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The effects of $d_{x^2-y^2}$–d_{xy} mixing on vortex structures and magnetization

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Abstract. The structure of an isolated single vortex and the vortex lattice, and the magnetization in a d-wave superconductor are investigated within a phenomenological Ginzburg–Landau (GL) model including the mixture of the $d_{x^2-y^2}$-wave and d_{xy}-wave symmetries. The isolated single-vortex structure in a weak magnetic field is studied both numerically and asymptotically. Near the upper critical field H_{c2}, the vortex lattice structure and the magnetization are calculated analytically.

1. Introduction

Since the discovery of the high-temperature superconductors (HTSCs), a great number of experimental and theoretical investigations have been carried out to identify the symmetry of the superconducting pairing state. Although there still remain controversies, it is believed that the $d_{x^2-y^2}$-wave symmetry is most probable in HTSCs; e.g. a series of strong pieces of evidence have been provided by phase-sensitive experiments [1].

In recent years, the structure of vortices in a $d_{x^2-y^2}$ superconductor has been of great interest. It was expected that the structure of d-wave vortices might be very different from that of s-wave vortices. And connected with the vortex structure, the question of order parameter symmetry admixture arose.

From the standpoint of the spontaneous symmetry breaking, in a bulk with a perfect crystal symmetry, the order parameter transforms according to an irreducible representation [2] of the crystallographic point group [3–5]. Thus in a crystal of tetragonal (D_4) symmetry, only one symmetry state (e.g. $d_{x^2-y^2}$-wave symmetry) is allowed. However, near interfaces, surfaces or impurities, the crystalline symmetry is not perfect, and the $d_{x^2-y^2}$-wave order parameter fluctuates spatially and hence induces components of other symmetry. This is also the case in the presence of vortices, to which we will confine ourselves in this work.

Soininen *et al* [6], starting from a simple microscopic model Hamiltonian and its Bogoliubov–de Gennes equation, found a substantial admixture of an induced s wave and the dominant $d_{x^2-y^2}$ wave. On the basis of that work, Berlinsky *et al* [7] and Franz *et al* [8] investigated the structure of d-wave vortices using the Ginzburg–Landau (GL) theory. Ren *et al* [9] derived the GL equation microscopically from the Gorkov equation of a continuum mean-field model, and it was studied in detail by Xu *et al* [10, 11] for the d-wave vortex structures. Joynt [12] also included the d–s mixing term in their phenomenological GL model, on the basis of symmetry arguments. Very recently, Maki and Béal-Monod [13] and Won and Maki [14] also incorporated d–s mixture. They used an interaction potential with

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the s-channel repulsive Coulomb interaction in their weak-coupling model. In most of the studies mentioned above, the investigators observed that the s-wave component induced near the vortex core causes the d-wave component to have fourfold anisotropy [7, 8, 10, 11], and that the vortices are arranged in an oblique lattice instead of a triangular one [7, 8, 11, 14].

Recently, the possibility of admixture of $d_{x^2-y^2}$ waves and d_{xy} waves was also suggested. Koyama and Tachiki [15] took into account the internal orbital motion of the pairing electrons in their linearized Gorkov-type gap equation near T_c. They found that the dominant $d_{x^2-y^2}$-wave symmetry was mixed with d_{xy}-wave symmetry, instead of the s-wave symmetry. The coupling of the two d-wave components led to a significant paramagnetic effect and to strong enhancement of the upper critical field at lower temperatures, which fits the experimental results on the overdoped cuprate superconductors $Bi_2Sr_2CuO_y$ and $Tl_2Ba_2CuO_6$ remarkably well. And Ichioka *et al* [16] considered both $d_{x^2-y^2}$–s mixing and $d_{x^2-y^2}$–d_{xy} mixing in the framework of the classical Eilenberger equations. They studied the isolated single-vortex structures and found that the amplitude of the d_{xy}-wave component has the shape of an octofoil.

As described above, for the case of d–s mixture, the single-vortex and/or vortex lattice structure have been extensively studied [7, 8, 14], but this is not so for the case of $d_{x^2-y^2}$–d_{xy} mixture. In this paper, we present analogous studies based on the GL theory which include the mixing of $d_{x^2-y^2}$ waves and d_{xy} waves, assuming $d_{x^2-y^2}$-wave symmetry of the superconducting ground state.

2. GL theory for a d-wave superconductor

We start with the GL free-energy functional proposed by Koyama and Tachiki:

$$\begin{aligned} G(H) = \int \mathrm{d}x \, \Bigg\{ & \frac{\hbar^2}{4m_+} \left| \left(-\mathrm{i}\boldsymbol{\nabla} + \frac{2\pi}{\phi_0}\boldsymbol{A} \right) \Psi_+ \right|^2 + \alpha_+(T)|\Psi_+|^2 + \frac{1}{2}\beta_+|\Psi_+|^4 \\ & + \frac{\hbar^2}{4m_-} \left| \left(-\mathrm{i}\boldsymbol{\nabla} + \frac{2\pi}{\phi_0}\boldsymbol{A} \right) \Psi_- \right|^2 + \alpha_-|\Psi_-|^2 + \frac{1}{2}\beta_-|\Psi_-|^4 \\ & + \beta_X|\Psi_+|^2|\Psi_-|^2 + \beta_Y(\Psi_+^{*}\Psi_-^2 + \mathrm{HC}) - \frac{1}{2}\gamma_p(\Psi_+^*\Psi_- + \mathrm{HC})B_z \\ & + \frac{B^2}{8\pi} - \frac{\boldsymbol{B}\cdot\boldsymbol{H}}{4\pi} \Bigg\} \end{aligned} \tag{1}$$

where the order parameter Ψ_+ (Ψ_-) corresponds to the $d_{x^2-y^2}$-wave (d_{xy}-wave) symmetry. As we previously assumed, in the Meissner state, the only non-vanishing component is ψ_+, and $\alpha_+(T) < 0$ at $T < T_c$. Other coefficients are assumed to be positive and independent of the temperature.

In passing, we make a couple of remarks. In equation (1) we included the coupling term $\sim(\Psi_+^{*2}\Psi_-^2 + \mathrm{HC})$, which was omitted in the model originally proposed by Koyama and Tachiki [15, 17]. This term is necessary in order to get the most general (up to the fourth order) free-energy functional from symmetry considerations [5]. The mixing term $\sim(\Psi_+^*\Psi_- + \mathrm{HC})B_z$ to quadratic order gives rise to a paramagnetic current [18]. As we will see below, it dominates other mixing terms and significantly affects the mixed-state properties of d-wave superconductors.

In the mean-field approximation, neglecting thermal fluctuation effects, physical properties are described by the corresponding GL equations. It is convenient to introduce dimensionless quantities by adopting as the fundamental length scale the GL coherence length ξ_+ of Ψ_+ (see table 1). In this case, the GL equations and Maxwell equations are

Table 1. Characteristic lengths, scales of physical quantities, and phenomenological parameters in the GL theory in question.

Characteristic lengths	$\xi_+^2 = \dfrac{\hbar^2}{4m_+\|\alpha_+\|}$, $\xi_-^2 = \dfrac{\hbar^2}{4m_-\alpha_-}$, $\lambda_+^2 = \dfrac{m_+c^2}{8\pi e^2\|\Psi_0\|^2}$
Characteristic field[a]	$H_{c2}^0 = \phi_0/2\pi\xi_+^2$
Fundamental parameters	$\Psi_0^2 = \|\alpha_+\|/\beta_+$, $\Phi_0/2\pi = \hbar c/2e$, $\kappa = \lambda_+/\xi_+$
Auxiliary parameters	$\Xi = \xi_+^2/\xi_-^2$, $\Upsilon = m_-\beta_-/m_+\beta_+$, $\mu = m_-/m_+$, $\nu_\pm = \gamma_p m_\pm c/e\hbar$, $\nu_p^2 = \nu_+\nu_-$, $\chi_+ = \beta_X/\beta$, $\chi_- = \mu\chi_+$ $\zeta_+ = \beta_Y/\beta$, $\zeta_- = \mu\zeta_+$
Reduced units	$\Psi_\pm/\Psi_0 = \psi_\pm$, $T/T_c \to T$, $\boldsymbol{r}/\xi_+ \to \boldsymbol{r}$, $\boldsymbol{B}/H_{c2}^0 \to \boldsymbol{B}$, $\boldsymbol{A}/\xi_+ H_{c2}^0 \to \boldsymbol{A}$, $\boldsymbol{J}/(cH_{c2}^0/4\pi\xi_+) \to \boldsymbol{J}$

[a] Here H_{c2}^0 is not the true upper critical field. The upper critical field can be substantially enhanced in this model.

written as

$$\Pi^2\psi_+ - \psi_+ + |\psi_+|^2\psi_+ + \chi_+|\psi_-|^2\psi_+ + \zeta_+\psi_+^*\psi_-^2 - \nu_+ B_z\psi_- = 0 \quad (2)$$

$$\Pi^2\psi_- + \Xi\psi_- + \Upsilon|\psi_-|^2\psi_- + \chi_-|\psi_+|^2\psi_- + \zeta_-\psi_-^*\psi_+^2 - \nu_- B_z\psi_+ = 0 \quad (3)$$

$$\kappa^2\boldsymbol{J} = -\frac{1}{2}(\psi_+^*\boldsymbol{\Pi}\psi_+ + \mathrm{HC}) - \frac{1}{2}\mu^{-1}(\psi_-^*\boldsymbol{\Pi}\psi_- + \mathrm{HC}) + \frac{1}{2}\nu_+\boldsymbol{\nabla}\times(\psi_+^*\psi_- + \mathrm{HC})\hat{\boldsymbol{z}} \quad (4)$$

where $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\boldsymbol{A} = \boldsymbol{J}$ and $\boldsymbol{\Pi} = (-\mathrm{i}\boldsymbol{\nabla} + \boldsymbol{A})$, and other parameters are defined in table 1. In equation (4), the last term is the paramagnetic current contribution.

3. Isolated single-vortex structure

Consider an isolated single vortex near the lower critical field H_{c1} [19]. For the problem of an isolated single vortex, it would be convenient to decompose the order parameter into the form $\psi_\pm = f_\pm \mathrm{e}^{+\mathrm{i}\varphi_\pm}$. Since the d_{xy}-wave component is induced through the direct coupling to the magnetic field, in the low field near H_{c1} its amplitude is expected to be very small compared with the $\mathrm{d}_{x^2-y^2}$-wave component. Thus, just for intuitive understanding, for the moment we neglect the effect of the coupling in the fourth order ($\chi_\pm \simeq 0$, $\zeta_\pm \simeq 0$). This effect will be considered below.

Let us first look at the phase distributions associated with the vortex. It is obvious from the rotational symmetry of the GL equations that the phases should have $\varphi(r,\theta)_\pm = -\theta$ up to an additive constant [20], which we take to be zero; the two d-wave components have the same winding. Thus, the differential equations are rewritten, in terms of $f_\pm$ only, as

$$\Pi^2 f_+ - f_+ + f_+^3 - \nu_+ B f_- = 0 \quad (5)$$

$$\Pi^2 f_- + \Xi f_- + \Upsilon f_-^3 - \nu_- B f_+ = 0 \quad (6)$$

$$\kappa^2\boldsymbol{J} = -(f_+^2 + \mu^{-1}f_-^2)(-1/r + A)\hat{\boldsymbol{\theta}} + \nu_+\boldsymbol{\nabla}\times(f_+f_-)\hat{\boldsymbol{z}} \quad (7)$$

where

$$\Pi^2 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} + \left(-\frac{1}{r} + A\right)^2$$

and where $\boldsymbol{A} = A(r)\hat{\boldsymbol{\theta}}$, $\boldsymbol{B} = B(r)\hat{\boldsymbol{z}}$, and $\boldsymbol{J} = J(r)\hat{\boldsymbol{\theta}}$.

Second, near the vortex centre ($r \to 0$), $B(r)$ and $f_\pm(r)$ have asymptotic behaviour of the following form:

$$B(r) = B_0 + B_2 r^2 + \mathcal{O}[r^4] \tag{8}$$

$$f_+(r) = C_0 r(1 + C_2 r^2 + \mathcal{O}[r^4]) \tag{9}$$

$$f_-(r) = D_0 r(1 + \mathcal{O}[r^4]) \tag{10}$$

where [21]

$$C_2 = -\frac{1}{8}(1 + B_0)\left[1 + \nu_p^2 \frac{B_0^2}{(\Xi - B_0)(1 + B_0)}\right] \tag{11}$$

$$D_0 = \nu_2 \frac{B_0}{\Xi - B_0} C_0 \tag{12}$$

$$B_2 = -\frac{1}{2}\frac{C_0^2}{\kappa^2}\left[1 - 2\nu_p^2 \frac{B_0}{\Xi - B_0} + \nu_p^2\left(\frac{B_0}{\Xi - B_0}\right)^2\right]. \tag{13}$$

Note that since $B_0 \sim 2/\kappa^2$, in the extreme type-II superconductors ($\kappa \gg 1$) the asymptotic behaviours of $B(r)$ and $f_+(r)$ deviate very little from those of the conventional s-wave GL theory ($C_2 \simeq -(1 + B_0)/8$, $B_2 \simeq -C_0^2/2\kappa^2$).

Next, consider the region far from the vortex centre ($r \gg \kappa$). Assuming the extreme type-II superconductor ($\kappa \gg 1$), we can treat $f_+ = 1$ and neglect $|\nabla^2 f|_- \sim f_-/\kappa^2 \ll f_-$. Then by taking the curl of equation (7) we get the usual London equation:

$$\kappa^2 \nabla \times \nabla \times \boldsymbol{B} + \boldsymbol{B} = 2\pi\delta^2(\boldsymbol{r})\hat{\boldsymbol{z}} \tag{14}$$

and from equation (6)

$$f_+(r) \simeq \frac{\nu_-}{\Xi} B(r) \sim \sqrt{\kappa/r}\, \mathrm{e}^{-r/\kappa} \qquad (r \gg \kappa). \tag{15}$$

Thus, far outside the core, only the pure $\mathrm{d}_{x^2-y^2}$-wave component remains.

Now we discuss the effect of the mixing terms in the fourth order, i.e. with finite $\chi_\pm$ and $\zeta_\pm$. In general, due to the coupling of the form $\psi_+^{*2}\psi_-^2 + \mathrm{HC}$ the GL equations do not have spherical symmetry. However, with the assumption of a small d_{xy}-wave component, we can apply a partial-wave expansion for ψ_-:

$$\psi_- = \sum_n f_-^{(n)}(r)\mathrm{e}^{\mathrm{i}n\theta}. \tag{16}$$

It is straightforward to show that the only non-vanishing component is that of $n = 1$, and that the asymptotic results given above are unchanged.

We also provide the numerical results for the distribution of the order parameter and the magnetic induction in figure 1. As shown in figure 1(a), the magnitude $f_-(r)$ for the d_{xy}-wave component increases as the $\mathrm{d}_{x^2-y^2}$–d_{xy} coupling strength ν_+ (ν_-) increases and as the temperature T decreases. However, $f_-(r)$ is so small that its effect on $f_+(r)$ and $B(r)$ is negligible; the isolated single-vortex structure of this model is very similar to that of the conventional s-wave GL theory.

4. The vortex lattice and magnetization near the upper critical field

In the vicinity of the upper critical field H_{c2}, the magnitudes of the order parameters are small, and thus the non-linear terms in the GL equations (2) and (3) are negligible. The magnetic fields are also assumed to be constant over the whole space since the inter-vortex

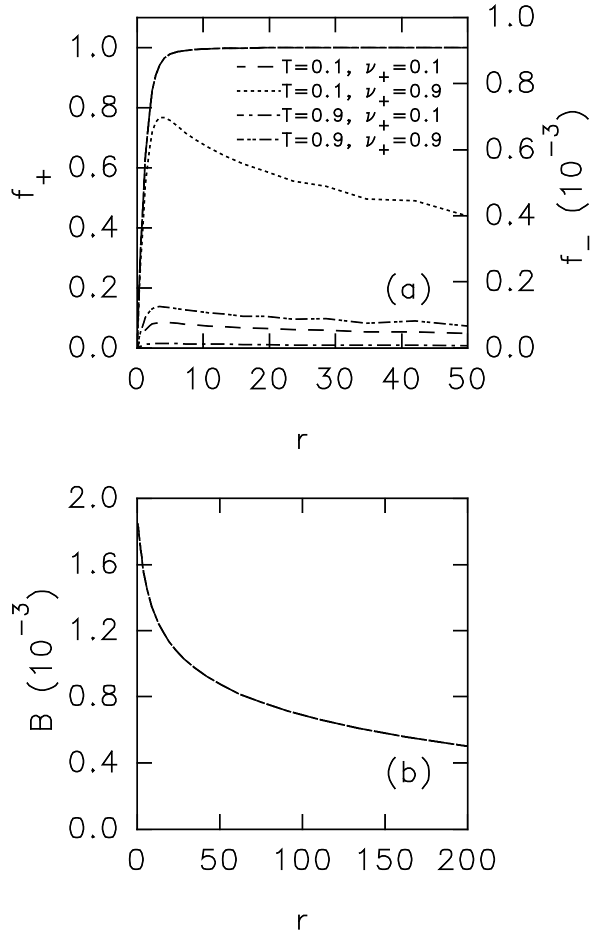

Figure 1. Distributions of the magnitudes of the order parameter and the magnetic induction associated with an isolated single vortex, for different values of T and ν_+: $T = 0.1, 0.9$ and $\nu_+ = 0.1, 0.9$. The other parameters are set as $\mu = 1.0$, $\Xi(0) = 1.0$, $\Upsilon = 1.0$, $\chi_+ = 0.8$.

spacing is much less than the penetration depth λ_+. Then the GL equations are reduced to a linearized form:

$$(\Pi^2 - 1)\psi_+ - \nu_+ B_z \psi_- = 0 \tag{17}$$

$$(\Pi^2 + \Xi)\psi_- - \nu_- B_z \psi_+ = 0. \tag{18}$$

Each of the solutions $\psi_{L\pm}$ is just a linear combination of the wave functions in the lowest Landau level, which is infinitely degenerate, and determined so as to minimize the GL free energy.

We minimize the free energy by generalizing Abrikosov's procedures [22, 23]. In these procedures, the two components of the order parameter satisfy

$$\frac{\psi_{L-}}{\psi_{L+}} = \frac{1}{\nu_+} \frac{H_{c2} - 1}{H_{c2}} \tag{19}$$

and the requirement that the current contribution is given by

$$\kappa^2 \boldsymbol{J}_L = -\frac{1}{2}\boldsymbol{\nabla} \times \left\{|\psi_{L+}|^2 + \mu^{-1}|\psi_{L-}|^2 - \nu_+(\psi^*_{L+}\psi_{L-} + \text{HC})\right\}\hat{\boldsymbol{z}}. \tag{20}$$

Then the magnetization [24] and the GL free energy are given by

$$4\pi M = -\frac{H_{c2} - H}{(2\kappa^2_{\text{eff}} - 1)\beta_A} \tag{21}$$

$$G_s(H) = G_n(H_{c2}) + 2\kappa^2 \left[(H^2_{c2} - H^2) - \frac{(H_{c2} - H)^2}{(2\kappa^2_{\text{eff}} - 1)\beta_A}\right] \tag{22}$$

where $\beta_A \equiv \langle f^4_+\rangle / \langle f^2_+\rangle^2$ is a still undetermined parameter, and $\kappa^2_{\text{eff}}(T) = \kappa^2 G(T)/F^2(T)$ with

$$R(T) = \frac{1}{\nu_+}\frac{H_{c2}(T) - 1}{H_{c2}(T)}$$

$$F(T) = 1 - 2\nu_+ R + \mu^{-1} R^2$$

$$G(T) = 1 + 2(\chi_+ + \zeta_+)R^2 + \mu^{-1}\Upsilon R^4.$$

The Abrikosov parameter β_A is concerned in the vortex lattice structure and is determined by minimizing the GL free energy. Since ψ_{L+} has the same form as the s-wave Abrikosov solution, it is obvious that the free energy is minimized for the triangular vortex lattice ($\beta_A = 1.16$) [25]. The magnetization in equation (22) shows the usual form of the conventional s-wave GL theory [22, 23], but the slope $4\pi\, \mathrm{d}M/\mathrm{d}H$ depends on the temperature.

5. Discussion

There has been no direct observation of the single-vortex structure in a HTSC, while Keimer *et al* [26] and Maggio-Aprile *et al* [27] observed oblique lattices in their SANS and STM experiments on YBCO compounds, respectively. Their result of an oblique lattice is not consistent with our result of a triangular lattice. Both the single-vortex structure and the vortex lattice structure are also different from theoretical predictions based on the $d_{x^2-y^2}$–s admixture scenario [7, 8, 10, 11, 14].

The single-vortex structure can have a significant influence on the structure of the vortex lattice in many-vortex problems. It is quite interesting to note that the fourfold symmetry of a d–s admixed vortex is an implication of the mixed-gradient coupling in the model. In our model, there is no mixed-gradient term up to quadratic order. Very recently, Ichioka *et al* [16] argued that a non-local correction is required and that the associated GL theory should include the fourth-order mixed-gradient term. They observed that the $d_{x^2-y^2}$-wave component has a four-lobe shape and that the d_{xy}-wave component has the shape of an octofoil. Although in this present paper we put emphasis on the effect of mixing through the direct coupling to the magnetic field, the result of Ichioka *et al* strongly suggests that $d_{x^2-y^2}$–d_{xy} admixture can lead to an oblique vortex lattice. Furthermore, even in the present GL model, for the intermediate-field regime away from the extreme regions near to H_{c1} or H_{c2}, the order parameter distribution is not spherically symmetric. Therefore further study is required for that region, because the non-spherical symmetry of the supercurrent distribution around a vortex is not compatible with the triangular lattice symmetry.

The strong temperature dependence of $\kappa_{\text{eff}}(T)$ in equation (22) (see figure 2) is reminiscent of that of $\kappa_2(T)$ found in the microscopic consideration of conventional superconductors by Maki and Tsuzuki [28] and Eilenberger [29]. Roughly speaking,

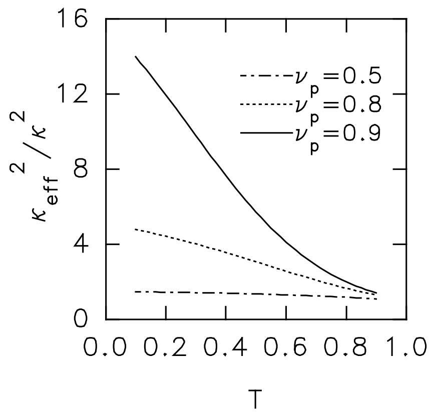

Figure 2. The temperature dependence of $\kappa_{\rm eff}^2$ for three different values of ν_p. The other parameters are set as $\mu = 1.0$, $\Xi(0) = 1.0$, $\Upsilon = 1.0$, $\chi_+ = 0.8$.

the difference between $\kappa_2(T)$ and κ for that case was due to the non-locality of the electromagnetic response of the superconductors. In our case, the strong T-dependence of $\kappa_{\rm eff}(T)$ has an interesting interpretation. In contrast to the case of the low-field limit, ψ_- is of the order of ψ_+ at high fields ($H \sim H_{c2}$) and low temperatures for $\nu_p \sim 1$, and the associated paramagnetic current significantly affects the magnetization curve $4\pi M(H)$ in the low-temperature region. Several experiments reported a strong temperature dependence of the slope $4\pi\, {\rm d}M/{\rm d}H$ near $H_{c2}(T)$ in HTSCs [15].

6. Conclusions

We have investigated a GL theory for vortex structures and magnetization in a d-wave superconductor. In the GL theory, we assumed the $d_{x^2-y^2}$-wave symmetry of the superconducting ground state, and the admixture of $d_{x^2-y^2}$-wave symmetry and d_{xy}-wave symmetry in the presence of the vortices. The structure of an isolated single vortex was studied asymptotically and numerically in the low-field region ($H \sim H_{c1}$). The isolated single vortex is similar to the conventional s-wave vortex, and has an almost spherically symmetric supercurrent distribution around it. The vortex lattice structure and magnetization were studied analytically at high fields near the upper critical field H_{c2}. The vortices are arranged in a triangular lattice, and the magnetization curve $4\pi M(H)$ shows a strong temperature dependence for $\nu_p \sim 1$ due to the paramagnetic current effect. Some physical implications of the results were discussed. The results were also compared with the experimental observations and with those of the d–s scenario. It was recognized that further study in the intermediate-field region would be valuable.

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