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

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state. Using the solutions, the density-density correlation function is calculated as a function of the distance from the vortex center. The charge profile and the screening effect are shown to have strong spatial dependence in the vortex state.

The BCS Hamiltonian for a charged superconductor is written as

$$H = H_{\rm BCS} + \int d\mathbf{r}\left\{e\hat{n}(\mathbf{r})\phi(\mathbf{r}) + \frac{\mathbf{E}^2(\mathbf{r})}{8\pi}\right\}, \tag{1}$$

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

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

where $\xi(\nabla) \equiv -\frac{\hbar^2}{2m}\nabla^2 - E_F$, and $\rho(\mathbf{r}) \equiv e\langle\hat{n}(\mathbf{r})\rangle$. These equations have to be self-consistently solved together with the gap equation $\Delta(\mathbf{r}) = g\sum_n u_n(\mathbf{r})v_n^*(\mathbf{r})$. In this Letter, we drop the vector potential $A(\mathbf{r})$ 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, $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$, which are classified in terms of the angular momentum μ, are expanded as

$$\begin{aligned} u_{n,\mu}(\mathbf{r}) &= \sum_i c_{n,i}\phi_{i,\mu-1/2}(r)\exp[i(\mu - 1/2)\theta],\\ v_{n,\mu}(\mathbf{r}) &= \sum_i d_{n,i}\phi_{i,\mu+1/2}(r)\exp[i(\mu + 1/2)\theta], \end{aligned} \tag{3}$$

where $\phi_{i,m}(r) \equiv [\sqrt{2}/RJ_{m+1}(\alpha_{im})]J_m(\alpha_{im}r/R)$, $|\mu| = 1/2, 3/2, 5/2\cdots$, and i is an integer ranging from $i = 1$ to N, depending on the value μ. 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, $\phi(r) = \sum_i f_i\phi_{i0}(r)$ for $\phi(\mathbf{r})[\equiv \phi(r)]$ and $\rho(r) = e\sum_n |v_n(r)|^2$.

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

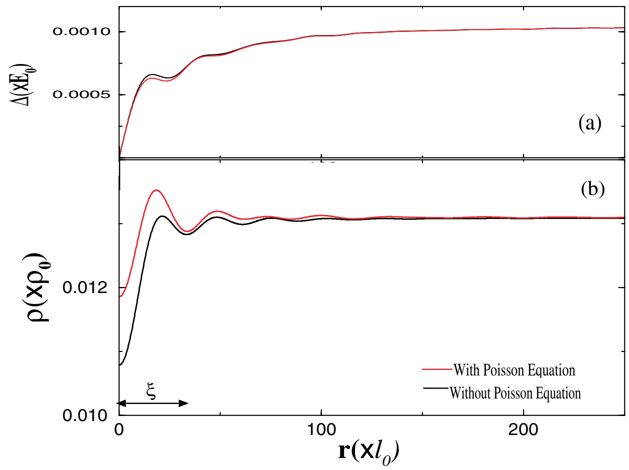

FIG. 1 (color). Spatial dependence of the gap function $\Delta(r)$ (a) and the charge density $\rho(r)$ (b) for $k_F\xi = 4$ with $\xi = 18.5$ Å. r is the distance from the vortex center, which is normalized in terms of the unit length l_0 ($\equiv 0.5292$ Å) in the atomic unit.

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 π/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 $\rho(\mathbf{r})$ 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 λ_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 ρ_∞ after about 5 times of oscillations. In Fig. 3 we plot the ratio λ_F/ξ 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 ξ in the case of $k_F\xi \approx 4$, 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.

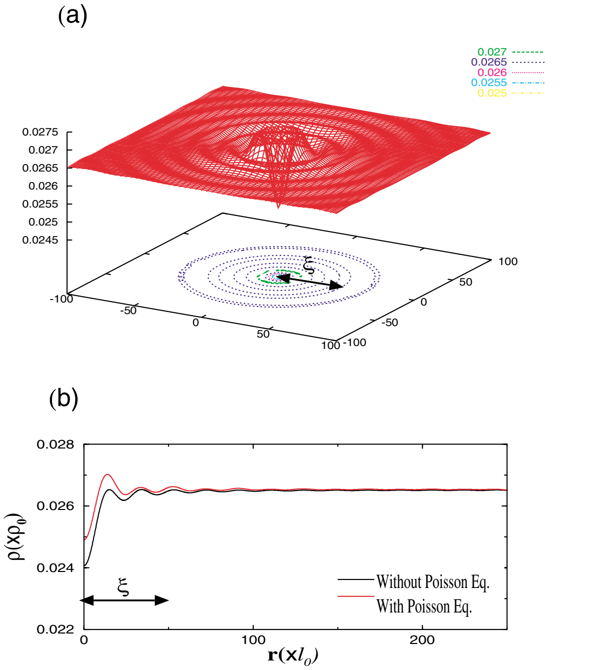

FIG. 2 (color). (a) 3D plot and contour map of the charge density profile in the case of $k_F\xi = 8$. The line with arrows at both ends gives a measure of the coherence length. (b) Spatial dependence of the charge density. The parameter values are the same as in (a).

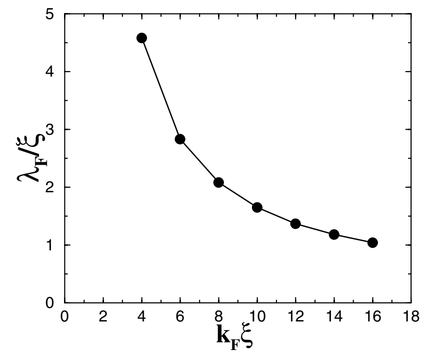

FIG. 3. $k_F\xi$ dependence of λ_F/ξ, where λ_F is the decay length of $\rho(r) - \rho_\infty$.

Let us next study the origin of the oscillations. As is well known, some of the wave functions for the qausi-particle 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. On 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 π/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 ξ 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 $n_{\rm in}$ at $T = 0$ K is expressed as

$$n_{\rm in}(\mathbf{r}) = \int d\mathbf{r}' K(\mathbf{r}, \mathbf{r}')\phi_{\rm ext}(\mathbf{r}'), \qquad K(\mathbf{r}, \mathbf{r}') = -e^2 \sum_{ij} \frac{F_{ij}(\mathbf{r}, \mathbf{r}') + F_{ij}^*(\mathbf{r}, \mathbf{r}')}{E_i + E_j},$$
$$F_{ij}(\mathbf{r}, \mathbf{r}') = 2[u_i(\mathbf{r})v_j(\mathbf{r})u_i^*(\mathbf{r}')v_j^*(\mathbf{r}') + u_i(\mathbf{r})v_j(\mathbf{r})u_j^*(\mathbf{r}')v_i^*(\mathbf{r}')], \tag{4}$$

where $\phi_{\rm ext}(\mathbf{r})$ 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, $K(\mathbf{r}, \mathbf{r}')$, depends only on the two spatial variables in the radial direction r and r', i.e., $K(\mathbf{r}, \mathbf{r}')$ [$\equiv K(r, r')$] [17]. Then, $K(r, r')$ is simplified as

$$K(r, r') = \sum_{n,m}\sum_{\mu} \frac{f_{n,m}^{\mu,-\mu}(r, r') + f_{m,n}^{-\mu,\mu}(r, r')}{E_{n,\mu} + E_{m,-\mu}}, \tag{5}$$

where

$$f_{n,m}^{\mu,-\mu} = u_{n,\mu}(r)u_{n,\mu}(r')v_{m,-\mu}(r')v_{m,-\mu}(r) + u_{n,\mu}(r)v_{n,\mu}(r')u_{m,-\mu}(r')v_{m,-\mu}(r). \tag{6}$$

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].

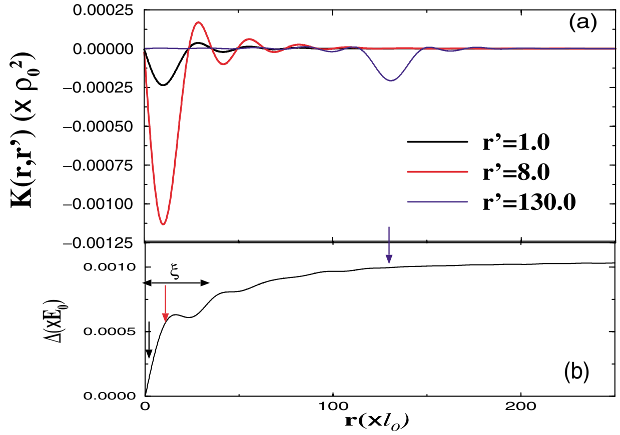

FIG. 4 (color). The spatial dependence of (a) the charge density correlation function $K(r, r')$ for fixed values r' ($=$ 1.0, 8.0, and 130.0) and (b) the gap function $\Delta(r)$ in the case of $k_F\xi = 4$. The black, red, and blue arrows, respectively, indicate the positions having the distances $r' = 1.0$, 8.0, and 130.0.

Let us next investigate the difference in the screening 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 develops 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 oscillatory 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 vortex core in high-T_c superconductors.

Finally we point out that the charging mechanism discussed in this Letter is close to that proposed by Koláček *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 intrinsic depletion cannot be supressed 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 calculations, 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 incorporated 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 understands that the sign of the charge emerging in the vortex core is almost uniquely determined in charged superconducting 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 correlation 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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