kT) \times \psi_n(r'_1, r'_2, r_3, \ldots, r_N) \psi_n^*(r_1, r_2, r_3, \ldots, r_N),
\]

where \(Z\) is the partition function, and \(T\) the temperature. Substituting \(\psi'_n\) for \(\psi_n\) makes no change for \(\rho_2\), since \(\rho_2\) is basis independent. So we also have

\[
\rho_2(r'_1, r'_2; r_1, r_2) = \int \cdots \int \frac{d\mathbf{r}_3 \cdots d\mathbf{r}_N}{(N-2)!} \frac{1}{Z} \sum_n \exp(-E_n/kT) \times \psi'_n(r'_1, r'_2, r_3, \ldots, r_N) \psi'_n^*(r_1, r_2, r_3, \ldots, r_N),
\]

Expressing the primed \(\psi'_n\) in (7) in terms of the non primed \(\psi_n\), we obtain

\[
\rho_2(r'_1, r'_2; r_1, r_2) = \exp\left\{\frac{ie}{\hbar} \left[\chi_\delta \theta(r'_1) + \chi_\delta \theta(r'_2) - \chi_\delta \theta(r_1) - \chi_\delta \theta(r_2)\right]\right\}
\]

\[
\times \int \cdots \int \frac{d\mathbf{r}_3 \cdots d\mathbf{r}_N}{(N-2)!} \frac{1}{Z} \sum_n \exp(-E_n/kT) \times \psi_n(r'_1 - \delta r_1, r'_2 - \delta r_2, r_3 - \delta r_3, \ldots, r_N - \delta r_N)
\]

\[
\times \psi_n^*(r_1 - \delta r_1, r_2 - \delta r_2, r_3 - \delta r_3, \ldots, r_N - \delta r_N).
\]

Shift the integration variables, \(\theta_i \rightarrow \theta_i + \delta \theta, i = 3, \ldots, N\). Note that \(r_i - \delta r_i = (R_i, \theta_i - \delta \theta, z_i)\). We obtain a relation for \(\rho_2\) at different space points:

\[
\rho_2(r'_1, r'_2; r_1, r_2) = \exp\left\{\frac{ie}{\hbar} \left[\chi_\delta \theta(r'_1) + \chi_\delta \theta(r'_2) - \chi_\delta \theta(r_1) - \chi_\delta \theta(r_2)\right]\right\}
\]

\[
\times \rho_2(r'_1 - \delta r_1, r'_2 - \delta r_2; r_1 - \delta r_1, r_2 - \delta r_2).
\]

By definition, the ODLRO in \(\rho_2\) means that

\[
\rho_2(r'_1, r'_2; r_1, r_2) \rightarrow \Phi(r'_1, r'_2)\Phi^*(r_1, r_2),
\]
as \(|r'_i - r'_j|, i, j = 1, 2,\) approaches macroscopic distances, and \(\Phi(r_1, r_2)\)
does not vanish as \(|r_1 - r_2|\) and \(|r'_1 - r'_2|\) remain finite in microscopic scale.
Where \(\Phi\) is the eigenfunction of \(\rho_2\) with the largest eigenvalue. If we assume
ODLRO in \(\rho_2\), (8) and (9) lead to

\[
\Phi(r_1, r_2) = \exp[i\alpha(\delta \theta)] \exp\left\{ \frac{ie}{\hbar} [\chi_{\delta \theta}(r_1) + \chi_{\delta \theta}(r_2)] \right\} 
\times \Phi(r_1 - \delta r_1, r_2 - \delta r_2),
\]

(11)

where \(\alpha(\delta \theta)\) is a real function of \(\delta \theta\), and it is independent of \(r_1, r_2\). It is easily
seen that \(\alpha(\delta \theta + \delta \theta') = \alpha(\delta \theta) + \alpha(\delta \theta')\), \(\alpha(0) = 0\).

Rotating the system successively, as \(\sum \delta \theta = 2\pi\), we have \(\sum \delta r_1 = \sum \delta r_2 = 0\). \(\Phi(r_1, r_2)\) is single-valued because \(\psi_n\) is single-valued. Thus, we obtain from
(10)

\[
\exp[i\alpha(2\pi)] \exp\left\{ \frac{ie}{\hbar} 2\pi \left[ \int_{R_0}^{R_1} RB(R) dR + \int_{R_0}^{R_2} RB(R) dR \right] \right\} = 1.
\]

(12)

(12) leads to

\[
\frac{\hbar}{e} \alpha(2\pi) + 2\pi \int_{R_0}^{R_1} RB(R) dR + \int_{R_0}^{R_2} RB(R) dR = n \frac{\hbar}{e}, \quad n = \text{integers}.
\]

(13)

On the left hand side of (13), \(R_1\) and \(R_2\) can be changed continuously. Let \(R_1 \to R_1 + dR_1\), the left hand of (13) gets an infinitesimal increment
\(2\pi R_1 B(R_1) dR_1\). On the other hand, the right hand side only takes discrete
values. To be consistent, we have to take \(B(R_1) = 0\). Since \(R_1\) is arbitrary
in the system, we obtain

\[
\mathbf{B}(r) = 0.
\]

(14)

Thus a non vanishing cylindrically symmetric magnetic field can not exist in
the system with ODLRO in \(\rho_2\). In other words, the magnetic field is expelled
from the system, i.e., there is the Meissner effect.
Electrons in the Magnetic Field Slowly Varying in Space

Consider the case of electrons in a magnetic field which is slowly varying in space. The vector potential can be written as

\[ A(r) = A_0(r) + \nabla \varphi(r), \]  

(15)

and \( B(r) = \nabla \times A_0(r) \). In general, \( \varphi(r) \) is multi-valued, however, \( \nabla \varphi(r) \) is single-valued.

Under an infinitesimal translation \( \delta r \),

\[ A(r) \to A_0(r - \delta r) + \nabla \varphi(r - \delta r) = A(r) - \delta r \cdot \nabla [A_0(r) + \nabla \varphi(r)]. \]  

(16)

In (16)

\[ \delta r \cdot \nabla A_0 = \nabla (\delta r \cdot A_0) - \delta r \times B \]

\[ = \nabla (\delta r \cdot A_0) - \nabla [\delta r \cdot (B \times r)] + [(\delta r \cdot \nabla)B] \times r + \delta r \times [(r \cdot \nabla)B]. \]  

(17)

Provided that \( B(r) \) is slowly varying, such that

\[ |\delta r \times B| >> \|[(\delta r \cdot \nabla)B] \times r + \delta r \times [(r \cdot \nabla)B]\| \]  

(18)

i.e., roughly speaking, \( |\nabla B_i| / |B|, i = x, y, z, \) is much less than \( L^{-1} \), where \( L \) is the linear dimension of the system. Under this condition, we can write

\[ \delta r \cdot \nabla A_0 = \nabla (\delta r \cdot A_0) - \nabla [\delta r \cdot (B \times r)], \]  

(19)

and (16) becomes

\[ A(r) \to A(r) + \nabla [\delta r \cdot (B \times r) - \delta r \cdot A_0 - \delta r \cdot \nabla \varphi(r)]. \]  

(20)
We see that the infinitesimal translation induces a gauge transformation. In the Hamiltonian of the system,

\[ H = \sum_j \frac{1}{2m} \left[ -i\hbar \nabla_j + \frac{e}{c} A(r_j) \right]^2 + U(r_1, ..., r_N), \]  

we assume that the potential \( U(r_1, ..., r_N) \) depends only on the distances between electrons. Suppose that \( \{\psi_n\} \) is a complete set of single-valued orthonormal eigenfunctions of the Hamiltonian. Then \( \{\psi'_n\} \) is also a complete set of single-valued orthonormal eigenfunctions of the Hamiltonian [3], where

\[ \psi'_n(r_1, ..., r_N) = e^{ie_c\bar{\hbar}\sum_j \chi_{\delta r}(r_j)}\psi_n(r_1 - \delta r, ..., r_N - \delta r), \]  

and

\[ \chi_{\delta r}(r_j) = \delta r \cdot [B(r_j) \times r_j - A_0(r_j) - \nabla_j \varphi(r_j)]. \]  

Repeating the discussion similar to that leads to (8) (see also [3]), we have

\[ \rho_2(r'_1, r'_2; r_1, r_2) = \exp\{\frac{ie}{\hbar}[\chi_{\delta r}(r'_1) + \chi_{\delta r}(r'_2) - \chi_{\delta r}(r_1) - \chi_{\delta r}(r_2)]\} \]
\[ \times \rho_2(r'_1 - \delta r, r'_2 - \delta r; r_1 - \delta r, r_2 - \delta r). \]  

If there is ODLRO in \( \rho_2 \), (10) is valid, and

\[ \Phi(r_1, r_2) = \exp[i\alpha(\delta r)] \exp\{\frac{ie}{\hbar}[\chi_{\delta r}(r_1) + \chi_{\delta r}(r_2)]\} \Phi(r_1 - \delta r, r_2 - \delta r), \]  

where \( \alpha(\delta r) \) is real, and not dependent on \( r_1, r_2 \). It is easily seen that \( \alpha(\delta r_1 + \delta r_2) = \alpha(\delta r_1) + \alpha(\delta r_2) \), and \( \alpha(0) = 0 \). Repeating successively for infinitesimal displacements along a closed path, and noting the single-valuedness of \( \Phi(r_1, r_2) \), we obtain from (25) the relation

\[ \exp\{i \sum \alpha(\delta r)\} \exp\{\frac{2ie}{\hbar} \oint dr \cdot [B(r) \times r - A_0(r) - \nabla \varphi(r)]\} = 1. \]
where the summation $\sum \alpha(\delta r)$ is over the closed path. In a simply connected region, around a sufficiently small contour, on which $\mathbf{B}$ can be considered as a constant vector, we have $\oint \mathbf{r} \cdot [\mathbf{B}(\mathbf{r}) \times \mathbf{r}] = 2\phi$, $\oint \mathbf{r} \cdot \mathbf{A}_0(\mathbf{r}) = \phi$, where $\phi$ is the magnetic flux through the surface spanned by the small contour, and $\oint \mathbf{r} \cdot \nabla \varphi(\mathbf{r}) = 0$, $\sum \alpha(\delta \mathbf{r}) = 0$. We obtain,

$$\exp\left\{\frac{2ie}{\hbar} \oint \mathbf{r} \cdot [\mathbf{B}(\mathbf{r}) \times \mathbf{r} - \mathbf{A}_0(\mathbf{r})]\right\} = \exp\left\{\frac{2ie}{\hbar} \phi\right\} = 1. \quad (27)$$

Thus

$$\phi = n\frac{\hbar}{2e}, \quad n = \text{integers}. \quad (28)$$

The contour can be deformed continuously. If $\mathbf{B} \neq 0$, the flux $\phi$ can be changed continuously. Which is in contradiction to the right hand side of (28). To be consistent, we conclude that $\mathbf{B} = 0$. It means that the system with ODLRO in $\rho_2$ can not support a magnetic field slowly varying in space, i.e., there is the Meissner effect.

Since $\mathbf{B} = 0$, we can take $\mathbf{A}_0 = 0$. When the path is not simply connected, e.g., it winds around an inaccessible tunnel, the path can not be deformed across this inaccessible region. In this case we still have $\sum \alpha(\delta \mathbf{r}) = 0\text{[3]}$, from (26), we obtain $\exp\left\{\frac{2ie}{\hbar} \oint \mathbf{r} \cdot \nabla \varphi(\mathbf{r})\right\} = 1$, thus

$$\oint \mathbf{r} \cdot \nabla \varphi(\mathbf{r}) = n\frac{\hbar}{2e}, \quad n = \text{integers}. \quad (29)$$

This equation shows that the magnetic flux trapped in the tunnel is quantized.

In summary, we have shown that if there is ODLRO in the reduced density matrix $\rho_2$, 1. the system can not support a cylindrically symmetric magnetic field; 2. the system can not support a slowly varying magnetic field. In these
two cases, we have derived the Meissner effect from the existence of ODLRO in $\rho_2$. Furthermore, in the latter case, we have shown that the magnetic flux trapped in the system is quantized. We know that the magnetic field is not vanishing, e.g., in the boundary region in superconductor. This fact is not in contradiction to our result, since the non vanishing magnetic field is in the region where it varies rapidly.

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[5] For a detail discussion about $\exp\{i \sum \alpha(\delta r)\} = 1$ on a closed path, see [2], where $\exp\{i \sum \alpha(\delta r)\}$ is written as $F(C)$. 

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