Friedel Oscillation in Charge Profile and Position Dependent Screening around a Superconducting Vortex Core

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We calculate microscopically the charge distribution around a vortex in type II superconductors by solving the Bogoliubov–de Gennes equation and the Poisson equation simultaneously. Our calculations show that the charge density depletion occurs in the vortex center and the Friedel oscillation appears over the coherence length when \( k_F \xi \) is small. We also calculate the density-density correlation function \( K(r, r') \) as a function of two spatial variables, \( r \) and \( r' \), and find that \( K(r, r') \) is strongly dependent on the distance from the vortex center. We clarify the spatial dependent screening properties on the basis of the correlation function in the core region.

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Recently, the electronic structure in a vortex core in type II superconductors has attracted a great interest in connection with the anomalous electronic states in high-\( T_c \) superconductors. It has been extensively discussed whether the vortex core has an electric charge or not [1–6] and also whether it is magnetized or not [7–9]. However, these issues have not yet been fully solved even within the conventional BCS theory. In this Letter we perform full microscopic calculations for the charge distribution around a vortex core and unveil the charge profile and the screening effect in the single-vortex state.

Since the observation of the anomalous Hall sign change in high-\( T_c \) cuprates [10], several mechanisms of charged vortices have been suggested [1,4,5]. Noting that the chemical potential in the superconducting state in superconductors breaking the particle-hole symmetry differs from that in the normal state, Khomskii and Freimuth pointed out that the chemical potential difference causes charge redistribution in between the normal region in a vortex core and the periphery superconducting region; that is, the vortex core should be charged up [1]. Blatter et al. calculated phenomenologically the charge profile around a vortex core on the basis of this charging mechanism [11]. On the other hand, Hayashi et al. showed that vortices are intrinsically charged up in superconductors having a small value of \( k_F \xi \), solving the Bogoliubov–de Gennes equation [4]. The charging mechanism in such a system is independent of whether the electron system has particle-hole symmetry or not; that is, the induced charge originates from the depletion of the matter density in a vortex core which is commonly observed in a neutral superfluid system. However, in their calculations the screening effect due to the Coulomb repulsion between superconducting electrons is neglected. Afterwards, Koláček et al. extended the Ginzburg-Landau theory to include the scalar potential and formulated phenomenologically the intrinsic depletion mechanism in charged superconductors [5]. Very recently, Matsumoto et al. also performed microscopic calculations, using the Bogoliubov–de Gennes equation coupled with the Poisson equation [12]. Although many studies concerning the vortex charge have so far been performed, its origin and also the charge profile around a vortex have not yet been solved completely on the basis of microscopic calculations. In this Letter we clarify how the vortex is charged up and unveil a novel feature in the charge profile in the vortex state.

In obtaining the charge profile in a superconductor the screening effect cannot be neglected [13]. The charge screening of the Thomas-Fermi type and the Friedel oscillations appearing in the induced charge profile are well known in the normal state of a charged Fermi liquid [13]. The former one works in a classical charged liquid, too, while the latter one has the quantum mechanical origin. Fetter investigated the screening effect in the superconducting state and showed that the Thomas-Fermi screening is dominant; that is, the Friedel oscillations diminish in the Meissner state [14]. This is because the Fermi surface becomes obscure in the presence of a superconducting gap. However, such a simple picture for the charge screening in the superconducting state breaks down in the vortex core region, since the low-energy quasiparticles in a vortex core behave like normal electrons, which implies that the Friedel oscillation appears around a vortex core. Hence, one understands that the Thomas-Fermi screening employed in previous phenomenological studies [5,11] is justified only in the region far from the vortex core and then a full microscopic treatment is required for obtaining the accurate charge profile in the vortex state. In this Letter, we perform extensive numerical studies for the Bogoliubov–de Gennes equation including the scalar potential in the single-vortex state.
Poisson equations are derived as follows:

\[ H = H_{BCS} + \int dr \left\{ e\hat{n}(r)\phi(r) + \frac{E^2(r)}{8\pi} \right\}, \]

where \( \hat{n}(r) \) is the density operator, \( \phi \) is the scalar potential, and \( E \) is the electric field. From Eq. (1) the BdG and Poisson equations are derived as follows:

\[
\begin{align*}
[\xi(\nabla) + e\phi]u_n(r) + \Delta(r)u_n(r) &= E_n u_n(r), \\
-\xi(\nabla) + e\phi]v_n(r) + \Delta^*(r)u_n(r) &= E_n v_n(r), \\
-\nabla^2 \phi(r) &= 4\pi \rho(r),
\end{align*}
\]

where \( \xi(\nabla) \equiv -\frac{\hbar^2}{2m} \nabla^2 - E_F \), and \( \rho(r) \equiv e\langle \hat{n}(r) \rangle \). These equations have to be self-consistently solved together with the gap equation \( \Delta(r) = g \sum_i u_{n_i}(r)v_{n_i}^*(r) \). In this Letter, we drop the vector potential \( A(r) \) since the effect of the superconducting current is small [4]. We also concentrate on the \( T = 0 \) case. Consider an isolated vortex in an s-wave superconductor. The eigenfunctions, \( u_n(r) \) and \( v_n(r) \), which are classified in terms of the angular momentum \( \mu \), are expanded as

\[
\begin{align*}
u_{n,\mu}(r) &= \sum_{l} c_{-l,1} \phi_{l,\mu-1/2}(r) \exp[i(\mu - 1/2)\theta], \\
\end{align*}
\]

for \( \phi_{l,m}(r) \equiv [\sqrt{2}/R]J_{m+1}(\alpha_{lm}r/R), \ |\mu| = 1/2, 3/2, 5/2 \cdots, \) and \( \ell \) is an integer ranging from \( \ell = 1 \) to \( N \), depending on the value \( \mu \). Thus, the BdG equation in Eq. (2) can be solved as an eigenvalue problem for \( 2N(\mu) \times 2N(\mu) \) matrices [15]. On the other hand, the Poisson equation, i.e., the third line of Eq. (2), is solved using the expansions, \( \phi(r) = \sum_l f_l \phi_{l,\mu}(r) \) for \( \phi(r)[= \phi(r)] \) and \( \rho(r) = e \sum_n |u_n(r)|^2 \).

Now we present the numerical results. Figures 1(a) and 1(b) show the dependence of the gap \( \Delta(r) \) and the charge density \( \rho(r) \) on the radial distance \( r \) from the vortex center in the case of \( k_F \xi = 4 \). Black and red lines in these figures represent the results, respectively, for the neutral \( (\phi = 0) \) and the charged \( (\phi \neq 0) \) cases. In the neutral case, the present calculation is essentially the same as that by Hayashi et al. in the quantum limit, i.e., in the small \( k_F \xi \) case [16]. In this limit \( \Delta(r) \) shows oscillatory behavior around a vortex core, as seen in Fig. 1(a). It is also noted that the gap suppression due to the Coulomb effect in the charged case is very tiny. On the other hand, as seen in Fig. 1(b), the charge distribution in the vortex core in the charged case is quantitatively very different from that in the neutral case, though in both cases the charge density is depleted near the vortex center. Note that the charge depletion in the vortex core is compensated so as to reduce the Coulomb energy and the strong oscillations with the sign changes appear in the charge density profile, \( |\rho(r) - \rho_{\infty}| \), in the charged case. This result is sharply contrasted with that in the neutral case; that is, \( |\rho(r) - \rho_{\infty}| \) does not show the change of signs. It is also noted that the oscillations in \( \rho(r) \) have the characteristic length \( \pi/k_F \) and survive over the coherence length. Such a charge profile is also seen for larger values of \( k_F \xi \), but the amplitude of the oscillations in \( |\rho(r) - \rho_{\infty}| \) shrinks for larger \( k_F \xi \). We have checked this tendency by performing calculations up to \( k_F \xi = 16 \).

From these results one notices that the simple screening of the Thomas-Fermi type does not work in the vortex state; that is, the oscillatory distribution appears in the induced charge profile, especially in the small \( k_F \xi \) cases. In Fig. 2(a) we present a 3D plot of \( \rho(r) \) to demonstrate the oscillatory behavior more clearly. \( \rho(r) \) vs \( r \) is also shown in Fig. 2(b). As seen in these figures, the oscillations extend over the coherence length even for \( k_F \xi = 8 \), though its extension is shortened compared to that in the case of \( k_F \xi = 4 \). Furthermore, we check how the range in which the oscillations appear varies with changing the values of \( k_F \xi \). We define the characteristic decay length \( \lambda_F \) at which the charge oscillation amplitude decreases below \( 10^{-2} \) of the maximum amplitude. It is seen that in all the cases the charge density attains \( \rho_{\infty} \) after about 5 times of oscillations. In Fig. 3 we plot the ratio \( \lambda_F/\xi \) as a function of \( k_F \xi \). The ratio decreases with increasing the value of \( k_F \xi \). Note that the decay length is much longer than \( \xi \) in the case of \( k_F \xi = 4 \), i.e., in the quantum limit. Since \( k_F \xi \) is ranging from 4 to 10 in high-\( T_c \) superconductors, one may expect that such charge density oscillations are observable in the vortex states.
Let us next study the origin of the oscillations. As is well known, some of the wave functions for the quasiparticle states in an s-wave superconductor are localized in a vortex core and they oscillate with periods of about $2\pi/k_F$ since their energy is in the very vicinity of the Fermi level. In the other hand, the extended quasiparticle states have the energy being scattered from $-E_F$ to 0 and therefore their wave functions oscillate with various periods. From this fact one may understand that the charge density oscillations are caused mainly by the localized quasiparticles; that is, the oscillations can be regarded as the Friedel oscillations produced by the core states. In fact, numerical calculations for various values of $k_F\xi$ reveal that the oscillations appear only around the vortex core and their period is nearly equal to $\pi/k_F$. One can also confirm this by comparing the oscillation periods in Figs. 1(b) and 2(b). The ratio of the period to $\xi$ given in Fig. 1(b) is about 2 times longer than that in Fig. 2(b). Note that the oscillatory charge distribution cannot be seen in the Meissner state in which the charge inhomogeneity is exponentially screened out, i.e., the Thomas-Fermi screening effect [14].

Now, let us study the screening properties near a vortex core in the presence of an external electric field on the basis of the linear response theory. The dielectric response to the external scalar potential in the vortex state is given in [17]. The induced electron density $n_{in}$ at $T = 0$ K is expressed as

$$n_{in}(r) = \int dr'K(r, r')\phi_{ext}(r'), \quad K(r, r') = -e^2\sum_{ij} F_{ij}(r, r') + F_{ij}^*(r, r')/E_i + E_j,$$

where $\phi_{ext}(r)$ is the external scalar potential. In this Letter we focus on the case in which the external scalar potential is rotationally invariant for simplicity. In this case the kernel, $K(r, r')$, depends only on the two spatial variables in the radial direction $r$ and $r'$, i.e., $K(r, r') \equiv K(r, r')$ [17]. Then, $K(r, r')$ is simplified as

$$K(r, r') = \sum_{n, m} \sum_{\mu} f_{n, m, -\mu}^{\mu}(r, r') + f_{n, m, -\mu}^{\mu}(r, r')/E_{n, \mu} + E_{m, -\mu},$$

where

$$f_{n, m, -\mu}^{\mu} = u_{n, \mu}(r)u_{n, \mu}(r')v_{m, -\mu}(r)v_{m, -\mu}(r) + u_{n, \mu}(r)u_{n, \mu}(r')u_{m, -\mu}(r)u_{m, -\mu}(r).$$

Figure 4(a) shows the spatial dependence of $K(r, r')$ for fixed values, $r' = 1, 8,$ and 130 in the atomic unit. The sites having distances $r' = 1$ and 8 are in the vortex core, while the points located at a distance $r' = 130$ are outside of it. It is noted that $|K(r, r')|$ does not take a maximum value at $r = r'$ in the case of $r' = 1$, i.e., $r'$ being fixed near a point close to the vortex center, which indicates the disappearance of the self-correlation in the neighborhood of the vortex center, though it takes the maximum at $r = r'$ for larger values, $r' = 8$ and 130. From these results one may conclude that the density depletion occurring in the core region cannot be compensated near the vortex center and, then, the charge redistribution due to the screening effect takes place mainly in the periphery region [18].
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 calculations, we employ the two-dimensional free electron


 Finally we point out that the charging mechanism
effect around the two sites, \( r' = 8 \) and 130. As seen in
Fig. 4(a), \( K(r, r') \) almost monotonically decays as \( r \) leaves
\( r' = 130 \), while it shows large oscillations, i.e., the
Friedel oscillations, around the core edge in the case of
\( r' = 8 \), which indicates that the Friedel oscillation devel-
ops in the vortex core region, while the Thomas-Fermi-
type screening is dominant in the region outside the
vortex core. Hence, one may conclude that the core states
in the vicinity of the Fermi level contribute to the oscil-
atory screening behavior near the core region. We also
note that the Friedel oscillation becomes more remarkable
in the quantum limit and also in the \( d \)-wave case. Since
the low-energy quasiparticles in the nodal directions also
contribute to the Friedel oscillation in the \( d \)-wave case
[19], one understands that the Friedel oscillation is an
essential character in the charge distribution near a vor-
tex core in high-\( T_c \) superconductors.

Finally we point out that the charging mechanism
discussed in this Letter is close to that proposed by
Kolářek et al. [5]; that is, the vortex charge is induced
mainly by the intrinsic density depletion in the vortex
core. Our microscopic calculation reveals that the intrin-
sic depletion cannot be suppressed near the vortex center
and then the strong Friedel oscillation appears in the core
region. Thus, the charge profile in the vortex state is
essentially different from that obtained in terms of the
simple Thomas-Fermi–type screening effect. In our cal-
culations, we employ the two-dimensional free electron
model having approximately the particle-hole symmetry.
The effect of the particle-hole asymmetry considered by
Khomskii et al. [1] and Blatter et al. [11] may be incorpo-
rated into our calculations by introducing the energy
dependent electron mass \([ m \rightarrow m^*(E) ] \) [3]. We have found
that the effect of the particle-hole asymmetry for the
vortex charge is very small within a reasonable range of
\( m^*(E) \), that is, the density depletion mechanism is always
dominant in small \( k_F \xi \) cases. From this result one under-
stands that the sign of the charge emerging in the vortex
core is almost uniquely determined in charged supercon-
dering systems with a small value of \( k_F \xi \) as long as other
strong charging mechanisms do not work. In fact,
Kumagai et al. have observed the carrier depletion in
the vortex core in the overdoped region, where the corre-
lation between electrons is relatively weak [6].

In summary, we microscopically calculated the charge
profile around a vortex in charged superconductors. For a
small value of \( k_F \xi \) the vortex is intrinsically charged up
due to the density depletion mechanism. The Friedel
oscillation appears in the charge profile in the region
near the vortex core, especially in the small \( k_F \xi \) case.
We believe that the Friedel oscillation plays an important
role in the formation of the vortex core states in high-\( T_c \)
superconductors.

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references therein.
(2002).
[18] M. Machida and T. Koyama, Physica (Amsterdam)
[19] In \( d \)-wave vortex, the low-lying excitations are aniso-
tropically distributed. Therefore, the anisotropic Friedel
oscillation is expected.