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2000 J. Phys.: Condens. Matter 12 8683

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## A simplified approach to non-collinear magnetism in amorphous transition metals

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Received 20 July 2000

**Abstract.** A theory of non-collinear magnetism in structurally disordered metals is presented on the basis of the Gaussian model for the distribution of the interatomic distance and the saddle-point approximation to the integral equation for the distribution of local magnetic moments. Simple self-consistent equations for the local moments, which significantly reduce the numerical calculations, are obtained. Magnetization and the spin-glass order parameters are calculated as a function of the d-electron occupation number  $N$  and temperature. It is shown that the theory describes the transition from the ferromagnetism to the non-collinear spin glass with decreasing  $N$ , which is expected experimentally. The calculated magnetic phase diagram is shown to be consistent with previous results based on the Monte Carlo sampling method as well as the recent experimental data on the quasi-binary amorphous Fe–Mn alloys.

### 1. Introduction

Structurally disordered metals and alloys often display magnetic properties which are quite different from their crystalline counterparts [1–3]. Iron-rich amorphous alloys are a typical example showing a drastic change of magnetism; the Curie temperatures rapidly decrease with increasing Fe concentration and the spin-glass phase (SG) appears beyond 90 at% Fe after complete disappearance of the ferromagnetism (F) [4, 5]. Since the experimental SG temperatures ( $T_g$ ) beyond 90 at% Fe are approximately constant ( $\approx 110$  K) irrespective of the second elements, the SG is considered to be inherent in the amorphous pure Fe.

The theory which explains the SG in amorphous Fe was first proposed by Kakehashi [6]. He constructed a finite temperature theory of amorphous metallic magnetism on the basis of the two-fields functional integral technique to the degenerate-band Hubbard model [7] and the distribution function method to treat the structural disorder of local moments (LM) [8]. Solving the self-consistent equations for the magnetization and the SG order parameter, he obtained the SG around the d-electron number  $N = 7.0$  (i.e. amorphous Fe), which is caused by the nonlinear magnetic couplings between Fe LM and the local environment effects on the amplitudes of Fe LMs. The volume dependence of the SG state and the influence of the degree of structural disorder on the magnetic phase diagram were investigated in [9, 10].

The ground-state calculations [11–14] for amorphous Fe reported the ferromagnetism at the early stage of their investigations. Later, the non-collinear ground-state calculations suggested the possibility of the SG in amorphous Fe. Krey *et al* [15] obtained two self-consistent solutions with magnetization  $1.17 \mu_B$  and  $0.2 \mu_B$  which are almost degenerate in energy, using the tight-binding supercell method with 54 atoms. Lorentz *et al* [16] performed detailed non-collinear calculations based on the self-consistent LMTO recursion method with 1728 atoms

in a cluster, and found that the ground-state magnetization decreases up to  $0.5 \mu_B$  with the SG-like random LM configuration. More recent non-collinear calculations by Liebs *et al* [17] with use of the LMTO supercell method with 32 Fe atoms in a unit cell showed that even the zero magnetic moment state (i.e. the SG) can become the ground state for amorphous Fe.

With the development of the ground-state theory, it has been desired to construct the non-collinear theory at finite temperatures. We proposed recently such a theory, extending the collinear theory of amorphous metallic magnetism to the non-collinear case [18]. We demonstrated using the non-collinear theory that the isotropic spin glass with the SG temperature being comparable with the experimental ones is realized in the vicinity of amorphous Fe as a function of the d-electron number. The non-collinear theory, however, uses the Monte Carlo sampling technique to treat a huge number of spin and structural configurations of surrounding atoms and LMs. The method requires a large amount of computing time for accurate calculations of the magnetization and the SG order parameters. Therefore it is not easy to obtain accurately the details of the magnetic phase diagram, to obtain the susceptibilities by taking the numerical derivative of the magnetization, and to apply the theory to more complex systems.

In the present paper, we propose an alternative theory which is more analytic and reduces the numerical calculations significantly. The difficulty in our previous theory was how to treat the  $4z$ -fold integrals in the integral equation for the distribution function of LMs. Here  $z$  is the number of nearest neighbours. We adopted in our previous paper [18] the decoupling approximation and the Monte Carlo sampling method to treat a large number of spin and structural configurations. In the present paper, we assume the Gaussian distribution with the width  $\sigma$  for the interatomic distance and perform the  $z$ -fold integrals analytically using the saddle point approximation which is exact in the large  $z/\sigma^2$  limit, so that we can reduce the  $4z$ -fold integral equation into the self-consistent equations for the magnetization and the SG order parameters with only 64 effective configurations.

In section 2.1, we present the basic expressions in the non-collinear theory of amorphous metallic magnetism. The microscopic expression of the LMs and the integral equation for the LM distribution will be presented there. In section 2.2, the Gaussian distribution for the interatomic distance will be introduced. It is shown that the central LM can be regarded as a function of the linear combinations of the deviations of the interatomic distances from their average value, so that the  $z$ -fold integrals in the kernel of the integral equation are performed analytically with use of the saddle point approximation. The remaining  $3z$ -fold integrals equation is transformed into a simplified self-consistent equation for the magnetization and the SG order parameter in section 2.3. In section 3, the numerical results for amorphous transition metals are presented to show the reliability and simplicity of the present theory. It is shown that an overall feature of the magnetic phase diagram is consistent with the previous results based on the Monte Carlo sampling method. The results are compared with recent experimental data on quasi-binary  $Y_{20}(\text{Mn}_{1-x}\text{Fe}_x)_{80}$  amorphous alloys. The last section is devoted to the summary of the present theory.

## 2. Formulation

### 2.1. Non-collinear theory of amorphous metallic magnetism

We start from the  $D$ -fold degenerate-band Hamiltonian with the intra-atomic Coulomb ( $U_i$ ) and exchange ( $J_i$ ) interactions as

$$H = \sum_{i\nu\sigma} \epsilon_i^0 \hat{n}_{i\nu\sigma} + \sum_{ij\nu\sigma} t_{ij} a_{i\nu\sigma}^\dagger a_{j\nu\sigma} + \frac{1}{4} \sum_i U_i \hat{n}_i^2 - \sum_i J_i \hat{S}_i^2. \quad (1)$$

Here  $\epsilon_i^0$  and  $t_{ij}$  are the atomic level on site  $i$  and the transfer integral between sites  $i$  and  $j$ , respectively.  $a_{i\nu\sigma}^\dagger$  ( $a_{i\nu\sigma}$ ) is the creation (annihilation) operator for an electron with spin  $\sigma$  and orbital  $\nu$  on site  $i$ ,  $\hat{n}_{i\nu\sigma} = a_{i\nu\sigma}^\dagger a_{i\nu\sigma}$  is the number operator of electrons on site  $i$ , orbital  $\nu$ , and spin  $\sigma$ . Furthermore,  $\hat{n}_i$  and  $\hat{S}_i$  denote the charge and spin density operators on site  $i$ , which are defined by  $\hat{n}_i = \sum_{\nu\sigma} \hat{n}_{i\nu\sigma}$ , and  $\hat{S}_i = \sum_{\nu\sigma\sigma'} a_{i\nu\sigma}^\dagger (\boldsymbol{\sigma})_{\sigma\sigma'} a_{i\nu\sigma'}/2$  with use of the Pauli spin matrices  $\boldsymbol{\sigma}$ , respectively.

After introducing the locally rotated coordinates into the intra-atomic interaction at each site in (1), we adopt the functional integral technique [7]. The method transforms the interacting Hamiltonian  $H$  into a one-electron Hamiltonian with time-dependent random charge and exchange fictitious fields acting on each site  $i$ . By making use of the static approximation, we obtain the expression of the local moment (LM) on site 0, which reduces to that of the generalized Hartree–Fock approximation at the ground state [19]

$$\langle m_0 \rangle = \frac{\int [\prod_j d\xi_j \xi_j^{-2}] (1 + \frac{4}{\beta \tilde{J}_0 \xi_0^2}) \xi_0 e^{-\beta E(\boldsymbol{\xi})}}{\int [\prod_j d\xi_j \xi_j^{-2}] e^{-\beta E(\boldsymbol{\xi})}} \quad (2)$$

$$E(\boldsymbol{\xi}) = \int d\omega f(\omega) \frac{1}{\pi} \text{Im Tr} \ln(L^{-1} - t) - \sum_i N_i w_i(\boldsymbol{\xi}) + \sum_i \frac{1}{4} \tilde{J}_i \xi_i^2. \quad (3)$$

Here  $\tilde{J}_i = U_i/2D + (1 + 1/2D)J_i$  is the effective exchange energy parameter,  $f(\omega)$  is the Fermi distribution function,  $(t)_{i\nu\sigma j\nu'\sigma'} = t_{ij} \delta_{\nu\nu'} \delta_{\sigma\sigma'}$ ,  $N_i$  is the neutral charge on site  $i$ , and  $w_i$  is the charge potential on the same site. The locator matrix  $L$  is defined by

$$(L^{-1})_{i\nu\sigma j\nu'\sigma'} = (\omega + i\delta - \epsilon_i^0 + \mu - w_i(\boldsymbol{\xi})) \delta_{ij} \delta_{\nu\nu'} \delta_{\sigma\sigma'} + \frac{1}{2} \tilde{J}_i \boldsymbol{\xi}_i \cdot (\boldsymbol{\sigma})_{\sigma\sigma'} \delta_{ij} \delta_{\nu\nu'} \quad (4)$$

$\delta$  being the infinitesimal positive number, and  $\mu$  being the chemical potential.

In what follows, we consider the amorphous metallic system. There are two kinds of disorder in this system; one is the diagonal disorder in  $L$  which is mainly caused by the thermal spin fluctuations, and the other is the off-diagonal disorder in  $t$  due to the fluctuation of the interatomic distance  $R$ . Since the amorphous metals and alloys form the well-defined nearest-neighbour (NN) shell [20], we treat the local environment effects due to the atoms and LMs on the NN shell directly, and describe the structural disorder outside the shell by means of the effective self-energy  $\mathcal{S}_\sigma$  and the thermal spin fluctuations by means of the effective locator  $\mathcal{L}_\sigma$ .

Let us introduce the inverse effective locator  $\mathcal{L}_\sigma^{-1}$  into the first term at the right-hand side (rhs) of (3) to describe the diagonal disorder as an average and expand the deviation with respect to the sites. We can then rewrite the energy (3) in the form

$$E(\boldsymbol{\xi}) = \int d\omega f(\omega) \frac{1}{\pi} \text{Im Tr} \ln(\mathcal{L}^{-1} - t) F + \sum_i E_i(\boldsymbol{\xi}_i) + \Delta E(\boldsymbol{\xi}). \quad (5)$$

Here the coherent Green function  $F$  is defined by

$$F_{i\sigma j\sigma'} = [(\mathcal{L}^{-1} - t)]_{i\sigma i\sigma} \delta_{ij} \delta_{\sigma\sigma'}. \quad (6)$$

The first term on the rhs of equation (5) is the zeroth-order term which is described by the effective medium only. This term could be dropped from the expression of energy, since it does not play any role in the thermal average. The second term is the first-order correction consisting of the sum of the single-site energy  $E_i(\boldsymbol{\xi}_i)$ . It is given by

$$E_i(\boldsymbol{\xi}_i) = \int d\omega f(\omega) \frac{D}{\pi} \text{Im} \ln \det(L_i^{-1} - \mathcal{L}^{-1} + F^{-1}) - N_i w_i(\boldsymbol{\xi}) + \frac{1}{4} \tilde{J}_i \xi_i^2 \quad (7)$$

where

$$L_i^{-1} = \omega + i\delta - \epsilon_i^0 + \mu - w_i(\boldsymbol{\xi}) + \frac{1}{2} \tilde{J}_i \boldsymbol{\xi}_i \cdot \boldsymbol{\sigma}. \quad (8)$$

The third term at the rhs of equation (5) is the higher-order correction.  $\Delta E(\xi)$  reduces to  $\sum_{(i,j)} \Phi_{ij}(\xi_i, \xi_j)$  in the pair approximation and all the higher-order terms are neglected by assuming small deviation from the effective medium. The pair energy functional  $\Phi_{ij}(\xi_i, \xi_j)$  between sites  $i$  and  $j$  is given by

$$\Phi_{ij}(\xi_i, \xi_j) = \int d\omega f(\omega) \frac{D}{\pi} \text{Im Tr}^{(ij)}[\ln(1 + \tilde{t}F')]. \quad (9)$$

Here  $\text{Tr}^{(ij)}$  denotes the trace over the subspace of sites  $i$  and  $j$ , the off-diagonal coherent Green function is defined by

$$F'_{i\sigma j\sigma'} = [(\mathcal{L}^{-1} - t)]_{i\sigma j\sigma'} (1 - \delta_{ij}) \delta_{\sigma\sigma'} \quad (10)$$

and  $\tilde{t}$  is the single-site  $t$  matrix defined by

$$\tilde{t} = [1 + (L^{-1} - \mathcal{L}^{-1})F]^{-1}(L^{-1} - \mathcal{L}^{-1}). \quad (11)$$

Equation (2) is then written as

$$\langle m_0 \rangle = \frac{\int d\xi_0 \xi_0^{-2} (1 + 4/\beta \tilde{J}_0 \xi_0^2) \xi_0 e^{-\beta E_0(\xi_0)} \langle \exp(-\beta \sum_{(i,j)} \Phi_{ij}(\xi_i, \xi_j)) \rangle'_0}{\int d\xi_0 \xi_0^{-2} e^{-\beta E_0(\xi_0)} \langle \exp(-\beta \sum_{(i,j)} \Phi_{ij}(\xi_i, \xi_j)) \rangle'_0}. \quad (12)$$

Here the average  $\langle (\sim) \rangle'_0$  is defined by

$$\langle (\sim) \rangle'_0 = \int \left[ \prod_{i=1}^{N-1} p_i(\xi_i) d\xi_i \xi_i^{-2} \right] (\sim) \quad (13)$$

and  $p_i(\xi_i)$  is the probability density for the single site energy  $E_i(\xi_i)$ ,

$$p_i(\xi_i) = \frac{e^{-\beta E_i(\xi_i)}}{\int d\xi_i \xi_i^{-2} e^{-\beta E_i(\xi_i)}}. \quad (14)$$

In the next step, we adopt in (12) the following decoupling approximation for arbitrary function  $f$ , which is correct up to the second moment:

$$\langle f(\xi_i) \rangle_0 \equiv \int d\xi_i p_i(\xi_i) f(\xi_i) \quad (15)$$

$$= \sum_{s_i} \frac{1}{8} \left( 1 + \frac{\langle \xi_{iz} \rangle_0}{a_{iz}} s_{iz} \right) f(\{s_{i\alpha} a_{i\alpha}\}) \quad (16)$$

where  $\sum_{s_i} = \sum_{s_{ix}=\pm 1} \sum_{s_{iy}=\pm 1} \sum_{s_{iz}=\pm 1}$  and  $a_{i\alpha} = \langle \xi_{i\alpha}^2 \rangle_0^{1/2}$ .

Taking the same steps as in [21], we reach

$$\langle m_0 \rangle = \frac{\int d\xi_0 \xi_0^{-2} \sum_{\{s_i\}} (1 + 4/\beta \tilde{J}_0 \xi_0^2) \xi_0 e^{-\beta \Psi(\xi_0, \{s_{i\alpha} a_{i\alpha}\})}}{\int d\xi_0 \xi_0^{-2} \sum_{\{s_i\}} e^{-\beta \Psi(\xi_0, \{s_{i\alpha} a_{i\alpha}\})}} \quad (17)$$

where

$$\Psi(\xi, \{s_{i\alpha} a_{i\alpha}\}) = E_0(\xi) - \beta^{-1} \sum_i s_{iz} \tanh^{-1} \frac{\langle \xi_{iz} \rangle_0}{a_{iz}} + \Delta E(\xi, \{s_{i\alpha} a_{i\alpha}\}) \quad (18)$$

$$\begin{aligned} \Delta E(\xi, \{s_{i\alpha} a_{i\alpha}\}) &= \sum_{i \neq 0} \Phi_{0i}^{(a)}(\xi) - \sum_{i \neq 0} \sum_{\alpha=x,y,z} \left[ \Phi_{0j\alpha}^{(e)}(\xi) + \sum_{j \neq 0, i} \mathcal{K}_{ij\alpha} \right] s_{i\alpha} \\ &+ \sum_{i \neq 0} \sum_{(\alpha, \gamma)} \Phi_{0j\beta}^{(b)}(\xi) s_{i\alpha} s_{i\gamma} + \sum_{(ij)} \frac{1}{64} \sum_{\mu_i \mu_j} \Phi_{ij}(\{\mu_{i\alpha} a_{i\alpha}\}, \{\mu_{j\alpha} a_{j\alpha}\}) \\ &- \sum_{(i\alpha, j\gamma)} \mathcal{J}_{ij\beta} s_{i\alpha} s_{j\gamma} + \sum_{(i\alpha, j\beta, k\gamma)} [\Phi_{0i}^{(c)}(\xi) \delta_{ij} \delta_{jk} + \mathcal{F}_{ij}^{(\beta, \gamma, \alpha)} \delta_{jk} \\ &+ \mathcal{F}_{jk}^{(\gamma, \alpha, \beta)} \delta_{ki} + \mathcal{F}_{ki}^{(\alpha, \beta, \gamma)} \delta_{ij}] s_{i\alpha} s_{j\beta} s_{k\gamma} + \dots \end{aligned} \quad (19)$$

In (17),  $s_{i\alpha}$  takes a value  $+1$  or  $-1$ , and  $\sum_{\{s_i\}}$  denote the sum over  $s_1, s_2, \dots$ .  $\sum'_{(\alpha,\gamma)}$  in (19) means a summation over all the cyclic pairs of  $x, y$  and  $z$ .  $\sum'_{(i\alpha,j\gamma)} (\sum'_{(i\alpha,j\beta,k\gamma)})$  denotes a summation over all the pairs (triplets) of sites and components with  $i \neq j$  and  $\alpha \neq \gamma$  ( $i \neq j \neq k$  and  $\alpha \neq \beta \neq \gamma$ ) which are not related to site 0. The pair interactions  $\Phi_{0i}^{(a)}(\xi)$ ,  $\Phi_{0i\alpha}^{(e)}(\xi)$ ,  $\Phi_{0j\alpha}^{(b)}(\xi)$ ,  $\Phi_{0i}^{(c)}(\xi)$ ,  $\mathcal{K}_{ij\alpha}$ ,  $\mathcal{J}_{ij\beta}$ , and  $\mathcal{F}_{ij}$  are defined, respectively as follows.

$$\Phi_{0j}^{(a)}(\xi) = \frac{1}{8} \sum_{\mu_j} \Phi_{0j}(\xi, \{\mu_{j\alpha} a_{j\alpha}\}) \quad (20)$$

$$\Phi_{0j\alpha}^{(e)}(\xi) = -\frac{1}{8} \sum_{\mu_j} \mu_{j\alpha} \Phi_{0j}(\xi, \{\mu_{j\gamma} a_{j\gamma}\}) \quad (21)$$

$$\Phi_{0j\beta}^{(b)}(\xi) = \frac{1}{8} \sum_{\mu_j} \mu_{j\alpha} \mu_{j\gamma} \Phi_{0j}(\xi, \{\mu_{j\delta} a_{j\delta}\}) \quad (22)$$

$$\Phi_{0j}^{(c)}(\xi) = \frac{1}{8} \sum_{\mu_j} \mu_{jx} \mu_{jy} \mu_{jz} \Phi_{0j}(\xi, \{\mu_{j\alpha} a_{j\alpha}\}) \quad (23)$$

$$\mathcal{K}_{ij\alpha} = \frac{1}{64} \sum_{\mu_i} \sum_{\mu_j} \mu_{i\alpha} \Phi_{ij}(\{\mu_{i\beta} a_{i\beta}\}, \{\mu_{j\gamma} a_{j\gamma}\}) \quad (24)$$

$$\mathcal{J}_{ij\beta} = \frac{1}{64} \sum_{\mu_i} \sum_{\mu_j} \mu_{i\alpha} \mu_{j\gamma} \Phi_{ij}(\{\mu_{i\lambda} a_{i\lambda}\}, \{\mu_{j\delta} a_{j\delta}\}) \quad (25)$$

$$\mathcal{F}_{ki}^{(\alpha,\beta,\gamma)} = \frac{1}{64} \sum_{\mu_i} \sum_{\mu_k} \mu_{i\alpha} \mu_{j\beta} \mu_{k\gamma} \Phi_{ik}(\{\mu_{i\delta} a_{i\delta}\}, \{\mu_{kv} a_{kv}\}). \quad (26)$$

In the following, we make a molecular-field approximation for the thermal averages of LMs on the NN shell. The variables  $s_{i\alpha}, s_{i\alpha} s_{j\gamma}, s_{i\alpha} s_{j\beta} s_{k\gamma}$  in (19) are replaced by their thermal averages.

$$\langle m_0 \rangle = \frac{\int d\xi \xi^{-2} (1 + 4/\beta \tilde{J} \xi^2) \xi e^{-\beta \Psi(\xi)}}{\int d\xi \xi^{-2} e^{-\beta \Psi(\xi)}} \quad (27)$$

$$\begin{aligned} \Psi(\xi) = E_0(\xi) + \sum_{j \neq 0}^z \left[ \Phi_{0j}^{(a)}(\xi) - \sum_{\alpha} \Phi_{0j\alpha}^{(e)}(\xi) \frac{\langle m_{j\alpha} \rangle}{\tilde{a}_{j\alpha}} + \sum_{(\alpha\gamma)} \Phi_{0j\delta}^{(b)}(\xi) \frac{\langle m_{j\alpha} \rangle \langle m_{j\gamma} \rangle}{\tilde{a}_{j\alpha} \tilde{a}_{j\gamma}} \right. \\ \left. + \Phi_{0j}^{(c)}(\xi) \frac{\langle m_{jx} \rangle \langle m_{jy} \rangle \langle m_{jz} \rangle}{\tilde{a}_{jx} \tilde{a}_{jy} \tilde{a}_{jz}} \right]. \end{aligned} \quad (28)$$

Here  $\sum_{\alpha} (\sum_{(\alpha\gamma)})$  denotes the sum over  $x, y, z$  components (( $yz$ ), ( $zx$ ), ( $xy$ ) pairs).  $\tilde{a}_{j\alpha} = (1 + 4/\beta \tilde{J}_j \langle \xi_j^2 \rangle_0) \langle \xi_{j\alpha}^2 \rangle_0^{1/2}$ ,  $\langle \rangle_0$  being the thermal average with respect to the single-site energy on site  $j$ .

The final expression of the single-site energy  $E_0(\xi)$  in (28) is given by

$$E_0(\xi) = \int d\omega f(\omega) \frac{D}{\pi} \text{Im} \ln[(\delta L_{0\uparrow}^{-1} + F_{00\uparrow}^{-1})(\delta L_{0\downarrow}^{-1} + F_{00\downarrow}^{-1}) - \frac{1}{4} \tilde{J}_0^2 \xi_{\perp}^2] - N_0 w_0(\xi) + \frac{1}{4} \tilde{J}_0 \xi^2 \quad (29)$$

where

$$\delta L_{j\sigma}^{-1} = (L^{-1})_{j\nu\sigma j\nu\sigma} - \mathcal{L}_{\sigma}^{-1} \quad (30)$$

and

$$\xi_{\perp}^2 = \xi_x^2 + \xi_y^2. \quad (31)$$

The pair energies  $\Phi_{0j}^{(a)}(\xi)$ ,  $\Phi_{0j\alpha}^{(e)}(\xi)$ ,  $\Phi_{0j\delta}^{(b)}(\xi)$ , and  $\Phi_{0j}^{(c)}(\xi)$  are calculated via (20)–(23) from  $\Phi_{0j}(\xi, \xi_j)$ , which is given by

$$\begin{aligned} \Phi_{0j}(\xi, \xi_j) = & \int d\omega f(\omega) \frac{D}{\pi} \operatorname{Im} \ln \left[ 1 - \sum_{\sigma} (\tilde{t}_0)_{\sigma\sigma} F'_{0j\sigma} F'_{j0\sigma} (\tilde{t}_j)_{\sigma\sigma} \right. \\ & - F'_{0j\uparrow} F'_{j0\downarrow} \frac{\tilde{J}_0 \tilde{J}_j}{2\tilde{R}_0 2\tilde{R}_j} (\xi_+ \xi_{j-} + \xi_- \xi_{j+}) \\ & \left. + (F'_{0j\uparrow} F'_{j0\downarrow})^2 \left\{ (\tilde{t}_0)_{\uparrow\uparrow} (\tilde{t}_0)_{\downarrow\downarrow} - \frac{\tilde{J}_0^2 \xi_{\perp}^2}{4\tilde{R}_0^2} \right\} \left\{ (\tilde{t}_j)_{\uparrow\uparrow} (\tilde{t}_j)_{\downarrow\downarrow} - \frac{\tilde{J}_j^2 \xi_{j\perp}^2}{4\tilde{R}_j^2} \right\} \right]. \end{aligned} \quad (32)$$

Here  $\xi_{j\pm} = \xi_{jx} \pm i\xi_{jy}$ ,  $(\tilde{t}_j)_{\sigma\sigma'}$  is the single-site  $t$  matrix whose diagonal component is given by

$$(\tilde{t}_j)_{\sigma\sigma} = \frac{\delta L_{j\sigma}^{-1} + (\delta L_{j\uparrow}^{-1} \delta L_{j\downarrow}^{-1} - \frac{1}{4} \tilde{J}_j^2 \xi_{j\perp}^2) F_{\sigma}}{\tilde{R}_j} \quad (33)$$

$$\tilde{R}_j = (1 + \delta L_{j\uparrow}^{-1} F_{\uparrow})(1 + \delta L_{j\downarrow}^{-1} F_{\downarrow}) - \frac{1}{4} \tilde{J}_j^2 \xi_{j\perp}^2 F_{\uparrow} F_{\downarrow}. \quad (34)$$

$(\tilde{t}_0)_{\sigma\sigma}$  and  $\tilde{R}_0$  are defined in the same way, but  $F_{\sigma}$  has been replaced by  $F_{00\sigma}$  in equations (33) and (34).

The coherent Green functions  $F_{00\sigma}$ ,  $F'_{0j\sigma}$ , and  $F_{\sigma} (= [(\mathcal{L}_{\sigma}^{-1} - t)^{-1}]_{j\sigma j\sigma})$  in (29), (32)–(34) are given in the Bethe approximation as

$$F_{00\sigma} = (\mathcal{L}_{\sigma}^{-1} - \theta \mathcal{K}_{\sigma})^{-1} \quad (35)$$

$$F'_{0j\sigma} = t_{0j} \mathcal{K}_{\sigma} F_{00\sigma} \quad (36)$$

and

$$F_{\sigma} = \int \frac{[\rho(\varepsilon)]_s d\varepsilon}{\mathcal{L}_{\sigma}^{-1} - \varepsilon}. \quad (37)$$

Here  $\theta = \sum_{j=1}^z t_{j0}^2$ ,  $\mathcal{K}_{\sigma} = (\mathcal{L}_{\sigma}^{-1} - \mathcal{S}_{\sigma})^{-1}$  and  $[\rho(\varepsilon)]_s$  is the structural average of the noninteracting density of states (DOS) for  $\{t_{ij}\}$ . Note that the transfer integral  $t_{j0}$  depends on the interatomic distance  $R_j$  between sites 0 and  $j$ ;  $t_{j0} = t_{j0}(R_j)$ . The self-energy  $\mathcal{K}_{\sigma}$  (or  $\mathcal{S}_{\sigma}$ ) is determined from the condition that

$$[(\mathcal{L}_{\sigma}^{-1} - \theta \mathcal{K}_{\sigma})^{-1}]_s = F_{\sigma}. \quad (38)$$

Here  $[\ ]_s$  denotes the structural average.

Equation (27) manifests that the central LM is determined by the coordination number  $z$  on the NN shell, the interatomic distances  $\{R_j\}$  between the central and neighbouring atoms, the LMs  $\{\langle m_j \rangle\}$  on the NN shell, when the two kinds of effective media  $\mathcal{L}_{\sigma}^{-1}$  and  $\mathcal{K}_{\sigma}$  are given. These variables randomly change in amorphous metals. We therefore introduce the distribution function  $p(z)$  which is the probability of finding a coordination number  $z$ , the probability  $g(\mathbf{m}) d\mathbf{m}$  of finding  $\langle m_j \rangle$  between  $\mathbf{m}$  and  $\mathbf{m} + d\mathbf{m}$ , and the probability  $p_s(R) dR$  of finding a neighbouring atom at the distance between  $R$  and  $R + dR$ . The distribution of the central LM is then given via (27) as follows since the distribution of the central LM is equivalent to those of the neighbouring ones [6, 8].

$$g(M) = \sum_z p(z) \int \delta(M - \langle m_0 \rangle) \prod_{j=1}^z [g(\mathbf{m}_j) d\mathbf{m}_j p_s(R_j) dR_j]. \quad (39)$$

We adopt in this paper the simplest form of  $p(z)$  given by

$$p(z) = ([z^*] + 1 - z^*) \delta_{z[z^*]} + (z^* - [z^*]) \delta_{z[z^*]+1}. \quad (40)$$

Here  $z^*$  is the average coordination number,  $[ ]$  denotes the Gauss's notation.

The above equation (39) forms the  $4z - 1$  fold integral equation for the distribution function  $g(\mathbf{m})$ . In our previous theory [6, 18], we introduced the distribution  $p'_s(y_j)$  for the square of the transfer integral  $y_j = t_{j0}^2(R_j)$  instead of that of the distance, and adopted the decoupling approximation to all the distributions at the rhs of (39), which corresponds to the two-delta approximation, e.g.  $p'_s(y) \approx [\delta(y + [(\delta y)^2]_s^{1/2}) + \delta(y - [(\delta y)^2]_s^{1/2})]/2$ . The resulting configurations at the rhs of (39) were of the order of  $10^7$ , therefore we estimated the rhs by means of the Monte Carlo sampling technique.

Although the method is useful for drawing the magnetic phase diagram and calculating the distribution of LMs, it is time-consuming when we increase the accuracy. To avoid the difficulty, we propose in the following subsection an alternative method which allows us to integrate the rhs of (39) over the variables  $\{R_j\}$ .

## 2.2. Gaussian distribution for the interatomic distance and saddle-point approximation

We adopt the Gaussian distribution for the probability of finding a neighbouring atom at  $R$

$$p_s(R) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(R-R_0)^2/2\sigma^2}. \quad (41)$$

Here  $\sigma$  ( $R_0$ ) denotes the width (average distance).

The distribution is much more reasonable when compared with the two-delta distribution adopted in the previous theory, as found in the radial distribution function in x-ray diffraction experiments [22]. It should be noted that the form (41) does not vanish at  $R = 0$ . It does not, however, introduce any difficulty since  $\sigma \ll R_0$  in amorphous system. In the following, we extend the range of integrations for (41) from  $[0, \infty]$  to  $[-\infty, \infty]$  assuming  $\sigma \ll R_0$ .

The energy  $\Psi(\xi)$  in (28) is regarded as the function of  $\theta$  and  $\{x_j = R_j - R_0\}$  because of (35) and (36);  $\Psi(\xi) = \Psi(\xi, \theta, \{x_j\})$ . In fact, one can assume [23] that  $t_{j0} = t(R_j) = t(R_0)(R_0/R_j)^\kappa$  ( $\kappa \approx 3.8$ ), and therefore  $t_{j0}^2$  and  $\theta$  are expanded as follows.

$$t_{j0}^2(R_j) = t(R_0)^2 \left( \frac{x_j + R_0}{R_0} \right)^{-2\kappa} \quad (42)$$

$$\theta = zt(R_0)^2 \left[ 1 - \frac{2\kappa}{R_0}u + \frac{\kappa(2\kappa + 1)}{R_0^2}v \right] \quad (43)$$

where

$$u = \frac{1}{z} \sum_{i=1}^z x_i \quad (44)$$

$$v = \frac{1}{z} \sum_{i=1}^z x_i^2. \quad (45)$$

Therefore, one can expand  $\Psi(\xi, \theta, \{x_j\})$  with respect to  $\{x_j\}$  as

$$\begin{aligned} \Psi(\xi, \theta, \{x_j\}) &= \Psi(\xi, \theta, 0) + z\Phi_1^{(a)}(\xi, \theta, 0)u - \sum_{\alpha} z\Phi_{\alpha 1}^{(e)}(\xi, \theta, 0)u_{\alpha} + \sum_{(\alpha\gamma)} z\Phi_{\delta 1}^{(b)}(\xi, \theta, 0)u_{\alpha\gamma} \\ &+ z\Phi_1^{(c)}(\xi, \theta, 0)u_{xyz} + \frac{1}{2}z\Phi_2^{(a)}(\xi, \theta, 0)v - \sum_{\alpha} \frac{1}{2}z\Phi_{\alpha 2}^{(e)}(\xi, \theta, 0)v_{\alpha} \\ &+ \sum_{(\alpha\gamma)} \frac{1}{2}z\Phi_{\delta 2}^{(b)}(\xi, \theta, 0)v_{\alpha\gamma} + \frac{1}{2}z\Phi_2^{(c)}(\xi, \theta, 0)v_{xyz}. \end{aligned} \quad (46)$$



Here  $\Phi_1^{(a)}(\xi, \theta, 0)$ ,  $\Phi_{\alpha 1}^{(e)}(\xi, \theta, 0)$ ,  $\Phi_{\delta 1}^{(b)}(\xi, \theta, 0)$  and  $\Phi_1^{(c)}(\xi, \theta, 0)$  are the first derivatives of  $\Phi_{0j}^{(a)}(\xi, \theta, x_j)$ ,  $\Phi_{0j\alpha}^{(e)}(\xi, \theta, x_j)$ ,  $\Phi_{0j\delta}^{(b)}(\xi, \theta, x_j)$ , and  $\Phi_{0j}^{(c)}(\xi, \theta, x_j)$  with respect to  $x_j$  at  $x_j = 0$ .  $\Phi_2^{(a)}(\xi, \theta, 0)$ ,  $\Phi_{\alpha 2}^{(e)}(\xi, \theta, 0)$ ,  $\Phi_{\delta 2}^{(b)}(\xi, \theta, 0)$  and  $\Phi_2^{(c)}(\xi, \theta, 0)$  are the second derivatives of the same pair energies.  $u_\alpha$ ,  $u_{\alpha\gamma}$ ,  $u_{xyz}$ ,  $v_\alpha$ ,  $v_{\alpha\gamma}$ , and  $v_{xyz}$  are defined by

$$u_\alpha = \frac{1}{z} \sum_j \frac{\langle m_{j\alpha} \rangle}{\tilde{a}_{j\alpha}} x_j \quad (47)$$

$$u_{\alpha\gamma} = \frac{1}{z} \sum_j \frac{\langle m_{j\alpha} \rangle \langle m_{j\gamma} \rangle}{\tilde{a}_{j\alpha} \tilde{a}_{j\gamma}} x_j \quad (48)$$

$$u_{xyz} = \frac{1}{z} \sum_j \frac{\langle m_{jx} \rangle \langle m_{jy} \rangle \langle m_{jz} \rangle}{\tilde{a}_{jx} \tilde{a}_{jy} \tilde{a}_{jz}} x_j \quad (49)$$

$$v_\alpha = \frac{1}{z} \sum_j \frac{\langle m_{j\alpha} \rangle}{\tilde{a}_{j\alpha}} x_j^2 \quad (50)$$

$$v_{\alpha\gamma} = \frac{1}{z} \sum_j \frac{\langle m_{j\alpha} \rangle \langle m_{j\gamma} \rangle}{\tilde{a}_{j\alpha} \tilde{a}_{j\gamma}} x_j^2 \quad (51)$$

$$v_{xyz} = \frac{1}{z} \sum_j \frac{\langle m_{jx} \rangle \langle m_{jy} \rangle \langle m_{jz} \rangle}{\tilde{a}_{jx} \tilde{a}_{jy} \tilde{a}_{jz}} x_j^2. \quad (52)$$

Equations (43) and (46) show that  $\langle \mathbf{m}_0 \rangle$  is a function of  $\{u, u_\alpha, u_{\alpha\gamma}, u_{xyz}\}$  and  $\{v, v_\alpha, v_{\alpha\gamma}, v_{xyz}\}$ ;  $\langle \mathbf{m}_0 \rangle = \langle \mathbf{m}_0 \rangle(\{u\}\{v\})$ .

We can now write the kernel of the integral equation (39) as

$$K(M, z, \{\mathbf{m}_j\}) \equiv \int \delta(M - \langle \mathbf{m}_0 \rangle) \left[ \prod_{j=1}^z p_s(R_j) dR_j \right] = \int d\mathbf{q} K(\mathbf{q}) \quad (53)$$

$$K(\mathbf{q}) = \int \left[ \prod_{j=1}^z dx_j \right] \frac{1}{(\sqrt{2\pi}\sigma)^z} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^z x_i^2 - \phi(\{u\}, \{v\})\right) \quad (54)$$

$$\phi(\{u\}, \{v\}) = 2\pi i \mathbf{q} \cdot (M - \langle \mathbf{m}_0 \rangle(\{u\}, \{v\})). \quad (55)$$

Here  $\{u_i\}$  ( $\{v_i\}$ ) ( $i = 1, 2, \dots, 8$ ) stands for a set of variables  $u, u_x, u_y, u_z, u_{yz}, u_{zx}, u_{xy}$  and  $u_{xyz}$  ( $v, v_x, v_y, v_z, v_{yz}, v_{zx}, v_{xy}$  and  $v_{xyz}$ ).

Since  $u_i$  and  $v_i$  are the linear combinations of the Gaussian variables  $\{x_j\}$  (or  $\{x_j^2\}$ ), their fluctuations may be suppressed in the large  $z/\sigma^2$  limit. We adopt therefore the saddle-point approximation for the evaluation of the integral (54) assuming large  $z/2\sigma^2$ . Using the identities such as  $\int du \delta(u - z^{-1} \sum_i x_i) = 1$ ,  $K(\mathbf{q})$  is expressed as follows.

$$K(\mathbf{q}) = \int \left[ \prod_{i=1}^8 du_i \right] \left[ \prod_{i=1}^8 dv_i \right] \exp[-\phi(\{u\}, \{v\}) - \psi(\{u\}, \{v\})] \quad (56)$$

$$\begin{aligned} \exp[-\psi(\{u\}, \{v\})] &= \int \left[ \prod_{j=1}^z dx_j \right] \left[ \prod_{i=1}^8 \delta\left(u_i - z^{-1} \sum_j c_{ij} x_j\right) \delta\left(v_i - z^{-1} \sum_j c_{ij} x_j^2\right) \right] \\ &\times \frac{1}{(\sqrt{2\pi}\sigma)^z} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^z x_i^2\right). \end{aligned} \quad (57)$$

Here  $\{c_{ij}\}$  are the coefficients which appear at the rhs of (47)–(49) or (50)–(52).

The saddle-point evaluation of (56) yields

$$K(\mathbf{q}) = \exp[-\phi(\{u\}, \{v\}) - \psi(\{u\}, \{v\})]. \quad (58)$$

Here  $\{u_i\}$  and  $\{v_i\}$  are determined by

$$\frac{\partial}{\partial u_i} [\phi(\{u\}, \{v\}) + \psi(\{u\}, \{v\})] = 0 \tag{59}$$

$$\frac{\partial}{\partial v_i} [\phi(\{u\}, \{v\}) + \psi(\{u\}, \{v\})] = 0. \tag{60}$$

The function  $\psi(\{u\}, \{v\})$  is obtained from the following integral.

$$\exp[-\Omega(\{\zeta\}, \{\eta\})] = \int \left[ \prod_{i=1}^8 du_i dv_i \right] \exp \left( - \sum_i \zeta_i u_i - \sum_i \eta_i v_i - \psi(\{u\}, \{v\}) \right). \tag{61}$$

The function  $\Omega(\{\zeta\}, \{\eta\})$  is a Gaussian integral as seen from (57) and (61), so that it is obtained exactly as

$$\Omega(\{\zeta\}, \{\eta\}) = - \sum_i \frac{\beta_i^2}{4\alpha_i} + \frac{1}{2} \sum_i \ln(2\sigma^2 \alpha_i) \tag{62}$$

$$\alpha_i = \frac{1}{2\sigma^2} + \frac{1}{z} \sum_j c_{ji} \eta_j \tag{63}$$

$$\beta_i = \frac{1}{z} \sum_j c_{ji} \zeta_j. \tag{64}$$

The saddle-point evaluation of  $\Omega$  via (61), on the other hand, yields

$$\Omega(\{\zeta\}, \{\eta\}) = \sum_i \zeta_i u_i + \sum_i \eta_i v_i + \psi(\{u\}, \{v\}) \tag{65}$$

$$\zeta_i + \frac{\partial}{\partial u_i} \psi(\{u\}, \{v\}) = 0 \tag{66}$$

$$\eta_i + \frac{\partial}{\partial v_i} \psi(\{u\}, \{v\}) = 0. \tag{67}$$

Note that  $\{\zeta_i\}$  and  $\{\eta_i\}$  are chosen so that the saddle-point values  $\{u_i\}$  and  $\{v_i\}$  in (65)–(67) agree with those in (58)–(60). Thus,  $\{u_i\}$  and  $\{v_i\}$  are connected to  $\{\zeta_i\}$  and  $\{\eta_i\}$  as

$$\begin{aligned} u_i(\{\zeta\}, \{\eta\}) &= \frac{\partial}{\partial \zeta_i} \Omega(\{\zeta\}, \{\eta\}) \\ &= -\frac{1}{2z} \sum_j \frac{c_{ij} \beta_j}{\alpha_j} \end{aligned} \tag{68}$$

$$\begin{aligned} v_i(\{\zeta\}, \{\eta\}) &= \frac{\partial}{\partial \eta_i} \Omega(\{\zeta\}, \{\eta\}) \\ &= \frac{1}{2z} \sum_j \frac{c_{ij}}{\alpha_j} \left( 1 + \frac{\beta_j^2}{2\alpha_j} \right). \end{aligned} \tag{69}$$

Moreover from (59) and (66) ((60) and (67)), we obtain

$$\begin{aligned} \zeta_i &= \frac{\partial}{\partial u_i} \phi(\{u\}, \{v\}) \\ &= -2\pi i \mathbf{q} \cdot \frac{\partial \langle \mathbf{m}_0 \rangle(\{u\}, \{v\})}{\partial u_i} \end{aligned} \tag{70}$$

$$\begin{aligned} \eta_i &= \frac{\partial}{\partial v_i} \phi(\{u\}, \{v\}) \\ &= -2\pi i \mathbf{q} \cdot \frac{\partial \langle \mathbf{m}_0 \rangle(\{u\}, \{v\})}{\partial v_i}. \end{aligned} \tag{71}$$

In summary,  $\psi(\{u\}, \{v\})$  in (58) is obtained from (65) and (62) as a Legendre transformation of the Gauss-type generating function  $\Omega$ . The parameters  $\{u\}$  and  $\{v\}$ , and their conjugate ones  $\{\zeta\}$  and  $\{\eta\}$  are determined self-consistently from (68)–(71).

In the limit  $\sigma^2/z \rightarrow 0$ , the self-consistent equations (68)–(71) are easily solved as

$$u_i = 0 \quad (72)$$

$$v_i = \langle v_i \rangle \equiv \frac{\sigma^2}{z} \left( \sum_{j=1}^z c_{ij} \right) \quad (73)$$

$$\psi(\{u\}, \{v\}) = 0. \quad (74)$$

Here the bracket  $\langle \cdot \rangle$  in (73) denotes the average with respect to  $\{x_j\}$ . We have then

$$K(\mathbf{q}) = e^{-\phi(\{0\}, \{v\})}. \quad (75)$$

This is the zeroth approximation in which the fluctuation of interatomic distance has completely been neglected.

To obtain the higher-order correction, we solve the self-consistent equations (68)–(71) expanding them with respect to  $\sigma^2/z$ . To the first order, we obtain

$$\begin{aligned} \phi(\{u\}, \{v\}) + \psi(\{u\}, \{v\}) &= \phi(\{0\}, \{v\}) - \frac{\sigma^2}{2z} \left[ \frac{1}{z} \sum_{j=1}^z \left( \sum_{i=1}^8 c_{ij} \frac{\partial \phi(\{0\}, \{v\})}{\partial u_i} \right)^2 \right] \\ &\quad - \frac{\sigma^4}{z} \left[ \frac{1}{z} \sum_{j=1}^z \left( \sum_{i=1}^8 c_{ij} \frac{\partial \phi(\{0\}, \{v\})}{\partial v_i} \right)^2 \right] + \dots \end{aligned} \quad (76)$$

Substituting (76) into (58), we reach

$$K(\mathbf{q}) = \exp \left[ -\pi \left( \sum_{\alpha\gamma} q_\alpha A_{\alpha\gamma} q_\gamma + \mathbf{q} \cdot \mathbf{b} \right) \right] \quad (77)$$

$$\begin{aligned} A_{\alpha\gamma} &= \frac{2\pi\sigma^2}{z} \frac{1}{z} \sum_{j=1}^z \left[ \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_\alpha \rangle(\{0\}, \{v\})}{\partial u_i} \right) \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_\gamma \rangle(\{0\}, \{v\})}{\partial u_i} \right) \right. \\ &\quad \left. + 2\sigma^2 \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_\alpha \rangle(\{0\}, \{v\})}{\partial v_i} \right) \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_\gamma \rangle(\{0\}, \{v\})}{\partial v_i} \right) \right] \end{aligned} \quad (78)$$

$$\mathbf{b} = 2i(\mathbf{M} - \langle \mathbf{m}_0 \rangle(\{0\}, \{v\})). \quad (79)$$

We adopt (77) in the following, and perform the integral in (53), so that the integral equation (39) is expressed as follows.

$$g(\mathbf{M}) = \sum_z p(z) \int K(\mathbf{M}, z, \{\mathbf{m}_j\}) \prod_{j=1}^z [g(\mathbf{m}_j) d\mathbf{m}_j] \quad (80)$$

$$K(\mathbf{M}, z, \{\mathbf{m}_j\}) = \frac{1}{\sqrt{\det A}} \exp[-\pi(\mathbf{M} - \langle \mathbf{m}_0 \rangle(\{0\}, \{v\})) A^{-1}(\mathbf{M} - \langle \mathbf{m}_0 \rangle(\{0\}, \{v\}))]. \quad (81)$$

The above expression is quite reasonable in a sense that the  $\delta$ -function  $\delta(\mathbf{M} - \langle \mathbf{m}_0 \rangle)$  in (53) has been changed into the Gaussian kernel  $K$  (equation (81)) due to the Gaussian fluctuations of  $\{R_j\}$  (equation (41)).

2.3. Decoupling approximation to the local-moment distribution

The distribution  $g(\mathbf{m})$  is expected to have the axial symmetry along the  $z$ -axis ( $\equiv$  the direction of magnetization). In this case, the following decoupling approximation is correct up to the second-order moment.

$$\int X(\mathbf{m})g(\mathbf{m}) d\mathbf{m} \approx \sum_{\mu_x\mu_y\mu_z} \frac{1}{8} \left( 1 + \mu_z \frac{[\langle m_z \rangle]_s}{[\langle m_z^2 \rangle]_s^{1/2}} \right) X(\mu_x[\langle m_x^2 \rangle]_s^{1/2}, \mu_y[\langle m_y^2 \rangle]_s^{1/2}, \mu_z[\langle m_z^2 \rangle]_s^{1/2}). \tag{82}$$

Here  $X(\mathbf{m})$  is an arbitrary function.  $\mu_x, \mu_y,$  and  $\mu_z$  take the values  $\pm 1$ .

Adopting the decoupling approximation (82) at the right-hand side of equation (80), we obtain

$$g(\mathbf{M}) = \sum_z p(z) \sum_{\{\mu_j\}} \left(\frac{1}{2}\right)^{3z} \prod_{j=1}^z \left( 1 + \mu_{jz} \frac{[\langle m_z \rangle]_s}{[\langle m_z^2 \rangle]_s^{1/2}} \right) K(\mathbf{M}, z, \{\mu_{j\alpha}[\langle m_\alpha^2 \rangle]_s^{1/2}\}). \tag{83}$$

Here  $\mu_j = (\mu_{jx}, \mu_{jy}, \mu_{jz})$  and  $\mu_{j\alpha} = 1$  or  $-1$ .

It should be noted that each  $\mu_j$  has one of the 8 configurations  $\hat{\nu}_1 = (1, 1, 1), \hat{\nu}_2 = (1, 1, -1), \hat{\nu}_3 = (1, -1, 1), \hat{\nu}_4 = (1, -1, -1), \hat{\nu}_5 = (-1, 1, 1), \hat{\nu}_6 = (-1, 1, -1), \hat{\nu}_7 = (-1, -1, 1)$  and  $\hat{\nu}_8 = (-1, -1, -1)$ . Moreover,  $K(\mathbf{M}, z, \{\mu_{j\alpha}[\langle m_\alpha^2 \rangle]_s^{1/2}\})$  is invariant for the rearrangement of  $\{\mu_1, \mu_2, \dots, \mu_z\}$ . Therefore, (83) is expressed by a polynomial distribution as follows

$$g(\mathbf{M}) = \sum_z p(z) \sum_{z=\sum_{n=1}^8 k_n} \frac{z!}{[\prod_{n=1}^8 k_n!]} \left[ \prod_{n=1}^8 q_n^{k_n} \right] K(\mathbf{M}, z, \{k_l\}). \tag{84}$$

Here  $k_n$  is the number of fictitious LMs  $\{\mu_i\}$  on the NN shell, which have the configuration  $\hat{\nu}_n$ . (Note that  $\sum_{n=0}^8 k_n = z$ .)  $q_n$  is defined by  $q_x \hat{\nu}_{nx} q_y \hat{\nu}_{ny} q_z \hat{\nu}_{nz}$ , where  $q_{x\pm} = q_{y\pm} = 1/2, q_{z\pm} = (1 \pm [\langle m_z \rangle]_s / [\langle m_z^2 \rangle]_s^{1/2})/2$  and  $\hat{\nu}_n = (\hat{\nu}_{nx}, \hat{\nu}_{ny}, \hat{\nu}_{nz})$ .  $K(\mathbf{M}, z, \{k_l\})$  stands for  $K(\mathbf{M}, z, \{\mu_{j\alpha}[\langle m_\alpha^2 \rangle]_s^{1/2}\})$  with configuration  $\{k_l\}$ .

The first and second moments,  $[\langle m_\alpha \rangle]_s$  and  $[\langle m_\alpha^2 \rangle]_s$  which appear in (84) are obtained from the following relation

$$[\langle m_\alpha \rangle^n]_s = \int M_\alpha^n g(\mathbf{M}) d\mathbf{M} = \sum_z p(z) \sum_{z=\sum_{n=1}^8 k_n} \frac{z!}{[\prod_{n=1}^8 k_n!]} \left[ \prod_{n=1}^8 q_n^{k_n} \right] \int M_\alpha^n K(\mathbf{M}, z, \{k_l\}) d\mathbf{M}. \tag{85}$$

The last integral is analytically obtained because of the Gaussian form, so that we reach the self-consistent equation

$$\left[ \begin{array}{c} [\langle m_\alpha \rangle]_s \\ [\langle m_\alpha^2 \rangle]_s \end{array} \right] = \sum_z p(z) \sum_{z=\sum_{n=1}^8 k_n} \frac{z!}{[\prod_{n=1}^8 k_n!]} \left[ \prod_{n=1}^8 q_n^{k_n} \right] \left[ \begin{array}{c} \langle m_\alpha \rangle(\{0\}, \{v\}) \\ \langle m_\alpha^2 \rangle(\{0\}, \{v\}) + A_\alpha(\{k_l\}) \end{array} \right]. \tag{86}$$

Here

$$\langle \mathbf{m} \rangle(\{0\}, \{v\}) = \left( 1 + \frac{4}{\beta \tilde{J} \langle \xi^2 \rangle(\{0\}, \{v\})} \right) \langle \xi \rangle(\{0\}, \{v\}) \tag{87}$$

$$\langle \xi^k \rangle(\{0\}, \{v\}) = \frac{\int d\xi \xi^{-2} \xi^k e^{-\beta \Psi(\xi, \{0\}, \{v\})}}{\int d\xi \xi^{-2} e^{-\beta \Psi(\xi, \{0\}, \{v\})}} \tag{88}$$

$$\begin{aligned}
\Psi(\xi, \{0\}, \{\langle v \rangle\}) &= E_0(\xi, \langle \theta \rangle) + z \left[ \Phi_{0j}^{(a)}(\xi, \langle \theta \rangle, 0) + \frac{\sigma^2}{2} \Phi_2^{(a)}(\xi, \langle \theta \rangle, 0) \right] \\
&\quad - \sum_{\alpha} \left[ \Phi_{0j}^{(e)}(\xi, \langle \theta \rangle, 0) + \frac{\sigma^2}{2} \Phi_{\alpha 2}^{(e)}(\xi, \langle \theta \rangle, 0) \right] \left( \sum_l k_l \hat{v}_{l\alpha} \right) \hat{v}_{\alpha} \\
&\quad + \sum_{(\alpha\gamma)} \left[ \Phi_{0j\delta}^{(b)}(\xi, \langle \theta \rangle, 0) + \frac{\sigma^2}{2} \Phi_{\delta 2}^{(b)}(\xi, \langle \theta \rangle, 0) \right] \left( \sum_l k_l \hat{v}_{l\alpha} \hat{v}_{l\gamma} \right) \hat{v}_{\alpha} \hat{v}_{\gamma} \\
&\quad + \left[ \Phi_{0j}^{(c)}(\xi, \langle \theta \rangle, 0) + \frac{\sigma^2}{2} \Phi_2^{(c)}(\xi, \langle \theta \rangle, 0) \right] \left( \sum_l k_l \hat{v}_{lx} \hat{v}_{ly} \hat{v}_{lz} \right) \hat{v}_x \hat{v}_y \hat{v}_z \quad (89)
\end{aligned}$$

$$\begin{aligned}
A_{\alpha\alpha}(\{k_l\}) &= \frac{A_{\alpha\alpha}(\{k_l\})}{2\pi} \\
&= \frac{\sigma^2}{z} \frac{1}{z} \sum_{i=1}^8 k_i \left[ \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_{\alpha} \rangle(\{0\}, \{\langle v \rangle\})}{\partial u_i} \right)_{\hat{v}_i}^2 + 2\sigma^2 \left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_{\alpha} \rangle(\{0\}, \{\langle v \rangle\})}{\partial v_i} \right)_{\hat{v}_i}^2 \right] \quad (90)
\end{aligned}$$

$$\begin{aligned}
\left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_{\alpha} \rangle}{\partial u_i} \right)_{\hat{v}_i} &= \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial u} + \sum_{\alpha} \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial u_{\alpha}} \hat{v}_{l\alpha} \hat{v}_{\alpha} \\
&\quad + \sum_{(\alpha\gamma)} \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial u_{\alpha\gamma}} \hat{v}_{l\alpha} \hat{v}_{l\gamma} \hat{v}_{\alpha} \hat{v}_{\gamma} + \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial u_{xyz}} \hat{v}_{lx} \hat{v}_{ly} \hat{v}_{lz} \hat{v}_x \hat{v}_y \hat{v}_z \quad (91)
\end{aligned}$$

$$\begin{aligned}
\left( \sum_{i=1}^8 c_{ij} \frac{\partial \langle m_{\alpha} \rangle}{\partial v_i} \right)_{\hat{v}_i} &= \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial v} + \sum_{\alpha} \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial v_{\alpha}} \hat{v}_{l\alpha} \hat{v}_{\alpha} \\
&\quad + \sum_{(\alpha\gamma)} \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial v_{\alpha\gamma}} \hat{v}_{l\alpha} \hat{v}_{l\gamma} \hat{v}_{\alpha} \hat{v}_{\gamma} + \frac{\partial \langle \mathbf{m} \rangle(\{0\}, \{\langle v \rangle\})}{\partial v_{xyz}} \hat{v}_{lx} \hat{v}_{ly} \hat{v}_{lz} \hat{v}_x \hat{v}_y \hat{v}_z. \quad (92)
\end{aligned}$$

Note that

$$\hat{v}_{\alpha} \equiv \frac{[\langle m_{\alpha} \rangle^2]_s^{1/2}}{\tilde{a}_{\alpha}} \quad (93)$$

and

$$\langle \theta \rangle = zt^2(R_0) \left[ 1 + (2\kappa + 1)\kappa \left( \frac{\sigma}{R_0} \right)^2 \right]. \quad (94)$$

It is desired to simplify further the self-consistent equation (86), since there are  $[\prod_{n=1}^7 (z+n)]/7!$  configurations (for example, 50 388 for  $z = 12$ ) at the rhs of (86). First, we neglect the interaction term  $\Phi_{0j}^{(c)}$  in (89), since the typical magnitude of the pair energies are  $\Phi_{0j}^{(a)} \sim \Phi_{0j}^{(e)} \sim 10^{-3}$  Ry,  $\Phi_{0j}^{(b)} \sim 10^{-6}$  Ry, and  $\Phi_{0j}^{(c)} \sim 10^{-8}$  Ry. Second, we note that  $\langle m_{\alpha} \rangle$  and  $A_{\alpha\alpha}$  at the rhs of (86) are the functions of

$$\hat{m}_{\alpha} = \sum_l k_l \hat{v}_{l\alpha} \quad (95)$$

$$\hat{m}_{\alpha\gamma} = \sum_l k_l \hat{v}_{l\alpha} \hat{v}_{l\gamma}. \quad (96)$$

The averages of the products among these variables with respect to the polynomial distribution are given by

$$\langle \hat{m}_{\alpha} \rangle_{\text{PD}} = z \frac{[\langle m_z \rangle]_s}{[\langle m_z \rangle^2]_s^{1/2}} \delta_{\alpha z} \quad (97)$$

$$\langle \hat{m}_{\alpha\gamma} \rangle_{\text{PD}} = 0 \quad (\alpha \neq \gamma) \tag{98}$$

$$\langle \hat{m}_{\alpha} \hat{m}_{\gamma} \rangle_{\text{PD}} = z(z-1) \frac{[\langle m_z \rangle_s]^2}{[\langle m_z^2 \rangle_s]} \delta_{\alpha z} \delta_{\gamma z} + z \delta_{\alpha\gamma} \tag{99}$$

$$\langle \hat{m}_{\alpha} \hat{m}_{\alpha'\gamma'} \rangle_{\text{PD}} = z \frac{[\langle m_z \rangle_s]}{[\langle m_z^2 \rangle_s]^{1/2}} (\delta_{\alpha x} \delta_{(\alpha'\gamma')(zx)} + \delta_{\alpha y} \delta_{(\alpha'\gamma')(yz)}) \tag{100}$$

$$\langle \hat{m}_{\alpha\gamma} \hat{m}_{\alpha'\gamma'} \rangle_{\text{PD}} = z \delta_{(\alpha\gamma)(\alpha'\gamma')} \tag{101}$$

Here  $\langle \rangle_{\text{PD}}$  denotes the average with respect to the polynomial distribution which appears in (84).

The above relations show that there are only two non-zero correlations among 15 different pair correlations between the variables  $\{\hat{m}_{\alpha}\}$  and  $\{\hat{m}_{\alpha\gamma}\}$ . This suggests that one can neglect the correlations between these variables, so that we adopt the decoupling approximation for each variable, which is correct up to the second order

$$\begin{aligned} \langle \Lambda(\{\hat{m}_{\alpha}\}, \{\hat{m}_{\alpha\gamma}\}) \rangle_{\text{PD}} &\approx \sum_{\{v_{\alpha}, v_{\alpha\gamma}\}} \left[ \prod_{\alpha} \frac{1}{2} \left( 1 + v_{\alpha} \frac{\langle \hat{m}_{\alpha} \rangle_{\text{PD}}}{\langle \hat{m}_{\alpha}^2 \rangle_{\text{PD}}^{1/2}} \right) \right] \left[ \prod_{(\alpha\gamma)} \frac{1}{2} \left( 1 + v_{\alpha\gamma} \frac{\langle \hat{m}_{\alpha\gamma} \rangle_{\text{PD}}}{\langle \hat{m}_{\alpha\gamma}^2 \rangle_{\text{PD}}^{1/2}} \right) \right] \\ &\times \Lambda(\{v_{\alpha} \langle \hat{m}_{\alpha}^2 \rangle_{\text{PD}}^{1/2}\}, \{v_{\alpha\gamma} \langle \hat{m}_{\alpha\gamma}^2 \rangle_{\text{PD}}^{1/2}\}). \end{aligned} \tag{102}$$

Here  $\Lambda$  is an arbitrary function of  $\{\hat{m}_{\alpha}\}$  and  $\{\hat{m}_{\alpha\gamma}\}$ .  $\{v_{\alpha}\}$  and  $\{v_{\alpha\gamma}\}$  take the values  $\pm 1$ .

Adopting the approximation (102), one can simplify the self-consistent equations (86) as follows

$$\begin{aligned} \frac{[\langle m_{\alpha} \rangle_s]}{[\langle m_{\alpha}^2 \rangle_s]} &= \sum_z p(z) \frac{1}{32} \sum_{\{v_{\alpha}, v_{\alpha\gamma}\}} \frac{1}{2} \left\{ 1 + v_z \frac{[\langle m_z \rangle_s]}{([\langle m_z \rangle_s]^2 + [(\delta \langle m_z \rangle_s)^2/z]^{1/2}} \right\} \\ &\times \left[ \frac{\langle m_{\alpha} \rangle(\{v\})}{\langle m_{\alpha} \rangle^2(\{v\}) + A_{\alpha}(\{v\})} \right]. \end{aligned} \tag{103}$$

The LM  $\langle m_{\alpha} \rangle(\{v\})$  in the upper part at the rhs of (103) is given as

$$\langle m_{\alpha} \rangle(\{v\}) = \left( 1 + \frac{4}{\beta \tilde{J} \langle \xi^2 \rangle(\{v\})} \right) \langle \xi_{\alpha} \rangle(\{v\}) \tag{104}$$

$$\langle \xi^n \rangle(\{v\}) = \frac{\int d\xi \xi^{-2} \xi^n e^{-\beta \Psi(\xi, \{v\})}}{\int d\xi \xi^{-2} e^{-\beta \Psi(\xi, \{v\})}} \tag{105}$$

$$\begin{aligned} \Psi(\xi, \{v\}) &= \tilde{E}_0(\xi) + z \tilde{\Phi}^{(a)}(\xi) - \sqrt{z} [\tilde{\Phi}_x^{(e)}(\xi) \hat{v}_x v_x + \tilde{\Phi}_y^{(e)}(\xi) \hat{v}_y v_y + \tilde{\Phi}_z^{(e)}(\xi) \hat{v}_z \hat{p} v_z] \\ &+ \sqrt{z} \sum_{(\alpha\gamma)}^{xyz} \tilde{\Phi}_{\delta}^{(b)}(\xi) \hat{v}_{\alpha} \hat{v}_{\gamma} v_{\alpha\gamma}. \end{aligned} \tag{106}$$

Here  $\tilde{E}_0(\xi)$  stands for  $E_0(\xi, \langle \theta \rangle)$ , and the pair energies  $\tilde{\Phi}^{(a)}(\xi)$ ,  $\tilde{\Phi}_{\alpha}^{(e)}(\xi)$ , and  $\tilde{\Phi}_{\delta}^{(b)}(\xi)$  are defined by

$$\tilde{\Phi}^{(a)}(\xi) = \Phi^{(a)}(\xi, \langle \theta \rangle, 0) + 2\kappa^2 \left( \frac{\sigma}{R_0} \right)^2 \hat{\Phi}_2^{(a)}(\xi, \langle \theta \rangle, 0) \tag{107}$$

$$\tilde{\Phi}_{\alpha}^{(e)}(\xi) = \Phi_{\alpha}^{(e)}(\xi, \langle \theta \rangle, 0) + 2\kappa^2 \left( \frac{\sigma}{R_0} \right)^2 \hat{\Phi}_{\alpha 2}^{(e)}(\xi, \langle \theta \rangle, 0) \tag{108}$$

$$\tilde{\Phi}_{\delta}^{(b)}(\xi) = \Phi_{\delta}^{(b)}(\xi, \langle \theta \rangle, 0) + 2\kappa^2 \left( \frac{\sigma}{R_0} \right)^2 \hat{\Phi}_{\delta 2}^{(b)}(\xi, \langle \theta \rangle, 0) \tag{109}$$

and

$$\hat{p} = \left[ 1 + (z-1) \frac{[\langle m_z \rangle_s]^2}{[\langle m_z^2 \rangle_s]} \right]^{1/2} \tag{110}$$

$$\left(\frac{\sigma}{R_0}\right)^2 = \frac{[(\delta R)^2]_s}{[R]_s^2}. \quad (111)$$

The fluctuation  $A_\alpha$  in the lower part at the rhs of equation (103) is expressed as

$$A_\alpha = \frac{1}{4} \left[ b^{(\alpha)}(\{v\}) + \frac{1}{\sqrt{z}} b_x^{(\alpha)}(\{v\}) v_x + \frac{1}{\sqrt{z}} b_y^{(\alpha)}(\{v\}) v_y \right. \\ \left. + \frac{1}{\sqrt{z}} b_z^{(\alpha)}(\{v\}) \hat{p} v_z + \frac{1}{\sqrt{z}} \sum_{(\alpha'\gamma')} b_{\alpha'\gamma'}^{(\alpha)}(\{v\}) v_{\alpha'\gamma'} \right]. \quad (112)$$

The expressions of  $b^{(\alpha)}$ ,  $b_\gamma^{(\alpha)}$ , and  $b_{\alpha'\gamma'}^{(\alpha)}$  are given in the appendix.

All the energies in  $\Psi(\xi, \{v\})$  are the functions of the two kinds of effective media  $\mathcal{L}_\sigma^{-1}$  and  $\mathcal{K}_\sigma$ . The former is determined by the CPA equation [24, 25]

$$\frac{1}{2} \sum_v \left( 1 + v \frac{[\langle \xi_z \rangle]_s}{[\langle \xi_z^2 \rangle]_s^{1/2}} \right) G_\sigma(\omega + i\delta, v[\langle \xi_z^2 \rangle]_s^{1/2}, [\langle \xi_\perp^2 \rangle]_s) = F_\sigma \quad (113)$$

$$G_\sigma(\omega + i\delta, \xi_z, \xi_\perp^2) = \frac{\delta \bar{L}_\sigma^{-1} + F_\sigma^{-1}}{(\delta \bar{L}_\uparrow^{-1} + F_\uparrow^{-1})(\delta \bar{L}_\downarrow^{-1} + F_\downarrow^{-1}) - \frac{1}{4} \tilde{J}^2 \xi_\perp^2}. \quad (114)$$

Here  $\delta \bar{L}_\sigma^{-1}$  is defined by (30) in which the charge potential  $w_i$  has been replaced by the single-site one, and the site indices have been omitted for simplicity.  $[\langle \xi_z^n \rangle]_s$  and  $[\langle \xi^2 \rangle]_s (= [\langle \xi_\perp^2 \rangle]_s + [\langle \xi_z^2 \rangle]_s)$  are obtained as follows by taking the same steps as those to obtain (103)

$$\left[ \frac{[\langle \xi_z^n \rangle]_s}{[\langle \xi^2 \rangle]_s} \right] = \sum_z p(z) \frac{1}{32} \sum_{\{v_\alpha, v_{\alpha\gamma}\}} \frac{1}{2} \left\{ 1 + v_z \frac{[\langle m_z \rangle]_s}{([\langle m_z \rangle]_s^2 + [(\delta \langle m_z \rangle)^2]_s/z)^{1/2}} \right\} \left[ \frac{\langle \xi_z^n \rangle(\{v\})}{\langle \xi^2 \rangle(\{v\})} \right]. \quad (115)$$

The medium  $\mathcal{K}_\sigma$  is obtained by applying the interpolation scheme [10] as

$$([\theta]_s \mathcal{K}_\sigma)^{-1} = \frac{\delta z_{ab}^* \theta_f}{\delta z_{fb}^* [\theta]_s} (\theta_f \mathcal{K}_{f\sigma})^{-1} + \frac{\delta z_{fa}^* \theta_b}{\delta z_{fb}^* [\theta]_s} (\theta_b \mathcal{K}_{b\sigma})^{-1} \\ + \frac{\delta z^*}{\delta z_{fb}^*} \left[ \frac{\theta_f}{[\theta]_s} (\theta_f \mathcal{K}_{f\sigma})^{-1} - \frac{\theta_b}{[\theta]_s} (\theta_b \mathcal{K}_{b\sigma})^{-1} \right] \\ + \frac{\Delta}{\Delta_a} \left[ \frac{\theta_a}{[\theta]_s} (\theta_a \mathcal{K}_{a\sigma})^{-1} - \frac{\delta z_{ab}^* \theta_f}{\delta z_{fb}^* [\theta]_s} (\theta_f \mathcal{K}_{f\sigma})^{-1} - \frac{\delta z_{fa}^* \theta_b}{\delta z_{fb}^* [\theta]_s} (\theta_b \mathcal{K}_{b\sigma})^{-1} \right]. \quad (116)$$

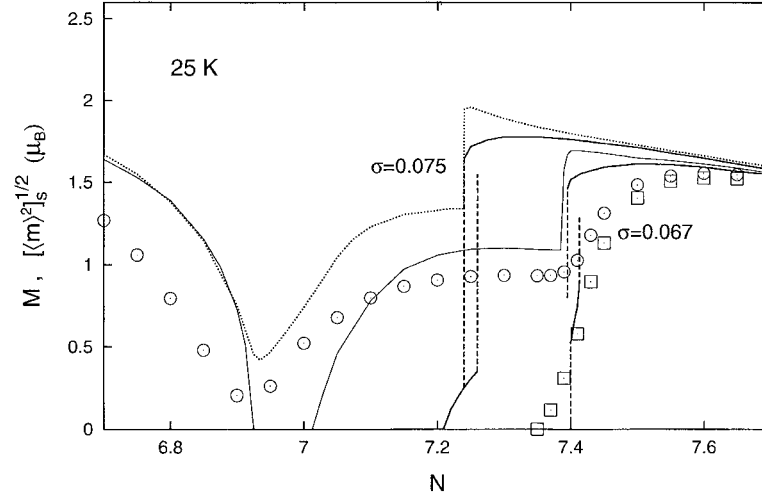
$$[\theta]_s = \frac{\delta z_{ab}^* \theta_f}{\delta z_{fb}^*} + \frac{\delta z_{fa}^* \theta_b}{\delta z_{fb}^*} + \frac{\delta z^*}{\delta z_{fb}^*} (\theta_f - \theta_b) + \frac{\Delta}{\Delta_a} \left( \theta_a - \frac{\delta z_{ab}^* \theta_f}{\delta z_{fb}^*} - \frac{\delta z_{fa}^* \theta_b}{\delta z_{fb}^*} \right). \quad (117)$$

Here the subscripts  $a, b$  and  $f$  denote the amorphous structure, the bcc structure, and the fcc structure as the reference systems. The differences in coordination numbers are defined by  $\delta z^* = z^* - z_a^*$  and  $\delta z_{ab}^* = z_a^* - z_b^*$ , for example.  $\theta_c$  ( $c = a, b, f$ ) are obtained from the DOS in non-interacting systems  $\rho_c(\epsilon)$  as

$$\theta_c = \int (\epsilon - \epsilon_c)^2 \rho_c(\epsilon) d\epsilon. \quad (118)$$

The medium of the reference system  $\mathcal{K}_{c\sigma}$  are given by

$$\theta_c \mathcal{K}_{c\sigma} = \mathcal{L}_\sigma^{-1} - F_{c\sigma}^{-1} \quad (119)$$



**Figure 1.** The magnetization  $M = [(m_z)]_s$  (thick full curves) and the spin glass order parameter  $[(m^2)_s]^{1/2}$  (thin full curve and dotted curve) at 25 K as a function of the d-electron number  $N$ , which are calculated for  $\sigma/R_0 = 0.067$  and  $0.075$ . The average coordination number is fixed to be  $z^* = 11.5$ . The open squares and circles are  $[(m_z)]_s$  and  $[(m^2)_s]^{1/2}$  obtained by the previous theory [18] with use of the Monte Carlo sampling technique at 35 K and  $\sigma/R_0 = 0.067$ , respectively.

for  $c = b$  and  $f$ , and

$$\theta_a \mathcal{K}_{a\sigma} = \frac{2F_{a\sigma} \mathcal{L}_\sigma^{-1} - 1 \pm \sqrt{1 + 4\{[(\delta\theta_a)^2]_s/[\theta_a]_s^2\} F_{a\sigma} \mathcal{L}_\sigma^{-1} (F_{a\sigma} \mathcal{L}_\sigma^{-1} - 1)}}{2(1 - \{[(\delta\theta_a)^2]_s/[\theta_a]_s^2\}) F_{a\sigma}}. \quad (120)$$

The sign of  $\mathcal{K}_{a\sigma}$  should be chosen to be  $\text{Im } \mathcal{K}_{a\sigma} < 0$ .

The coherent Green functions  $F_{c\sigma}$  ( $c = a, b, f$ ) in (119) and (120) are defined by (37) in which  $[\rho(\epsilon)]_s$  has been replaced by  $\rho_c(\epsilon)$ . Moreover, the fluctuation  $[(\delta\theta_a)^2]_s/[\theta_a]_s^2$  is obtained from the relation

$$\frac{[(\delta\theta_a)^2]_s}{[\theta_a]_s^2} = \frac{([z_a^*] + 1 - z_a^*)(z_a^* - [z_a^*])}{z^{*2}} + \frac{4\kappa^2[1 + \frac{1}{2}(2\kappa + 1)^2(\sigma_a/R_0)^2]}{z^*[1 + \kappa(2\kappa + 1)(\sigma_a/R_0)^2]} \left(\frac{\sigma_a}{R_0}\right)^2 \quad (121)$$

where  $(\sigma_a/R_0)^2$  is given by (111).

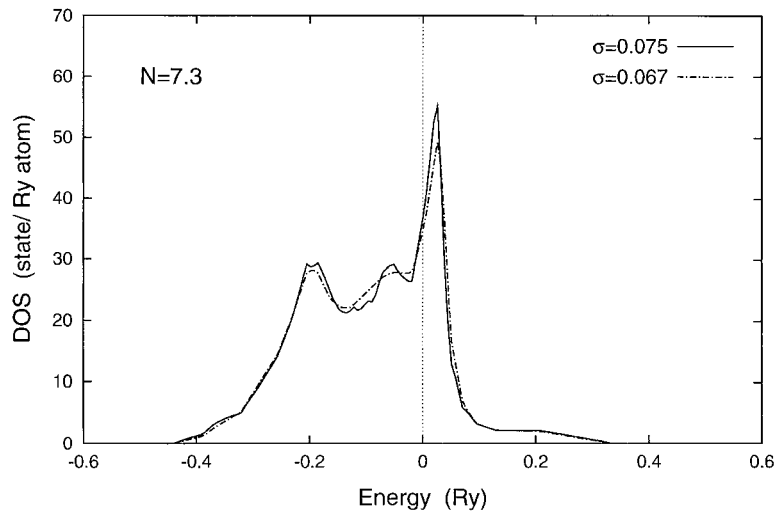
Equations (103), (113), and (116) determine self-consistently  $[(m_z)]_s$ ,  $[(m_z)^2]_s$ ,  $[(m_x)^2]_s$ ,  $[(m_y)^2]_s$  and the effective media  $\mathcal{L}_\sigma^{-1}$  and  $\mathcal{K}_\sigma$ . Note that the number of effective configurations in (103) has been reduced from  $10^4$  to 64, so that the numerical calculations have been much simplified as compared with the previous theory.

### 3. Numerical results

We have performed the numerical calculations for amorphous transition metals to examine the overall features of the present theory. We adopted the input DOS  $\rho_a(\epsilon)_s$  and  $\rho_b(\epsilon)_s$  calculated by Fujiwara [26],  $\rho_f(\epsilon)_s$  calculated by Moruzzi *et al* [27], and the effective exchange energy parameter  $\tilde{J} = 0.059$  Ry, all of which have been used in our previous calculations [6, 10, 18]. We verified that the computing time to solve the self-consistent equations is only one-tenth of the previous scheme based on the Monte Carlo sampling method.

Figure 1 shows the magnetic moments as a function of the d-electron number  $N$  calculated at  $z^* = 11.5$  and  $T = 25$  K. In the case of  $\sigma/R_0 = 0.067$ , the ferromagnetism (F) is realized





**Figure 2.** Non-interacting densities of states (DOS) for  $N = 7.3$ . The solid curve:  $\sigma/R_0 = 0.075$ , dot-dashed curve:  $0.067$ . The vertical dashed line shows the Fermi level.

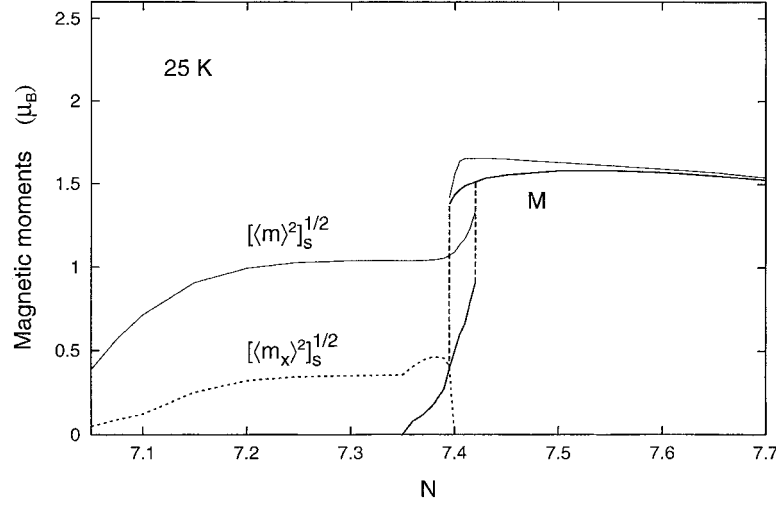
in the region  $N > 7.4$ , and the transition from the ferromagnetism to the non-collinear spin glass occurs at  $N = 7.4$ ; the magnetization  $[\langle m_z \rangle]_s$  suddenly drops there with decreasing the d-electron number  $N$ , but the spin glass order parameter  $[\langle m \rangle^2]_s^{1/2}$  remains below  $N = 7.4$ . This feature is consistent with the previous results obtained by the Monte Carlo sampling and the decoupling approximation to the distribution for the transfer integrals, as shown by circles and open squares.

The SG state in the present theory disappears around  $N = 6.95$  for  $\sigma/R_0 = 0.067$  at 25 K, while it remains in the previous method. This is because the decoupling approximation to the distribution of the transfer integrals, which was used in the previous theory, overestimates the fluctuations of the interatomic distance and therefore those of the magnetic couplings, so that the approximation enhances the SG order in the critical region where the average magnetic couplings almost disappear. The difference, however, is of the quantitative problem, since we found that the SG order persists at 20 K even around  $N = 6.95$  in the present theory.

When we adopt larger fluctuation  $\sigma/R_0 = 0.075$ , the ferromagnetic region for  $\sigma/R_0 = 0.075$  is extended to the region of smaller  $N$  as shown in figure 1. This is simply explained by the enhancement of the DOS at the Fermi level due to the increasing structural disorder (see figure 2). The SG order remains near  $N = 6.95$  even at 25 K as shown on figure 1, so that the SG order parameter  $[\langle m \rangle^2]_s^{1/2}$  shows the behaviour similar to the results obtained by the previous theory.

The previous theory with use of the Monte Carlo sampling yields the second-order transition from the F to the SG at least above 30 K as a function of  $N$ . The present result shows the first-order transition and the metastable ferromagnetic state near the boundary, which is often found in the crystalline close-packed systems [28] such as  $\gamma$ -Fe. It is possible that the crystalline feature still remains at the transition point for a small value of  $\sigma/R_0$ . Although the present theory is valid in the limit of small  $\sigma/R_0$ , it is difficult at the present stage to conclude whether or not the first-order transition persists for a larger strength of  $\sigma/R_0$ .

It should be noted that the nature of the transition at the F-SG boundary seems to be sensitive to the approximation. For example, we made a decoupling approximation (102). This neglects the fluctuations  $\langle \hat{m}_x \hat{m}_{zx} \rangle_{PD} - \langle \hat{m}_x \rangle_{PD} \langle \hat{m}_{zx} \rangle_{PD} = z \hat{u}_z$  and  $\langle \hat{m}_y \hat{m}_{yz} \rangle_{PD} -$



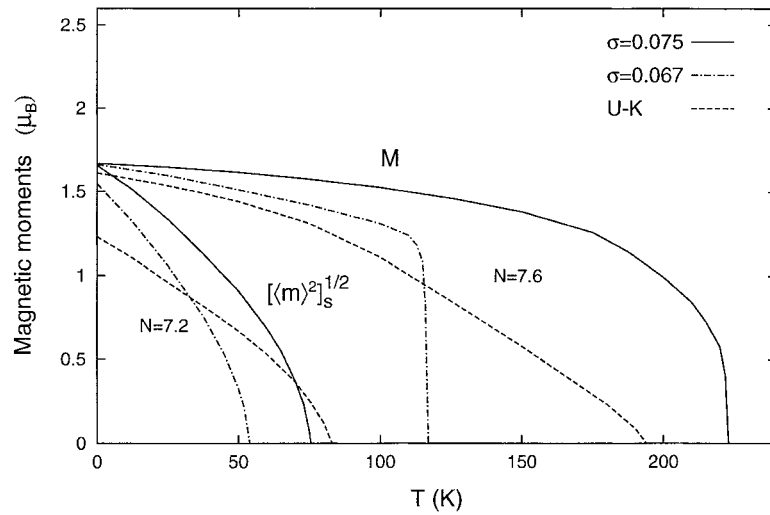
**Figure 3.** The magnetization  $M$  (thick full curve), the spin glass order parameter  $[(m)^2]_s^{1/2}$  (thin full curve), and its  $x$  component  $[(m_x)^2]_s^{1/2}$  (broken curve) for  $\sigma/R_0 = 0.067$ ,  $z^* = 11.5$ , and 25 K, which are calculated with use of the modified decoupling approximation.

$\langle \hat{m}_y \rangle_{\text{PD}} \langle \hat{m}_{yz} \rangle_{\text{PD}} = z \hat{u}_z \cdot \hat{u}_z$  being defined by  $[(m_z)^2]_s / [(m_z)^2]_s^{1/2}$ . If we adopt the decoupling approximation to the new variables  $\tilde{m}_x = (\hat{m}_x + \hat{m}_{zx})/\sqrt{2}$ ,  $\tilde{m}_y = (\hat{m}_y + \hat{m}_{yz})/\sqrt{2}$ ,  $\tilde{m}_z = \hat{m}_z$ ,  $\tilde{m}_{yz} = (\hat{m}_y - \hat{m}_{yz})/\sqrt{2}$ ,  $\tilde{m}_{zx} = (\hat{m}_x - \hat{m}_{zx})/\sqrt{2}$ , and  $\tilde{m}_{xy} = \hat{m}_{xy}$ , this problem is removed since  $\langle \tilde{m}_\alpha \tilde{m}_\gamma \rangle_{\text{PD}} = \langle \tilde{m}_\alpha^2 \rangle_{\text{PD}} \delta_{\alpha\gamma}$ ,  $\langle \tilde{m}_\alpha \tilde{m}_{\alpha'\gamma'} \rangle_{\text{PD}} = 0$ , and  $\langle \tilde{m}_{\alpha\gamma} \tilde{m}_{\alpha'\gamma'} \rangle_{\text{PD}} = \langle \tilde{m}_{\alpha\gamma}^2 \rangle_{\text{PD}} \delta_{(\alpha\gamma)(\alpha'\gamma')}$  are satisfied. The resulting self-consistent equations (103) remain unchanged, but  $\{v_\alpha\}$  in (106) are replaced by  $\tilde{v}_x = (\sqrt{1 + \hat{u}_z v_x} + \sqrt{1 - \hat{u}_z v_{zx}})/\sqrt{2}$ ,  $\tilde{v}_y = (\sqrt{1 + \hat{u}_z v_y} + \sqrt{1 - \hat{u}_z v_{yz}})/\sqrt{2}$ ,  $\tilde{v}_z = v_z$ ,  $\tilde{v}_{yz} = (\sqrt{1 + \hat{u}_z v_y} - \sqrt{1 - \hat{u}_z v_{yz}})/\sqrt{2}$ ,  $\tilde{v}_{zx} = (\sqrt{1 + \hat{u}_z v_x} - \sqrt{1 - \hat{u}_z v_{zx}})/\sqrt{2}$ , and  $\tilde{v}_{xy} = v_{xy}$ . The magnetic moments against  $N$  curves calculated with use of the modified decoupling approximation are presented in figure 3. The non-collinear ferromagnetic state appears between  $N = 7.35$  and  $N = 7.40$  near the boundary, though the other features hardly change.

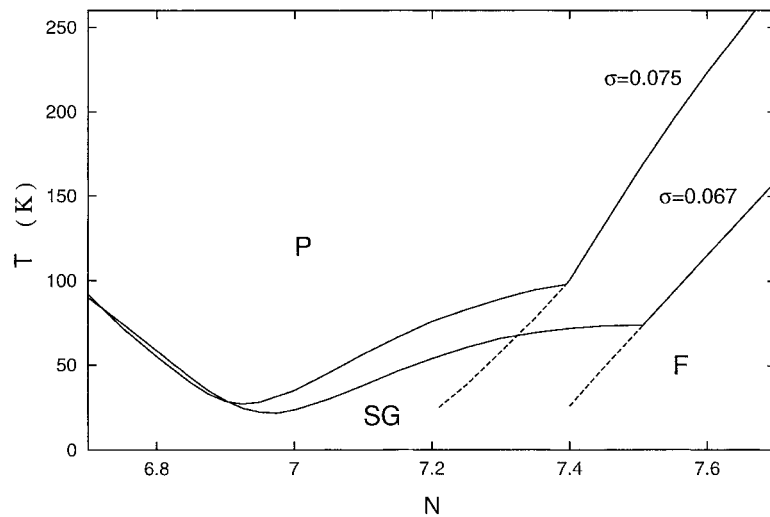
We have also examined the temperature dependence of the magnetization and the SG order parameter as shown in figure 4. The latter monotonically decreases with increasing temperature, and shows the second-order transition to the paramagnetic state. The SG temperature  $T_g$  is increased when  $\sigma/R_0$  is increased since the fluctuations of the interatomic distance increase those of the magnetic couplings, therefore  $T_g$ .

The magnetization for  $N = 7.6$  and  $\sigma/R_0 = 0.067$  rapidly decreases near the Curie temperature  $T_C$ , showing a behaviour similar to the first-order transition as often found in the crystalline counterparts with the same  $d$ -electron number. When we increase  $\sigma/R_0$ , we obtain higher  $T_C$  and the Brillouin-like curve leading to the second-order transition as shown in figure 3. Both  $T_C$  and  $T_g$  in the present scheme qualitatively agree with those obtained by the Monte Carlo sampling (see the broken curves in figure 4).

The calculated  $T_C$  and  $T_g$  are presented in figure 5 as a function of  $d$ -electron number. The Curie temperature monotonically decreases with decreasing the  $d$  electron number for both  $\sigma/R_0 = 0.067$  and  $0.075$ , and shows an instability leading to the SG. The spin glass temperature shows a minimum as a function of  $N$  around  $N = 6.9$ , where the average NN magnetic interactions change the sign. It should be noted that  $T_C$  and  $T_g$  in the present calculations are underestimated by a factor of two due to the classical treatment of spin fluctuations. The quantum treatment would enhance  $T_C$  and  $T_g$  by a factor of two, and the magnetic short-



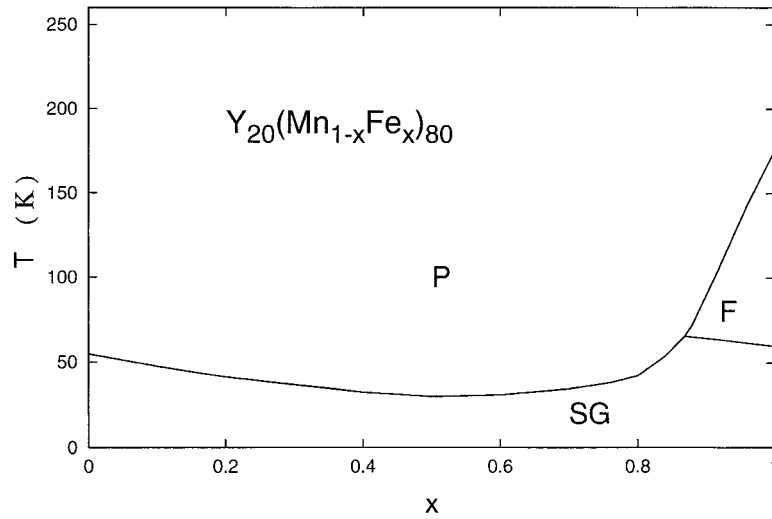
**Figure 4.** The temperature dependence of the magnetization  $[(m_z)_s]$  and the SG order parameter  $[(m_z)_s]^{1/2}$  for  $N = 7.6$  and  $7.2$ , respectively. Chain curves:  $\sigma/R_0 = 0.067$ , the full curves:  $\sigma/R_0 = 0.075$ . The broken curves represent the temperature dependence of  $[(m_z)_s]$  and  $[(m_z)_s]^{1/2}$  obtained by the Monte Carlo sampling method [18].



**Figure 5.** The Curie temperatures and the SG temperatures as a function of the d-electron number  $N$  for  $\sigma/R_0 = 0.067$  and  $0.075$ . F, SG and P denote the ferromagnetic state, the spin-glass state, and the paramagnetic one, respectively. The broken curves show the upper limit of the ferromagnetic state.

range order effects (i.e. the long-range spin fluctuations) can reduce them further. The phase boundary between F and SG cannot be determined by the present theory since the first-order phase transition takes place at the boundary. For the determination one needs the explicit expression of free energy, which is left for future work.

The d-electron number dependence of  $T_C$  and  $T_g$  shown in figure 5 seems to be consistent with the recent experimental data by Ohta *et al* [29]. They obtained the magnetic phase diagram



**Figure 6.** Experimental phase diagram for  $Y_{20}(Mn_{1-x}Fe_x)_{80}$  quasi-binary amorphous alloys obtained by Ohta *et al* [29]. The Fe concentration  $x$  is regarded as a parameter controlling the  $d$ -electron number  $N$ .

of  $Y_{20}(Mn_{1-x}Fe_x)_{80}$  quasi-binary amorphous alloys to investigate the average electron number dependence of the phase diagram. The ferromagnetism is stabilized in  $Y_{20}Fe_{80}$  alloys due to the atomic size effects [30]. The Fe concentration may be regarded as a parameter changing the average  $d$ -electron number. With decreasing Fe concentration, the Curie temperature rapidly decreases, and the SG state is stabilized. The SG temperature show a minimum at  $x = 0.5$ . This feature is consistent with our phase diagram given in figure 5, although the re-entrant behaviour around  $x = 0.9$  is not explained by the present theory.

#### 4. Summary

We have presented a simplified theory of non-collinear magnetism in amorphous transition metals. The theory is based on the functional integral technique describing the thermal spin fluctuations and the distribution function method dealing with the random LMs due to structural disorder. The distribution of LMs is given by the  $4z$ -fold integral equation. Adopting the Gaussian model to the distribution for the interatomic distance and making use of the saddle-point approximation, we performed analytically the  $z$ -fold integrals of the kernel in the integral equations, so that we derived the simplified equations for the magnetization and the SG order parameters with only 64 configurations of the surrounding effective spins. This enabled us to calculate the magnetic moments without introducing statistical errors, and to reduce the computing time by a factor of ten.

Solving the self-consistent equations for amorphous transition metals, we have demonstrated that the theory describes the transition from the ferromagnetism to the SG with decreasing the  $d$ -electron number and verified that the theory leads to qualitatively the same  $T_C$  and  $T_g$  against  $N$  curves as in the previous theory based on the Monte Carlo sampling method. The  $N$  dependence of  $T_C$  and  $T_g$  is consistent with the recent experimental data for  $Y_{20}(Mn_{1-x}Fe_x)_{80}$  quasi-binary amorphous alloys.

The behaviour near the boundary between F and SG is sensitive to the approximation. The present theory causes the first-order F-SG transition or the first-order transition

from the high-spin F to the low-spin non-collinear F state, while the previous theory leads to the second-order transition from the non-collinear F to the SG at least above 30 K. The former should be valid for small  $\sigma/R_0$ , and the latter may be reasonable for larger values of  $\sigma/R_0$ . The details of the phase diagram near the F–SG boundary and the description of the reentrant SG behaviour in metallic systems are left for future theoretical investigations. Furthermore, it is possible that the well-defined long-range non-collinear magnetic orders such as the helical structure develop in the small  $\sigma/R_0$  region. The present theory does not distinguish such ordered states from the SG. For their description, one has to extend the theory introducing a site-dependent effective medium which is off-diagonal in the spin space and a site-dependent distribution function. Apart from these difficulties, the present theory is useful for a qualitative or semi-quantitative understanding of the non-collinear magnetism of amorphous metals and allow us to treat more complex systems which cannot be analysed by the previous theory. The application to amorphous rare-earth transition metal alloys is one of the possible works left in the future investigations.

### Appendix. Expressions of $b^{(\alpha)}$ , $b_{\gamma}^{(\alpha)}$ , and $b_{\alpha'\gamma'}^{(\alpha)}$

We derive here the expressions of  $b^{(\alpha)}$ ,  $b_{\gamma}^{(\alpha)}$ , and  $b_{\alpha'\gamma'}^{(\alpha)}$  in equation (112).

Substituting (91) and (92) into (90), and expanding the squares of them, we obtain

$$A_{\alpha} = \frac{1}{4z} \left[ zb^{(\alpha)} + \sum_{\alpha'} b_{\alpha'}^{(\alpha)} \sum_l k_l \hat{v}_{l\alpha'} + \sum_{(\alpha'\gamma')} b_{\alpha'\gamma'}^{(\alpha)} \sum_l k_l \hat{v}_{l\alpha'} \hat{v}_{l\gamma'} \right]. \quad (\text{A1})$$

Here

$$b^{(\alpha)} = \frac{4\sigma^2}{z} (b^{(\alpha 1)} + 2\sigma^2 b^{(\alpha 2)}) \quad (\text{A2})$$

$$b_{\alpha'}^{(\alpha)} = \frac{4\sigma^2}{z} (b_{\alpha'}^{(\alpha 1)} + 2\sigma^2 b_{\alpha'}^{(\alpha 2)}) \quad (\text{A3})$$

$$b_{\alpha'\gamma'}^{(\alpha)} = \frac{4\sigma^2}{z} (b_{\alpha'\gamma'}^{(\alpha 1)} + 2\sigma^2 b_{\alpha'\gamma'}^{(\alpha 2)}) \quad (\text{A4})$$

$$b^{(\alpha 1)} = \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \right)^2 + \sum_{\alpha'} \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{\alpha'}} \right)^2 + \sum_{(\alpha'\gamma')} \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{\alpha'\gamma'}} \right)^2 \quad (\text{A5})$$

$$b_x^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_x} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_y} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{xy}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_z} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{zx}} \right) \quad (\text{A6})$$

$$b_y^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_y} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_z} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{yz}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_x} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{xy}} \right) \quad (\text{A7})$$

$$b_z^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_z} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_x} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{zx}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_y} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{yz}} \right) \quad (\text{A8})$$

$$b_{yz}^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{yz}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_y} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_z} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{xy}} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{zx}} \right) \quad (\text{A9})$$

$$b_{zx}^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{zx}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_z} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_x} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{yz}} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{xy}} \right) \quad (\text{A10})$$

$$b_{xy}^{(\alpha 1)} = 2 \left( \frac{\partial \langle m_{\alpha} \rangle}{\partial u} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{xy}} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_x} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_y} + \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{zx}} \frac{\partial \langle m_{\alpha} \rangle}{\partial \tilde{u}_{yz}} \right). \quad (\text{A11})$$

The variables  $\tilde{u}_\alpha$  and  $\tilde{u}_{\alpha\gamma}$  are defined by  $\tilde{u}_\alpha = u_\alpha/\hat{v}_\alpha$  and  $\tilde{u}_{\alpha\gamma} = u_{\alpha\gamma}/\hat{v}_\alpha\hat{v}_\gamma$ , respectively.  $b^{(\alpha 2)}$ ,  $b_x^{(\alpha 2)}$ ,  $b_y^{(\alpha 2)}$ ,  $b_z^{(\alpha 2)}$ ,  $b_{yz}^{(\alpha 2)}$ ,  $b_{zx}^{(\alpha 2)}$  and  $b_{xy}^{(\alpha 2)}$  are defined by (A5)–(A11) in which  $u$  has been replaced by  $v$ .

When we adopt the decoupling approximation (102), (A1) reduces to

$$A_\alpha(\{v\}) = \frac{1}{4z} \left[ z b^{(\alpha)} + \sqrt{z} b_x^{(\alpha)} v_x + \sqrt{z} b_y^{(\alpha)} v_y + \sqrt{z} b_z^{(\alpha)} \hat{p} v_z + \sqrt{z} \sum_{(\alpha'\gamma')} b_{\alpha'\gamma'}^{(\alpha)} v_{\alpha'\gamma'} \right] \quad (\text{A12})$$

which is identical to (112).

The derivatives of local moments in (A5)–(A11) often make the self-consistent equation (103) unstable due to their nonlinearity. We therefore replace them with the finite differences in the fluctuation range:

$$\begin{aligned} \frac{\partial \langle m_\alpha \rangle}{\partial u_i} &= \frac{\delta \langle m_\alpha \rangle_{u_i}}{2 \langle (\delta u_i)^2 \rangle^{1/2}} \\ &\equiv \frac{\langle m_\alpha \rangle \langle u_i \rangle + \langle (\delta u_i)^2 \rangle^{1/2} - \langle m_\alpha \rangle \langle u_i \rangle - \langle (\delta u_i)^2 \rangle^{1/2}}{2 \langle (\delta u_i)^2 \rangle^{1/2}} \end{aligned} \quad (\text{A13})$$

$$\begin{aligned} \frac{\partial \langle m_\alpha \rangle}{\partial v_i} &= \frac{\delta \langle m_\alpha \rangle_{v_i}}{2 \langle (\delta v_i)^2 \rangle^{1/2}} \\ &\equiv \frac{\langle m_\alpha \rangle \langle v_i \rangle + \langle (\delta v_i)^2 \rangle^{1/2} - \langle m_\alpha \rangle \langle v_i \rangle - \langle (\delta v_i)^2 \rangle^{1/2}}{2 \langle (\delta v_i)^2 \rangle^{1/2}}. \end{aligned} \quad (\text{A14})$$

Here  $\langle m_\alpha \rangle \langle u_i \rangle \pm \langle (\delta u_i)^2 \rangle^{1/2}$  denotes the LM at  $u_1 = \langle u_1 \rangle, \dots, u_i = \langle u_i \rangle + \langle (\delta u_i)^2 \rangle^{1/2}, \dots, u_8 = \langle u_8 \rangle$ , and  $v_1 = \langle v_1 \rangle, \dots, v_8 = \langle v_8 \rangle$ ,  $\langle \rangle$  being the average over  $\{R_j\}$  given by

$$\langle \dots \rangle \equiv \int (\dots) \left[ \prod_{j=1}^z p_s(R_j) dR_j \right]. \quad (\text{A15})$$

Substituting (A13) and (A14) into (A2)–(A11), we obtain

$$b^{(\alpha)} = \hat{b}^{(\alpha 1)} + \hat{b}^{(\alpha 2)} \quad (\text{A16})$$

$$b_{\alpha'}^{(\alpha)} = \hat{b}_{\alpha'}^{(\alpha 1)} + \hat{b}_{\alpha'}^{(\alpha 2)} \quad (\text{A17})$$

$$b_{\alpha'\gamma'}^{(\alpha)} = \hat{b}_{\alpha'\gamma'}^{(\alpha 1)} + \hat{b}_{\alpha'\gamma'}^{(\alpha 2)} \quad (\text{A18})$$

$$\hat{b}^{(\alpha 1)} = (\delta \langle m_\alpha \rangle_u)^2 + \sum_{\alpha'} (\delta \langle m_\alpha \rangle_{u_{\alpha'}})^2 + \sum_{(\alpha'\gamma')} (\delta \langle m_\alpha \rangle_{u_{\alpha'\gamma'}})^2 \quad (\text{A19})$$

$$\hat{b}_x^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_x} + \delta \langle m_\alpha \rangle_{u_y} \delta \langle m_\alpha \rangle_{u_{xy}} + \delta \langle m_\alpha \rangle_{u_z} \delta \langle m_\alpha \rangle_{u_{zx}}) \quad (\text{A20})$$

$$\hat{b}_y^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_y} + \delta \langle m_\alpha \rangle_{u_z} \delta \langle m_\alpha \rangle_{u_{yz}} + \delta \langle m_\alpha \rangle_{u_x} \delta \langle m_\alpha \rangle_{u_{xy}}) \quad (\text{A21})$$

$$\hat{b}_z^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_z} + \delta \langle m_\alpha \rangle_{u_x} \delta \langle m_\alpha \rangle_{u_{zx}} + \delta \langle m_\alpha \rangle_{u_y} \delta \langle m_\alpha \rangle_{u_{yz}}) \quad (\text{A22})$$

$$\hat{b}_{yz}^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_{yz}} + \delta \langle m_\alpha \rangle_{u_y} \delta \langle m_\alpha \rangle_{u_z} + \delta \langle m_\alpha \rangle_{u_{xy}} \delta \langle m_\alpha \rangle_{u_{zx}}) \quad (\text{A23})$$

$$\hat{b}_{zx}^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_{zx}} + \delta \langle m_\alpha \rangle_{u_z} \delta \langle m_\alpha \rangle_{u_x} + \delta \langle m_\alpha \rangle_{u_{yz}} \delta \langle m_\alpha \rangle_{u_{xy}}) \quad (\text{A24})$$

$$\hat{b}_{xy}^{(\alpha 1)} = 2(\delta \langle m_\alpha \rangle_u \delta \langle m_\alpha \rangle_{u_{xy}} + \delta \langle m_\alpha \rangle_{u_x} \delta \langle m_\alpha \rangle_{u_y} + \delta \langle m_\alpha \rangle_{u_{zx}} \delta \langle m_\alpha \rangle_{u_{yz}}). \quad (\text{A25})$$

Here we used the relations

$$\langle (\delta u)^2 \rangle^{1/2} = \frac{\sigma}{\sqrt{z}} \quad (\text{A26})$$

$$\langle (\delta u_\alpha)^2 \rangle^{1/2} = \hat{v}_\alpha \frac{\sigma}{\sqrt{z}} \quad (\text{A27})$$

$$\langle (\delta u_{\alpha\gamma})^2 \rangle^{1/2} = \hat{v}_\alpha \hat{v}_\gamma \frac{\sigma}{\sqrt{z}} \quad (\text{A28})$$

$$\langle (\delta v_i)^2 \rangle^{1/2} = \sqrt{2} \sigma \langle (\delta u_i)^2 \rangle^{1/2}. \quad (\text{A29})$$

The expressions of  $\hat{b}^{(\alpha 2)}$ ,  $\{\hat{b}_\gamma^{(\alpha 2)}\}$ , and  $\{\hat{b}_{\alpha'\gamma'}^{(\alpha 2)}\}$  are also given by (A19)–(A25) in which subscript  $u$  has been replaced by  $v$ .

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