

# Magnetic Field Induced Antiferromagnetism in a Two-Dimensional Hubbard Model: analysis of CeRhIn<sub>5</sub>

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We propose the mechanism for the magnetic field induced AFM state in a two-dimensional Hubbard model in the vicinity of the antiferromagnetic (AFM) quantum critical point (QCP), using the fluctuation-exchange (FLEX) approximation by taking the Zeeman energy due to magnetic field  $\mathbf{B}$  into account. In the vicinity of the QCP, we find that the AFM correlation perpendicular to  $\mathbf{B}$  is enhanced, whereas that parallel to  $\mathbf{B}$  is reduced. This fact means that the finite magnetic field enhances  $T_N$ , with the AFM order perpendicular to  $\mathbf{B}$ . The increment of  $T_N$  can be understood in terms of the reduction of both the quantum and the thermal fluctuations due to the magnetic field, which is brought by the self-energy effect within the FLEX approximation. The present study naturally explains the increment of  $T_N$  in CeRhIn<sub>5</sub> under the magnetic field found recently.

KEYWORDS: field induced magnetism, FLEX, antiferromagnetic fluctuations, CeRhIn<sub>5</sub>

Recently, critical phenomena in the vicinity of the magnetic quantum critical point (QCP) attract much interest in strongly correlated metals. Experimentally, outer magnetic field is frequently used to change the distance from the QCP. As for the antiferromagnetic (AFM) QCP, the magnetic field is believed to enlarge the distance to the QCP in general. Spin fluctuation theories such as the SCR theory<sup>1)</sup> or the fluctuation-exchange (FLEX) approximation,<sup>2)</sup> have been succeeded in describing various critical phenomena in metals close to the AFM-QCP, such as the non-Fermi liquid like behaviors of various transport coefficients.<sup>3,4)</sup> However, previous studies on the effect of the magnetic field based on the spin fluctuation theory were limited.<sup>5)</sup>

CeMIn<sub>5</sub> (M=Rh, Co, Ir) is a well-known quasi two-dimensional heavy fermion compounds, where single conductive CeIn-layers stack perpendicular to the  $c$ -axis. CeCoIn<sub>5</sub> is a superconductor with  $T_c = 2.3\text{K}$  at ambient pressure.<sup>6)</sup> In CeRhIn<sub>5</sub>, the AFM order emerges at  $T_N = 3.8\text{K}$  at ambient pressure, and the superconductivity emerges at  $T_c \approx 2\text{K}$  below  $P = 1.6\text{GPa}$ .<sup>7,8)</sup> Recent experiments reveals that the  $T_N$  *increases* under the magnetic field along  $a(b)$ -axis. When  $B = 9\text{T}$ , the increment of  $T_N$  is about  $0.15\text{K}$ . A tiny increment of  $T_N$  is also observed in Ce<sub>2</sub>RhIn<sub>8</sub> which is composed of double CeIn-layers. However, there has been no theoretical explanation for this phenomenon.

In the present letter, we study the two-dimensional Hubbard model under the uniform magnetic field  $\mathbf{B}$  along  $x$ -axis, based on the FLEX approximation. In the vicinity of the AFM-QCP, we find that the AFM spin correlation of  $y(z)$ -component is *enhanced* by the applied magnetic field. In the obtained phase diagram, the magnetic transition temperature  $T_N$ , below which the staggered magnetism emerges on the  $yz$ -plane, increases with the magnetic field. The mechanism of the

field induced antiferromagnetism proposed in the present work will be universal in low-dimensional metals close to the AFM-QCP, contrary to the fact that the magnetic field suppresses  $T_N$  in usual models by the mean-field approximation. The present study naturally explains the enhancement of  $T_N$  under the magnetic field in CeRhIn<sub>5</sub>.

Here we analyze the following two-dimensional Hubbard model:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}'-\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow}, \quad (1)$$

where  $\sigma = 1(-1)$  corresponds to the  $\uparrow$ - ( $\downarrow$ -) spin state and  $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + \sigma B$ , where the factor  $\sigma B$  represents the Zeeman energy. The spin quantization axis is  $x$ -axis. Here, we study the square lattice tight-binding model with the nearest neighbor hopping ( $t$ ) and the next-nearest one ( $t'$ ). The dispersion of the electron is given by  $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x k_y$ . Hereafter, we study the case of  $(t, t') = (1, -0.25)$  with the electron density  $n = 0.90$  ( $n = 1.20$ ) per site, which corresponds to a hole-doped (electron-doped) high- $T_c$  cuprates. In the case of  $n = 0.90$ , the Fermi surface (FS) is very close to the van-Hove singular point (at  $(\pi, 0)$  in this case; see Fig.3), and it is similar to the largest (main) cylindrical FS in CeMIn<sub>5</sub> (M=Co, Ir, Rh).<sup>9)</sup> Assuming a similar single cylindrical FS, many aspects of CeMIn<sub>5</sub>, especially the  $d_{x^2-y^2}$ -wave superconductivity, are reproduced by the perturbation study.<sup>10,11)</sup>

In the presence of the magnetic field along  $x$ -axis, the dynamical spin susceptibilities within the FLEX approximation (or random phase approximation (RPA)),  $\chi_x^s(q)$  and  $\chi_{y(z)}^s(q)$ , are given by

$$\chi_y(q) = \chi_z(q) = (\chi_{\uparrow,\downarrow}(q) + \chi_{\downarrow,\uparrow}(q))/4 \quad (2)$$

$$\chi_x(q) = [\chi_{\uparrow,\uparrow}(q) + \chi_{\downarrow,\downarrow}(q)]/4 + U \chi_{\uparrow,\uparrow}(q) \chi_{\downarrow,\downarrow}^0(q)/2, \quad (3)$$

$$\chi_{\sigma,-\sigma}(q) = \frac{\chi_{\sigma,-\sigma}^0(q)}{1 - U\chi_{\sigma,-\sigma}^0(q)}, \quad (4)$$

$$\chi_{\sigma,\sigma}(q) = \frac{\chi_{\sigma,\sigma}^0(q)}{1 - U^2\chi_{\sigma,\sigma}^0(q)\chi_{-\sigma,-\sigma}^0(q)}, \quad (5)$$

$$\chi_{\sigma,\sigma'}^0(q) = -T \sum_k G_{\sigma}(k+q)G_{\sigma'}(k). \quad (6)$$

We note that  $\chi_{\uparrow,\downarrow}(q) = \{\chi_{\uparrow,\uparrow}(q)\}^*$ . Here and hereafter, we promise that  $q \equiv (\mathbf{q}, i\omega_n) = (\mathbf{q}, 2\pi in)$  and  $k \equiv (\mathbf{k}, i\epsilon_n) = (\mathbf{k}, \pi i(2n+1))$ . Apparently, both  $\chi_x(q)$  and  $\chi_{y(z)}(q)$  are even-functions of  $B$ , reflecting the reflectional symmetry in the spin space. Apparently,  $\chi_x(q) = \chi_y(q)$  when  $B = 0$ .

The self-energy in the FLEX approximation is given by

$$\begin{aligned} \Sigma_{\sigma}(k) = U^2 T \sum_q [G_{\sigma}(k-q)(\chi_{-\sigma,-\sigma}(q) - \chi_{-\sigma,-\sigma}^0(q)) \\ + G_{-\sigma}(k-q)\chi_{\sigma,-\sigma}(q)] + Un_{-\sigma}, \end{aligned} \quad (7)$$

where  $n_{\sigma} = T \sum_k \text{Im}G_{\sigma}(k)e^{-i\epsilon_n \cdot 0^+}/\pi$  is the density of electrons with  $\sigma$ -spin. Here, we solve the eqs. (2)-(7) together with the Dyson equation  $G_{\sigma}^{-1}(k) = i\epsilon_n + \mu - \epsilon_{\mathbf{k}} - \sigma B - \Sigma_{\sigma}(k)$  numerically, by adjusting the chemical potential  $\mu$  so as to  $n = \sum_{\sigma} n_{\sigma}$ .

Here, we discuss the numerical results obtained by the FLEX approximation. We use  $64 \times 64$   $\mathbf{k}$ -meshes and 1028 Matsubara frequencies in the present numerical study by FLEX approximation. Figure 1 shows obtained static staggered spin susceptibilities:  $\chi_{\alpha}^{\max} \equiv \max_{\mathbf{q}} \chi_{\alpha}(\mathbf{q}, 0)$  where  $\alpha = x, y, z$ .  $\alpha_S \equiv \max_{\mathbf{q}} U\chi^0(\mathbf{q}, 0)$  is the Stoner factor without  $B$ . In the FLEX approximation,  $\alpha_S < 1$  is always satisfied at finite  $T$  in two-dimensional systems, so the Marmin-Wagner-Hohenberg theorem is satisfied.<sup>12,13</sup> The momentum dependence of  $\chi_{\alpha}(\mathbf{q}, 0)$  ( $\alpha = x, z$ ) and the splitting of the FS under the magnetic field are given in figs.2 and 3, respectively, in the case of  $n = 0.90$ .

In fig. 1,  $\chi_x^{\max}$  decreases whereas  $\chi_y^{\max}$  increases with  $\mathbf{B} \parallel \hat{x}$  in both cases of  $n = 0.90$  and  $n = 1.20$  by FLEX approximation. Their field dependence becomes more prominent as  $U$  increases, that is, as  $\alpha_S$  approaches to one. This results mean that the distance to the AFM-QCP decreases owing to the uniform magnetic field. In the FLEX approximation, the field dependence of the susceptibility is caused by (i) the change of the nesting conditions owing to the Zeeman splitting of the FS, and (ii) the self-energy effect (or mode-mode coupling effect) which represents the reduction of  $\chi^{\max}$  and its Curie-Weiss like temperature dependence owing to the spin-fluctuations. In the FLEX approximation, large  $\text{Im}\Sigma(\mathbf{k}, -i\delta)$  caused by spin fluctuations reduces density of states (DOS) at  $\mu$ , which makes  $\chi^{\text{FLEX}} \gg \chi^{\text{RPA}}$ . Below, we will discuss that the effect (ii), which is absent in the RPAs is important to explain why  $\chi_{y(z)}^{\max}$  is enhanced under the magnetic field parallel to  $x$ -axis.

We discuss the physical reason for the field enhancement of the AFM correlation: First, the uniform magnetization induced by  $\mathbf{B} \parallel \hat{x}$  will reduce the AFM correlation along  $x$ -direction. It leads to the enhancement

of  $\chi_y^{\max}$  by contraries, as a result of solving the confliction between spin-fluctuations with different components. The enhancement of  $\chi_y^{\max}$  will be more prominent in lower dimensional systems because the reduction of  $T_N$  due to fluctuations is large in general. Note that the reduction of the staggered moment at  $T = 0$  owing to the quantum fluctuations is about 40%(15%) in two (three) dimensional  $S = 1/2$  Heisenberg model without magnetic field.

Consistently with the above discussion,  $\chi_{y(z)}^{\max}$  increases whereas  $\chi_x^{\max}$  decreases under  $\mathbf{B} \parallel \hat{x}$  in the present model by the FLEX approximation. We have checked that it is an universal behavior in two-dimensional systems close to the AFM-CQP, by studying various types of the Hubbard models. Here, we briefly discuss the self-energy effect for susceptibilities, which will give the dominant field-dependence of the magnetic susceptibility when  $1 - \alpha_S \ll 1$ . When  $\mathbf{B} = 0$ , the modification of  $\chi_{\uparrow,\downarrow}^0(\mathbf{q}, 0)$  from the RPA's result within the lowest order with respect to the self-energy, under the condition that  $1 - \alpha_S \ll 1$ , is given by

$$\begin{aligned} \delta' \chi_{\uparrow,\downarrow}^0(\mathbf{q}, 0) \approx -T^2 \sum_{k,q'} G^0(k)^2 G^0(k+\mathbf{q}) G^0(k+q') \\ \times 2U^2(\chi_x(q') + 2\chi_y(q')), \end{aligned} \quad (8)$$

which is mainly brought by the reduction of DOS owing to the large  $\text{Im}\Sigma$  caused by spin-fluctuations. Because  $\delta' \chi_{\uparrow,\downarrow}^0(\mathbf{Q}, 0) < 0$ ,  $\chi_y^{\max}$  in the FLEX approximation becomes smaller than that in RPA. The reduction of  $\chi_x(q')$  owing to the field-induced uniform magnetization along  $x$ -axis will make  $|\delta' \chi_{\uparrow,\downarrow}^0(\mathbf{Q}, 0)|$  smaller. As a result,  $\chi_y^{\max}$  is expected to increase in proportion to  $B^2$  as far as only the self-energy effect is taken into account.

On the other hand, unphysical results are obtained by RPA, where all  $G$ 's in eqs.(2)-(7) are replaced with  $G_0$ 's. In the case  $n = 0.90$ , both  $\chi_x^{\max}$  and  $\chi_y^{\max}$  by RPA increases with  $B$  as shown in fig.1, possibly reflecting the fact that the FS is close to the van-Hove singularity. On the contrary, both  $\chi_x^{\max}$  and  $\chi_y^{\max}$  decreases with  $\mathbf{B}$  when  $n = 1.20$ . Thus, results given by the RPA are not universal, depending sensitively on the shape of the FS. As a result, the self-energy effect included in the FLEX approximation is indispensable to reproduce a physically reasonable behavior of the two-dimensional nearly AFM metals (i.e.,  $\alpha_S \gtrsim 0.98$ ) under the magnetic field.

In the next stage, we study the magnetic-field dependence of the Néel temperature  $T_N$  by assuming a weak three-dimensional coupling.<sup>12,13</sup> To simplify the analysis, we define  $T_N$  in the presence of the magnetic field under the condition that  $\max_{\mathbf{q}} U\chi_{\uparrow,\downarrow}^0(\mathbf{q}, 0) = \alpha_S^0$ , where  $\alpha_S^0$  is a constant which is slightly smaller than one. By putting  $\alpha_S^0 = 1 - J_{\perp}/U \sim 0.99$  ( $J_{\perp}$  denotes the inter-layer magnetic coupling strength), we obtained the reasonable Néel temperature of  $\kappa$ -(BEDT-TTF)<sub>2</sub>X and TMTSF based on the dimer model.<sup>12,13</sup> Figure 4 shows the field dependence of  $T_N$  given by the FLEX approximation, for several choice of  $\alpha_S^0$ 's. We find that the field-enhancement of the Néel temperature in nearly AFM metals in two dimensions, which has been pointed out in the present work for the first time. In Fig. 4,

$T_N$  starts to increase in proportion to  $B^2$ , and it almost saturates around  $B^* \sim 0.3$ . This result also means that the system approaches to the AFM-QCP by applying the magnetic field.

Here, we comment that in the antiferromagnetic isotropic Heisenberg chain under the magnetic field along  $x$ -axis,  $\langle S_i^x S_j^x \rangle - M^2 \propto (-1)^{i-j} |i-j|^{-1/\eta} \cos(2\pi M(i-j))$  and  $\langle S_i^y S_j^y \rangle \propto (-1)^{i-j} |i-j|^{-\eta}$ , where  $\eta$  decreases from 1 with the magnetic field.<sup>14)</sup> Their field dependencies are consistent with the present study on a two dimensional Hubbard model. In the XXZ-Heisenberg chain, an infinitely small magnetic field along  $x$ -axis induces the staggered magnetization of  $y$ -component in the case of  $J_z < J_x$ .<sup>15,16)</sup> In the opposite case,  $J_z > J_x$ , the staggered magnetization along  $z$ -axis, which exists without the field, is enhanced by  $\mathbf{B} \parallel \hat{x}$ .<sup>17)</sup> We also point out that Ref. 18 studied a localized electron model with interactions between quadrupole moments by a local approximation, and found the field enhancement of  $T_Q$  due to the suppression of fluctuations.

We also comment that the field-induced SDW is realized in quasi-one dimensional metal, TMTSF, owing to the orbital motion of electrons, free from the Zeeman effect.<sup>19)</sup> However, various characters of the field induced magnetism in CeRhIn<sub>5</sub> do not coincide with that observed in TMTSF. In fact, CeRhIn<sub>5</sub> possesses both cylindrical and spherical FS's. They are naturally explained in terms of the Zeeman effect as discussed in the present study.

From now on, we discuss experimental results of CeMIn<sub>5</sub> based on the present study. The bandwidth of the present model is  $\sim 10$ . If we estimate the renormalized quasiparticle bandwidth of CeMIn<sub>5</sub> is  $\sim 1000\text{K}$ ,<sup>20)</sup> the temperature  $T = 0.02$  corresponds to  $\sim 2\text{K}$ , which is close to  $T_c$  in CeCoIn<sub>5</sub>.<sup>21)</sup> The magnetic field  $B = 0.1$  in the present work corresponds to  $\sim 5\text{T}$  for the  $M = \pm 5/2$  Kramers doublet (KD), because the Zeeman energy for  $\text{Ce}^{3+}$  is  $(6/7)\mu_B M H$  ( $6/7$  is the  $g$ -value of  $\text{Ce}^{3+}$ ). Note that the renormalization factor averaged over the FS is 0.217 in the present FLEX approximation for  $U = 5$  at  $T = 0.02$ . References 7,8 reports that  $T_N$  in CeRhIn<sub>5</sub> continues to increase with the magnetic field parallel to  $ab$ -plane, at least below 9T.  $T_N = 3.8\text{K}$  at 0T, and  $T_N(9\text{T}) - T_N(0\text{T}) \approx 0.15\text{K}$ . Whereas  $T_N$  decreases monotonously when  $\mathbf{B} \parallel \hat{c}$  as is observed in usual 3D heavy Fermion systems. It is naturally understood because the orbital motion of electrons, which is absent in the present study where  $\mathbf{B}$  is parallel to the 2D system, will destroy the AF state to earn the energy due to the Landau diamagnetism.

Furthermore, we discuss the anisotropy of  $\hat{\chi}(q)$  in CeRhIn<sub>5</sub>: The lowest KD of  $\text{Ce}^{3+}$ -ion in CeRhIn<sub>5</sub> is  $\Gamma_7^{(2)}$ ;  $|z; \pm\rangle \equiv \beta |M_z = \pm 5/2\rangle - \alpha |M_z = \mp 3/2\rangle$ ,<sup>22,23)</sup> which is about 70K lower than the second lowest KD. If we put  $(\alpha, \beta) \approx (0.44, 0.9)$ ,<sup>23)</sup>  $\langle z; \pm | J_z | z; \pm \rangle = \pm(2.5\beta^2 - 1.5\alpha^2) \approx \pm 1.74$ . On the other hand,  $\langle x; \pm | J_x | x; \pm \rangle = \pm\sqrt{5}\alpha\beta \approx \pm 0.885$  where  $|x; \pm\rangle \equiv (|z; +\rangle \mp |z; -\rangle)/\sqrt{2}$ . Then, the anisotropy of the susceptibility of a single  $\text{Ce}^{3+}$ -ion is  $\chi_a/\chi_c \approx 1.74/0.885 = 1.97$ , which is similar to the experimental ratio. On the other hand, sev-

eral neutron experiments on CeRhIn<sub>5</sub> revealed that the magnetic moments on Ce sites lie on the  $ab$ -plane below  $T_N$ , whose effective moment is  $\mu_{\text{eff}} = 0.264\mu_B$ .<sup>22,23)</sup> It will suggest that the antiferromagnetic RKKY interaction between nearest neighbor Ce sites is XY-like;  $J_{a,b} > J_c$ .<sup>24)</sup> Then, the magnetic field along  $a$ -axis will enhance the AFM correlation along  $b$ -axis as a result of the reduction of fluctuations, which is similar to the behavior of the XXZ-Heisenberg chain under  $\mathbf{B}$ .<sup>15,16)</sup> In fact,  $\mu_{\text{eff}}$  is much smaller than  $(6/7)\mu_B(x; + | J_x | x; +) \approx 0.76\mu_B$ , which suggests that the quantum fluctuations are strong in CeRhIn<sub>5</sub>, reflecting its two-dimensionality. As a result, the field-enhancement of  $T_N$  observed in CeRhIn<sub>5</sub> is well understood in terms of the reduction of the spin-fluctuations by the magnetic field.

In summary, based on the FLEX approximation, we found the field-induced antiferromagnetism in a two-dimensional Hubbard model, as a result of solving the confliction of fluctuation by magnetic field. This phenomenon is expected to be prominent and universal in the vicinity of the QCP, irrespective of the fact that the field-induced uniform magnetization tends to reduce the AFM moment. The induced AFM moments are almost on the plane perpendicular to the applied magnetic field, to earn the Zeeman energy by canting. Experimentally, the enhancement of  $T_N$  will be realized in two dimensional systems under  $\mathbf{B}$  parallel to the system, because the reduction of  $T_N$  caused by the orbital motion effect (Landau quantization) is absent.

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quasiparticles given by the  $c$ - $f$  mixing is larger than 1000K. Here, we analyze the “renormalized band” owing to the many-body effect, using the FLEX approximation in terms of the “residual interaction”; see ref.<sup>11)</sup>

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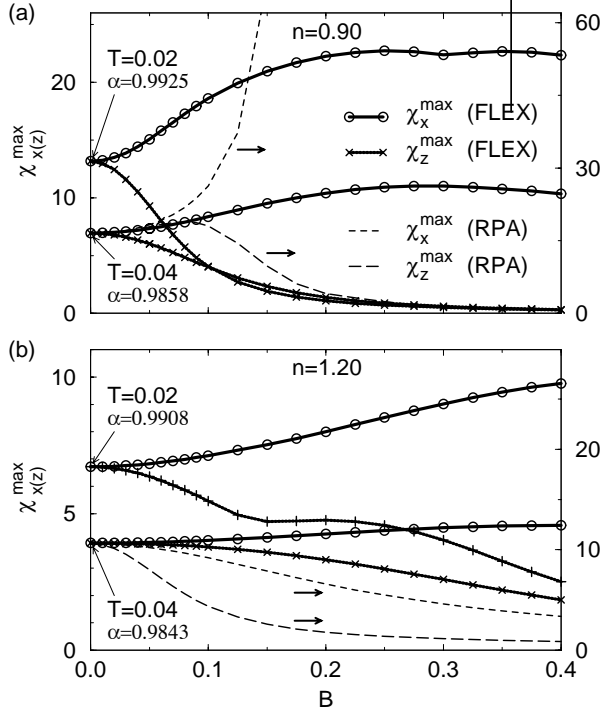


Fig. 1. Field dependence of  $\chi_x^{\max}$  and  $\chi_y^{\max}$  by the FLEX approximation (RPA), under the condition (a)  $n = 0.90$ ,  $U = 5$  ( $U = 2.10$ ) and (b)  $n = 1.20$ ,  $U = 8$  ( $U = 2.96$ ), at  $T = 0.02$ . In the numerical study by RPA,  $256 \times 256$   $\mathbf{k}$ -meshes and 256 Matsubara frequencies are used. In (a),  $\chi_x^{\max}$  ( $\chi_y^{\max}$ ) by RPA diverges at  $B = 0.08$  ( $B = 0.1$ ).

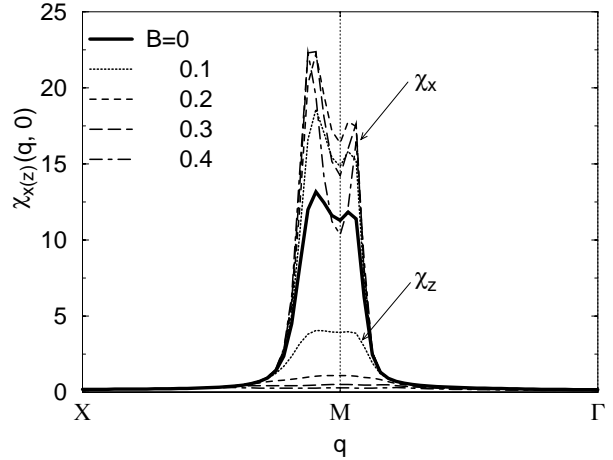


Fig. 2.  $\chi_x(\mathbf{q}, 0)$  and  $\chi_y(\mathbf{q}, 0)$  under finite  $B$  for  $n = 0.90$  at  $T = 0.02$ .

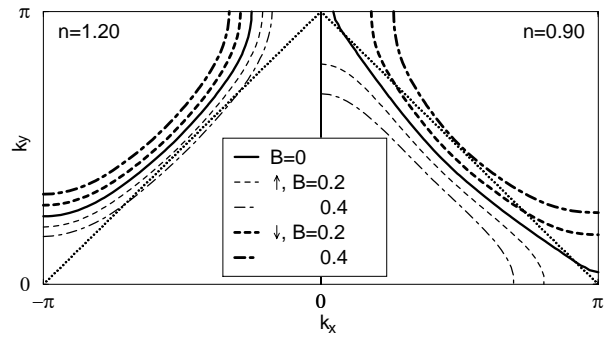


Fig. 3. FS's for  $\uparrow$ - and  $\downarrow$ -electrons under various magnetic field  $B$  for  $n = 0.90$  at  $T = 0.02$ .

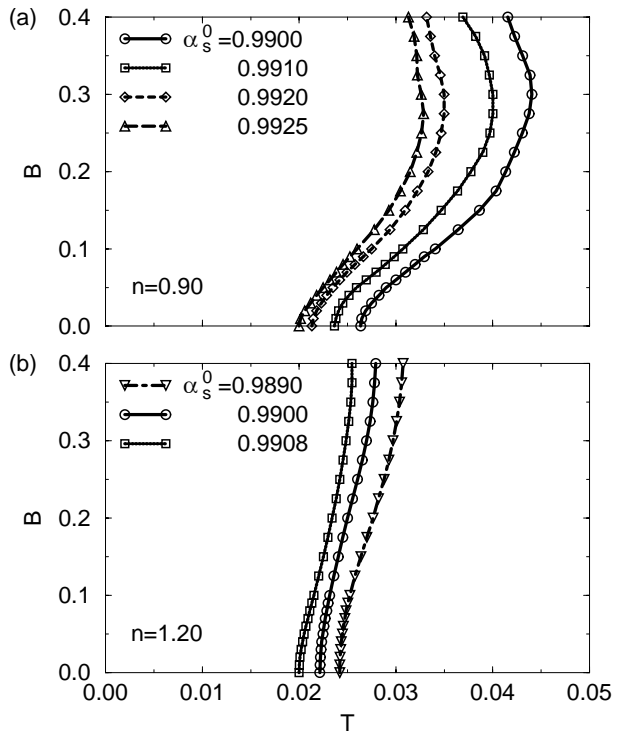


Fig. 4. Obtained phase diagram for  $T_N$  versus  $B$  for various  $\alpha_S^0$ 's.