

Friedel Oscillation in Charge Profile around Superconducting Vortex Core

Masahiko Machida ^{a,1}, Tomio Koyama ^b

^a *CCSE, Japan Atomic Energy Research Institute, 6-9-3 Higashi-Ueno Taito-ku, Tokyo 110-0015, Japan*

^b *IMR, Tohoku University, 2-1 Katahira Aoba-ku, Sendai 980-8577, Japan*

Abstract

We numerically perform microscopic calculations for charge distributions around a superconducting vortex core on the basis of the BdG formalism including the Poisson equation for the scalar potential. The numerical results reveal that the charge distribution shows the Friedel oscillation around a vortex core and the oscillation survives over the coherence length in small $k_F \xi$ cases, i.e. the quantum limit. To clarify the origin of the oscillation we study the charge screening properties by calculating the charge density correlation function around a vortex core. The correlation function strongly depends on the position from the vortex center and remarkably oscillates around the vortex core. This result indicates that the Thomas-Fermi type screening is broken in the vortex core.

Key words: Vortex Charge Profile; Friedel Oscillation ; Charge Screening ;

1. Introduction

It has been extensively discussed whether the vortex core has an electric charge or not [1],[2]. However, these problems have not yet been solved even within the conventional BCS theory. In this paper we perform full microscopic calculations for the charge distribution around a vortex core in s-wave case to unveil the charge-profile and the screening effect around a single vortex core.

In obtaining the charge-profile in a superconductor the screening effect cannot be neglected. The Thomas-Fermi type screening and the Friedel oscillations are known to appear in the induced charge-profile in the normal state of a charged Fermi-liquid. 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 [3] since the Fermi surface becomes ob-

scure in the presence of a superconducting gap. However, one may expect that such a simple picture breaks down in the vortex core region and the Friedel oscillation appears around a vortex core, which is caused by the low-lying core states. Hence, one understands that the Thomas-Fermi screening 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 paper, we perform numerical studies for the BdG equation including the scalar potential and clarify the charge-profile in the single vortex state. Using the solutions the density-density correlation function is calculated as a function of the distance from the vortex center. The strong spatial-dependence appears in the screening properties in the vortex state.

2. Numerical Calculations

The BCS Hamiltonian for a charged superconductor is written as

¹ Corresponding author, E-mail: mac@koma.jaeri.go.jp

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

where $\hat{n}(\mathbf{r})$ is the density operator, φ is the scalar potential and \mathbf{E} is the electric field. From the Hamiltonian (1) the BdG equation and the Poisson equation are derived. The BdG equation is solved as an eigenvalue problem for $2N(\mu) \times 2N(\mu)$ matrices by using the method given in Ref.[4]. Then, using the Poisson equation, in which the charge density $\rho(r) = e \sum_n |v_n(r)|^2$ is expressed in terms of the solution of the BdG equation $v_n(r)$, we calculate the scalar potential. The calculations are repeated until the self-consistent solutions for $u_n(r)$, $v_n(r)$ and $\varphi(r)$ are obtained.

Fig.1 shows a result for $\rho(\mathbf{r})$ in the case of $k_F\xi = 8$. As seen in this figure, the oscillations extend over the coherence length for $k_F\xi = 8$. We find that the range in which the oscillation survives increases with decreasing $k_F\xi$.

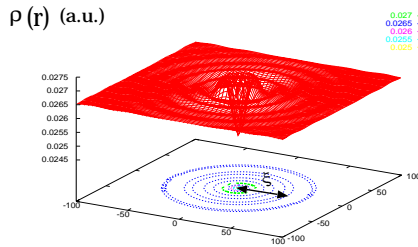


Fig. 1. 3D plot of the charge density profile in the case of $k_F\xi = 8$. The line with arrows at both ends gives a measure of the coherence length.

Let us now study the origin of the oscillations. The wave functions for the localized core states in a s-wave superconductor locally oscillate with periods of about $2\pi/k_F$ since they are located near the Fermi level. Thus, the presence of these wave functions is expected to cause π/k_F oscillations in the charge density-profile inside the core, that is, local Friedel oscillations generated by the core-states. In fact, our numerical calculations reveal that the oscillations appear only around the vortex core and their period is nearly equal to π/k_F which is a given parameter in the calculations.

Let us next investigate the screening properties near a vortex core using the function $K(\mathbf{r}, \mathbf{r}')$ defined as the static limit of the density-density correlation function, $K(\mathbf{r}, \mathbf{r}', t - t') = -i \frac{e^2}{\hbar} \theta(t - t') < [n(\mathbf{r}, t), n(\mathbf{r}', t')] >$, which characterizes the charge screening effect in the present system. Fig.2 shows the spatial dependence of $K(r, r')$ for fixed values, $r' = 1, 8$ and 130 (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 the core. 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. This result indicates that the self-correlation disappears in the neighborhood of the vortex center, though it takes maximum at $r = r'$ for larger values, $r' = 8$, and 130 . From these results one understand that the intrinsic density depletion 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 [5]. Finally, we focus on the difference in the screening effect around the two sites, $r' = 8$ and 130 . As seen in Fig.2, the correlation function, $K(r, r')$, almost monotonically decays as r leaves $r' = 130$, while it shows large oscillations around the core edge in the case of $r' = 8$. From this result one may conclude that the Friedel oscillation strongly develops in the core region, while the Thomas-Fermi type screening recovers in the region outside the vortex core.

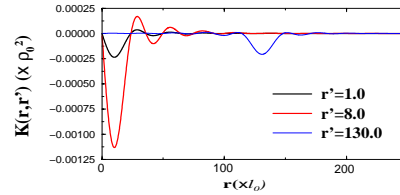


Fig. 2. The spatial dependence of the charge density correlation function $K(r, r')$ for fixed points located at distances, $r' (= 1.0, 8.0$ and $130.0)$, in the case of $k_F\xi = 4$ where $\xi = 37$. The atomic unit ($l_0 = 0.5292 \text{ \AA}$) is used.

In summary, we clarified the microscopic charge-profile in charged superconductors, studying the screening properties around a vortex core. We found that the Friedel oscillation appears in the region near the vortex core.

Acknowledgements

M.M. thanks CCSE staff for supporting our numerical calculations.

References

- [1] D.I.Khomskii and A.Freimuth, *Phys.Rev.Lett.* **75**, 1384(1995); M.V.Feigel'man et al., *JETP Lett.* **62**, 834(1995).; G.Blatter et al., *Phys.Rev.Lett.* **77**, 566(1996).; N.Hayashi et al.*J.Phys.Soc.Jpn.* **67**, 3368(1998);Kolacek et al. *Phys.Rev.Lett.* **86**, 312(2001)
- [2] K.Kumagai et al. *Phys.Rev.B* **63**,144502(2001).
- [3] A.L.Fetter *Phys.Rev.* **140**,1921(1965).
- [4] F.Gygi and M.Schlüter *Phys.Rev.B* **43**,7609(1991).
- [5] M.Machida and T.Koyama *Physica C* (To be published); M.Machida and T.Koyama (Unpublished).