

Magnetic Field Induced Antiferromagnetism in a Two-Dimensional Hubbard Model: analysis of CeRhIn₅

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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 CeRhIn₅ under the magnetic field found recently.

KEYWORDS: field induced magnetism, FLEX, antiferromagnetic fluctuations, CeRhIn₅

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 theory¹⁾ or the fluctuation-exchange (FLEX) approximation,²⁾ 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.^{3,4)} However, previous studies on the effect of the magnetic field based on the spin fluctuation theory were limited.⁵⁾

CeMIn₅ (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. CeCoIn₅ is a superconductor with $T_c = 2.3\text{K}$ at ambient pressure.⁶⁾ In CeRhIn₅, 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 $P = 1.6\text{GPa}$.^{7,8)} 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 0.15K . A tiny increment of T_N is also observed in Ce₂RhIn₈ 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 CeRhIn₅.

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 σB 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 CeMIn₅ (M=Co, Ir, Rh).⁹⁾ Assuming a similar single cylindrical FS, many aspects of CeMIn₅, especially the $d_{x^2-y^2}$ -wave superconductivity, are reproduced by the perturbation study.^{10,11)}

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 σ -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 μ so as to $n = \sum_{\sigma} n_{\sigma}$.

Here, we discuss the numerical results obtained by the FLEX approximation. We use 64×64 \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.^{12,13} 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, χ_x^{\max} decreases whereas χ_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 α_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 χ^{\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 μ , 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 χ_y^{\max} by contraries, as a result of solving the confliction between spin-fluctuations with different components. The enhancement of χ_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 χ_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 $\delta' \chi_{\uparrow,\downarrow}^0(\mathbf{Q}, 0) < 0$, χ_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, χ_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 χ_x^{\max} and χ_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 χ_x^{\max} and χ_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.^{12,13} 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 α_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 κ -(BEDT-TTF)₂X and TMTSF based on the dimer model.^{12,13} Figure 4 shows the field dependence of T_N given by the FLEX approximation, for several choice of α_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 η decreases from 1 with the magnetic field.¹⁴⁾ 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 $J_z < J_x$.^{15,16)} In the opposite case, $J_z > J_x$, the staggered magnetization along z -axis, which exists without the field, is enhanced by $\mathbf{B} \parallel \hat{x}$.¹⁷⁾ 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.¹⁹⁾ However, various characters of the field induced magnetism in CeRhIn₅ do not coincide with that observed in TMTSF. In fact, CeRhIn₅ 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 CeMIn₅ based on the present study. The bandwidth of the present model is ~ 10 . If we estimate the renormalized quasiparticle bandwidth of CeMIn₅ is $\sim 1000\text{K}$,²⁰⁾ the temperature $T = 0.02$ corresponds to $\sim 2\text{K}$, which is close to T_c in CeCoIn₅.²¹⁾ 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 Ce^{3+} is $(6/7)\mu_B M H$ ($6/7$ is the g -value of 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 CeRhIn₅ 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 CeRhIn₅: The lowest KD of Ce^{3+} -ion in CeRhIn₅ is $\Gamma_7^{(2)}$; $|z; \pm\rangle \equiv \beta |M_z = \pm 5/2\rangle - \alpha |M_z = \mp 3/2\rangle$,^{22,23)} which is about 70K lower than the second lowest KD. If we put $(\alpha, \beta) \approx (0.44, 0.9)$,²³⁾ $\langle z; \pm | J_z | z; \pm \rangle = \pm(2.5\beta^2 - 1.5\alpha^2) \approx \pm 1.74$. 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 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 CeRhIn₅ revealed that the magnetic moments on Ce sites lie on the ab -plane below T_N , whose effective moment is $\mu_{\text{eff}} = 0.264\mu_B$.^{22,23)} It will suggest that the antiferromagnetic RKKY interaction between nearest neighbor Ce sites is XY-like; $J_{a,b} > J_c$.²⁴⁾ 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} .^{15,16)} In fact, μ_{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 CeRhIn₅, reflecting its two-dimensionality. As a result, the field-enhancement of T_N observed in CeRhIn₅ 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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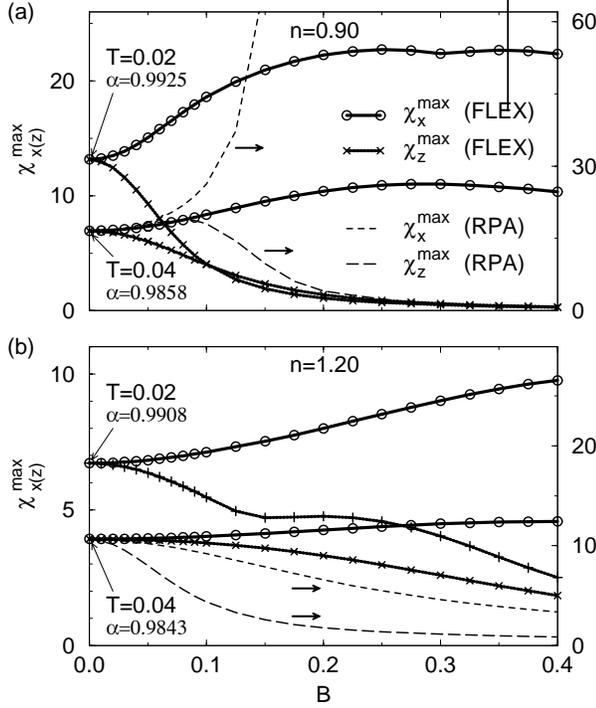


Fig. 1. Field dependence of χ_x^{\max} and χ_y^{\max} by the FLEX approximation (RPA), under the condition (a) $n = 0.90$, $U = 5$ ($U = 2.10$) and (b) $n = 1.20$, $U = 8$ ($U = 2.96$), at $T = 0.02$. In the numerical study by RPA, 256×256 \mathbf{k} -meshes and 256 Matsubara frequencies are used. In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

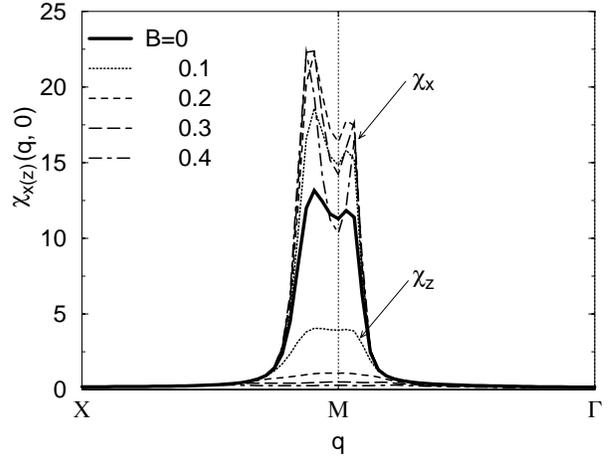


Fig. 2. $\chi_x(\mathbf{q}, 0)$ and $\chi_y(\mathbf{q}, 0)$ under finite B for $n = 0.90$ at $T = 0.02$.

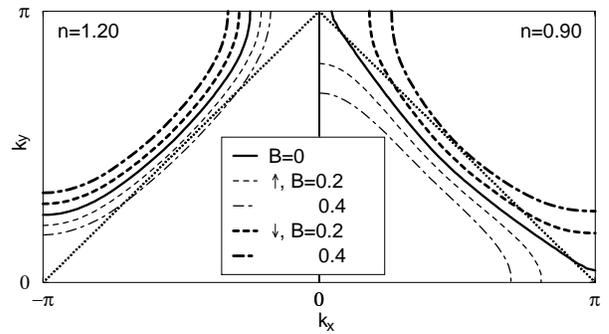


Fig. 3. FS's for \uparrow - and \downarrow -electrons under various magnetic field B for $n = 0.90$ at $T = 0.02$.

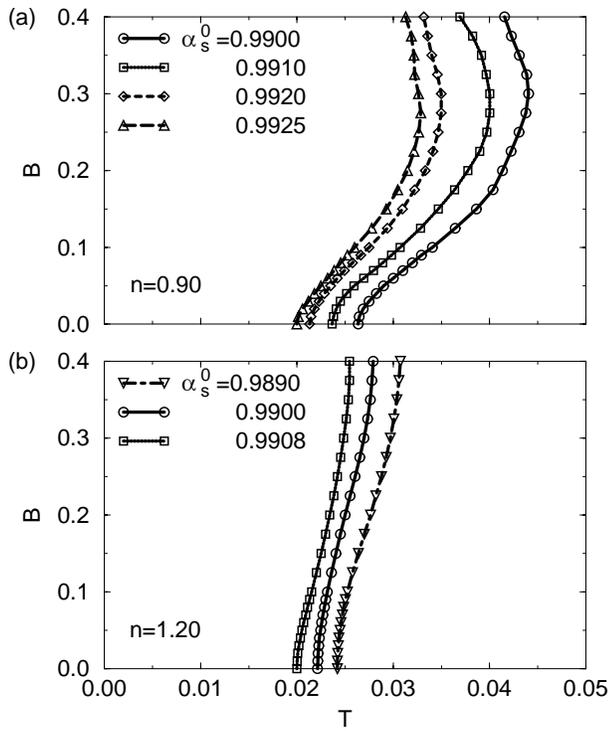


Fig. 4. Obtained phase diagram for T_N versus B for various α_S^0 's.