Disorder-induced fluctuations in the magnetic properties of an Anderson-Hubbard model

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We present a microscopic description of the inhomogeneous magnetic response of a disordered, interacting system, with local susceptibilities determined via a random-phase-approximation-type approach about stable, inhomogeneous mean-field ground states. A careful treatment of the role of disorder is vital in describing: the phase boundary to local moment formation; site-differential inhomogeneity in the distribution of local susceptibilities in a local moment regime, and its marked disorder-induced enhancement; and, on the length scales probed, large disorder-induced fluctuations in the total magnetic susceptibility.

A theoretical description of local magnetic moments in disordered metals, and their role in the approach to a metal-insulator transition, is a problem of great current interest (see, e.g., Refs. 1–6). Milovanović, Sachdev, and Bhatt[1] have shown clearly the importance of disorder in accounting for the instability of a disordered, interacting Fermi liquid towards the formation of local moment states, by treating the disorder exactly via a numerical calculation and interactions at the mean-field level of Hartree-Fock. But granted local moment formation—occurring necessarily on an inhomogeneous scale due to disorder—what are the properties of the resultant local moment phases themselves? In particular, what is their inhomogeneous magnetic response, it evolution with disorder and interaction strength, and how does the site-differential character of the local magnetic response dictate bulk behavior? These questions are of central importance to the wide range of systems wherein both local moments and disorder are simultaneously present, and are the subject of the present paper.

For specificity we consider a site-disordered Anderson-Hubbard model (AHM) in $d=3$ on a simple cubic lattice,

$$H=\sum_{i,\sigma}\epsilon_i n_{i\sigma}-t\sum_{\langle ij\rangle,\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_i n_{i+}n_{i-}\ ,$$

where the $\langle ij\rangle$ sum is over nearest-neighbor sites; $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ and $\sigma=\pm$ denotes the spin. The site energies $\{\epsilon_i\}$ are drawn randomly from a common Gaussian distribution $g(\epsilon)$ of variance Δ^2. We consider half-filling, $y=1$. With $B=12t$ the simple cubic bandwidth, the model is specified simply by the scaled interaction and disorder strengths, $\tilde{U}=U/B$ and $\tilde{\Delta}=\Delta/B$, respectively. A *site*-disordered AHM is chosen because ϵ_i provides a clear and natural site-differential measure for resolving the inhomogeneous distribution of, e.g., local magnetization[5] and magnetic susceptibilities.

Self-consistent, fully unrestricted Hartree-Fock (UHF) was recently used[5] to find locally stable, inhomogeneous mean-field ground states for all local moment phases at $T=0$ in the disorder-interaction plane. Since the magnetic response of the system reflects collective excitations about such states, we first review briefly this work. The resultant diagram[5] in the $(\tilde{\Delta},\tilde{U})$ plane, shown as part of Fig. 1 (for $N=512$ sites), arises from direct sampling of a wide range of possible self-consistent UHF states. All broken-symmetry mean-field phases for $y=1$ are found to be Ising-like, with $S_z^{\rm tot}=0$; and all phase boundaries occur for relatively weak coupling $\tilde{U}$, where UHF for the ground state is likely to be reasonable. The mean-field ground state is determined on energetic grounds, with its magnetic character deduced by examination of $S_z(\mathbf{k})=N^{-1}\sum_i\mu_i e^{i\mathbf{k}\cdot\mathbf{R}_i}$ where $\mu_i=2\langle\hat{s}_{iz}\rangle_{\rm HF}$ is the UHF site local moment. Three distinct magnetic phases are thereby found at half-filling: disordered paramagnetic (P), antiferromagnetic (AF) and spin-glass-like (SG) phases. In the P phase, $\mu_i=0$ for all sites. In the two broken-symmetry phases the distribution of moment magnitudes $\{|\mu_i|\}$ is site disordered, but different magnetic ordering occurs. For the AF, $S_z(\mathbf{k})$ is sharply peaked at $\mathbf{k}=\boldsymbol{\pi}$, on the order of the mean moment magnitude per site $(N^{-1}\sum_i|\mu_i|)$, indicating AF long-ranged order; while in

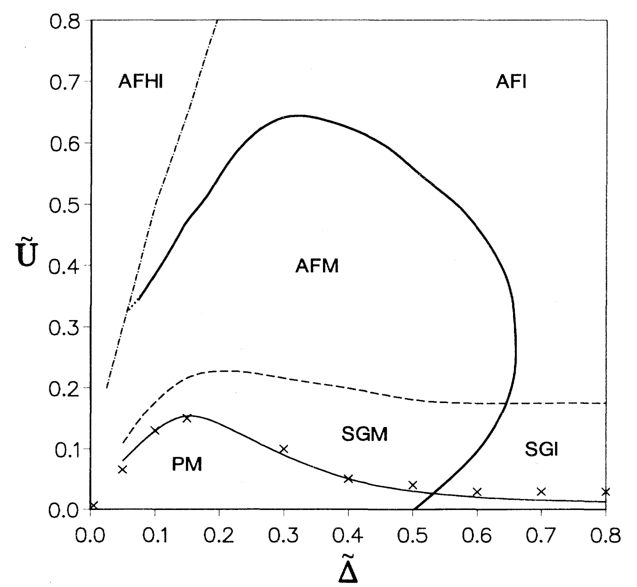

FIG. 1. Mean-field phase diagram at half filling (Ref. 5). AF: antiferromagnet; SG: spin glass; P: paramagnet; M: metal; I: gapless insulator; HI: Mott-Hubbard insulator. The P-SG phase boundary obtained here is indicated by crosses.

the SG phase, $S_z(\mathbf{k})$ shows small peaks of magnitude $O(1/N)$ at numerous $\mathbf{k}$ vectors, and no hint of long-ranged order. The metallic (M) or insulating character of the mean-field states is also shown in Fig. 1. The dominant insulating phase is a gapless insulator (I), although a disordered Hubbard (gapped) insulator (HI) is also found at low $\tilde{\Delta}$; and the location of the metal-gapless insulator transition (MIT) was obtained by considering localization properties of single-particle states in the pseudogap at the Fermi level.

To examine the inhomogeneous magnetic response of the disordered mean-field states in any of the phases, we employ a random-phase approximation (RPA). Since the UHF states are Ising-like, transverse-spin excitations decouple from longitudinal spin and charge excitations. We consider here the static magnetic susceptibilities, their site-differential character and disorder-induced fluctuations therein. Broken-symmetry phases are found to undergo a zero-field spin-flop transition, such that the Ising spin axis lies perpendicular to a uniform applied magnetic field. Thus, only the transverse static susceptibility $\boldsymbol{\chi}^{-+}=\boldsymbol{\chi}^{+-}\equiv\boldsymbol{\chi}$ is probed. For any disorder realization the RPA $\chi_{ij}=[\boldsymbol{\chi}]_{ij}$ is given by

$$\boldsymbol{\chi}=\boldsymbol{\chi}^0[\mathbf{1}-U\boldsymbol{\chi}^0]^{-1} \tag{1}$$

with $[\mathbf{1}]_{ij}=\delta_{ij}$. $\boldsymbol{\chi}^0$ is the UHF transverse susceptibility given (for $T=0$) by

$$\chi^0_{ij}=\sum_{\sigma}\sum_{\substack{\alpha>F\\ \beta<F}}\frac{a_{i\alpha\sigma}a_{j\alpha\sigma}a_{i\beta-\sigma}a_{j\beta-\sigma}}{E_{\alpha\sigma}-E_{\beta-\sigma}} . \tag{2}$$

$\{E_{\alpha\sigma}\}$ are the energies of the UHF single-particle states, with eigenvectors $|\Psi_{\alpha\sigma}\rangle=\sum_i a_{i\alpha\sigma}|\phi_{i\sigma}\rangle$ expanded in a site basis. $\boldsymbol{\chi}^0$ is real symmetric; it may thus be diagonalized (with eigenvalues $\{\lambda_\gamma\}$) by an orthogonal matrix $\mathbf{v}$ such that, for any λ_γ, $\boldsymbol{\chi}^0\mathbf{v}_\gamma=\lambda_\gamma\mathbf{v}_\gamma$. From (1) the RPA $\boldsymbol{\chi}$ is *also* diagonalized by $\mathbf{v}$, and has eigenvalues $\lambda_\gamma/(1-U\lambda_\gamma)$, i.e.,

$$\chi_{ij}=\sum_{\gamma}v_{i\gamma}\frac{\lambda_\gamma}{1-U\lambda_\gamma}v_{j\gamma} . \tag{3}$$

The above procedure is, in principle, simple: first solve the UHF problem to obtain $\{E_{\alpha\sigma},a_{i\alpha\sigma}\}$, then diagonalize $\boldsymbol{\chi}^0$; the RPA $\boldsymbol{\chi}$ follows from (3). But this should be done for each disorder realization at a given $(\tilde{\Delta},\tilde{U})$ point; and the disorder "averaging" is delicate. For example, $\bar{\boldsymbol{\chi}}$, the disorder averaged $\boldsymbol{\chi}$, has the translational invariance of the lattice, as does $\bar{\boldsymbol{\chi}}^0$; and we denote $\delta\boldsymbol{\chi}^0=\boldsymbol{\chi}^0-\bar{\boldsymbol{\chi}}^0$. If, following Singh,[7] (1) is iterated in powers of $\boldsymbol{\chi}^0$ and all fluctuation moments $[\delta\boldsymbol{\chi}^0]^m$ *neglected,* then a Fourier transform yields the purely algebraic $\bar{\chi}(\mathbf{q})\simeq\bar{\chi}^0(\mathbf{q})/[1-U\bar{\chi}^0(\mathbf{q})]$. Use of this to find magnetic phase boundaries amounts to a generalized Stoner criterion: at some critical $U_c(\tilde{\Delta}),\bar{\chi}(\mathbf{q})$ will diverge. But this will occur at a *single* $\mathbf{q}$ vector, implying a transition to a magnetically *ordered* phase for *any* disorder $\tilde{\Delta}$. For example, the resultant phase boundary to local moment formation with increasing $\tilde{U}$, coming from a nonmagnetic (P) regime, is always found to be to an AF (as indeed found in Ref. 7), with *increasing* stability of the P phase at large disorder $\tilde{\Delta}$ (where $U_c\sim\Delta$). This disagrees strongly with Fig. 1, obtained by direct sampling of lowest energy UHF states.[5]

Neglect of the disorder-induced fluctuations $[\delta\boldsymbol{\chi}^0]^m$ is, however, found to be wholly inadequate. For example, from (3) the boundary to local moment formation may be obtained by finding $U_c(\tilde{\Delta})$ at which, for a given disorder realization, an eigenvalue of $\boldsymbol{\chi}$ first diverges, i.e., $\max(\lambda_\gamma)\rightarrow U^{-1}$; and *then* sampling disorder realizations. The results of such are shown by crosses in Fig. 1 (also for $N=512$ sites); variation of $\tilde{U}_{\text{crit}}$ with disorder realizations is small, within ±0.02 of the mean for all $\tilde{\Delta}$. Full agreement with the UHF boundary is found, in all cases within the error bars of Ref. 5. Fourier resolution of the divergent Goldstone eigenvector $\{v_{i\gamma}\}$ further shows uniform contributions from most $\mathbf{q}$ values, i.e., a magnetically disordered SG phase, as opposed to an AF. This occurs for $\tilde{\Delta}$ as low as 0.005, suggesting that for all $\tilde{\Delta}>0$ a SG moment phase is first accessed; (for $\tilde{\Delta}=0$ we find correctly $\tilde{U}_{\text{crit}}=0$ and an AF stable for all $\tilde{U}>0$, as the lattice is bipartite[8]).

Incipient local moment formation, and hence the P-SG border, is thus accessible via the *restricted* HF states appropriate to the P phase. However, Eqs. (1)–(3) hold equally well for magnetic phases *provided* the specific broken-symmetry UHF states are stable: this requires[9] $\lambda_\gamma<U^{-1}$ for all γ other than the characteristic Goldstone mode $[\max(\lambda_\gamma)=U^{-1}]$. To examine the magnetic phases we consider the total uniform static susceptibility $\chi_u=N^{-1}\sum_{i,j}\chi_{ij}\equiv N^{-1}\sum_i\chi_i$, with $\chi_i=\sum_j\chi_{ij}$ the local susceptibility of site i. We write

$$\chi_u=\int\chi(\epsilon)g(\epsilon)d\epsilon , \tag{4}$$

where, for any disorder realization, $\chi(\epsilon)=N_\epsilon^{-1}\sum_{i:\epsilon_i=\epsilon}\chi_i$ is the mean local susceptibility per site of *given* site energy ϵ; and $N_\epsilon/N=g(\epsilon)d\epsilon$. Note that the Goldstone mode, corresponding to a global spin rotation, does not contribute to $\{\chi_i\}$ for $S_z^{\text{tot}}=0$ Ising-like UHF states; its occurrence is thus not a practical problem.

The ϵ dependence of $\chi(\epsilon)$ reflects the inhomogeneous magnetic response of the disordered local moment distribution, itself embodied at the UHF level[5] in the ϵ-differential distribution of local moment magnitudes: $|\mu(\epsilon)|=N_\epsilon^{-1}\sum_{i:\epsilon_i=\epsilon}|\mu_i|$. To show the evolution of $\chi(\epsilon)$ with disorder, we consider a fixed interaction strength $\tilde{U}=\frac{1}{2}$ with increasing disorder, $\tilde{\Delta}=0,\frac{1}{8},\frac{1}{4},\frac{1}{2}$; Fig. 2 shows $\chi(\epsilon)$ and $|\mu(\epsilon)|$ vs $\tilde{\epsilon}=\epsilon/B$ for $\tilde{\Delta}=\frac{1}{8}$ (a) and $\frac{1}{2}$ (b), averaged over several typical realizations for $N=216$ sites. For the $\tilde{\Delta}=0$ pure Hubbard model the UHF ground state is a Hubbard insulator (HI) and a uniform two-sublattice Néel AF,[8] with $\chi_i\equiv\chi_u$ for all sites i and the RPA $\chi_u=0.39/t$ (the $N\rightarrow\infty$ limit which, for $\tilde{U}=\frac{1}{2}$, is reproduced for N as low as 64). With $\tilde{\Delta}>0$ the UHF $\{\mu_i\}$ are again "phase-locked" to produce AF ordering, but the distribution of moment magnitudes is site disordered (Fig. 2) with $|\mu(\epsilon)|$ largest for sites with $|\tilde{\epsilon}|\lesssim\frac{1}{2}\tilde{U}\equiv\tilde{E}_F$,[5] and the moment carrying sites are randomly located in space. At $\tilde{\Delta}=\frac{1}{8}$ the system is a gapless insulator (I); by $\tilde{\Delta}=\frac{1}{4}$ it is safely metallic (M), and as $\tilde{\Delta}$ increases further

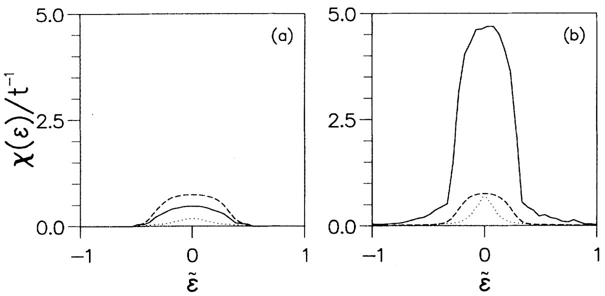

FIG. 2. Distribution of local susceptibilities $\chi(\epsilon)$ vs $\tilde{\epsilon}=\epsilon/B$ (solid lines), for disorder realizations yielding typical total susceptibilities, for $\tilde{U}=\frac{1}{2}$ and $\tilde{\Delta}=\frac{1}{8}$ (a) and $\frac{1}{2}$ (b). Also shown are the corresponding local moment distributions $|\mu(\epsilon)|$ (dashed lines) and the noninteracting $\tilde{U}=0$ Pauli local susceptibilities $D(\epsilon;E_F)$ (dotted lines).

it is driven towards a M-(gapless)I transition (MIT) at $\tilde{\Delta}\simeq 0.56$; see Fig. 1.

For low disorder, $\tilde{\Delta}=\frac{1}{8}$, Fig. 2(a) shows strong local moment sites to have $\chi(\epsilon)$'s close to the $\tilde{\Delta}=0$ pure Hubbard limit of $0.39/t$. Likewise, $\chi(\epsilon)$ is only slightly enhanced over the $\tilde{U}=0$ noninteracting limit, where $\chi_u=D(E_F)$ (Pauli) with $\chi(\epsilon)=D(\epsilon;E_F)$ the corresponding local density of Fermi level states,[5] also shown. However, although the local moment profile $|\mu(\epsilon)|$ varies little over the $\tilde{\Delta}$ range shown, *a pronounced ϵ-differential susceptibility enhancement for strong local moment carrying sites occurs with increasing disorder.* This is already evident by $\tilde{\Delta}=\frac{1}{4}$ in the M phase, but it increases markedly with disorder until [Fig. 2(b)] by $\tilde{\Delta}=\frac{1}{2}$—close to the MIT—$\chi(\epsilon)$ for the strong local moment sites, is well over an order of magnitude larger than that for the $\tilde{\Delta}=0$ nondisordered limit; and is similarly in excess of that for the $\tilde{U}=0$ limit. That $\chi(\epsilon)$ is largest for strong local moment sites reflects appreciable overlap, on such sites, of low-ω transverse-spin excitations; these, being spin-wave-like, naturally have largest weight on the moment carrying sites. [This is evident from the Lehmann representation of $\chi_i\equiv\sum_j\chi_{ij}^{-+}(\omega)$; and has been confirmed directly by analysis of the ω-dependent RPA transverse-spin excitations.[10]]

The above effect has significant implications. First, *all* sites contribute to the total susceptibility χ_u, Eq. (4); and the disorder-induced enhancement of $\chi(\epsilon)$ for strong local moment sites leads to a net *increase* in χ_u as $\tilde{\Delta}$ is increased towards the MIT. This occurs even though, for fixed $\tilde{U}$ in the site-disordered AHM, the fraction of moment carrying sites decreases with increasing $\tilde{\Delta}$. Secondly, the local NMR Knight shift under the electron-nuclear contact interaction, K_i, is proportional to the local site susceptibility χ_i; site-differential inhomogeneity in $\{\chi_i\}$, reflected in $\chi(\epsilon)$, will thus lead to a distribution of Knight shifts. In practice however, only nuclei resonant within a machine-dictated field range are detected experimentally, the observed Knight-shift range being typical of Pauli susceptibilities. Thus, as disorder is increased towards the MIT, the strong local moment sites whose large disorder-induced $\chi(\epsilon)$ enhancements dominate the total χ_u, may by the same token ultimately be "projected out" of the Knight-shift signal—which will thus be dominated by sites outside the strong local moment range, whose $\chi(\epsilon)$'s have Pauli-like values; further, as shown in Ref. 5, it is precisely the latter sites which participate most significantly in Fermi-level single-particle states, and which thus dominate charge transport in the metal. The above behavior is qualitatively akin to that observed by Alloul and Dellouve in Si:P;[6] and although the present study is of course for a site-disordered AHM, which differs in several important respects from the positionally disordered AHM directly applicable[1] to doped semiconductors, we believe it likely that the effects described here, together with the important role of density fluctuations and temperature,[4] will also be relevant in that case.

The $\chi(\epsilon)$ enhancement for strong local moment sites is further manifest in *disorder-induced fluctuations in the total uniform RPA susceptibility* χ_u, whose probability density over disorder realizations we denote by $P(\chi_u)$. We consider again $\tilde{U}=\frac{1}{2}$, with increasing disorder $\tilde{\Delta}=\frac{1}{8},\frac{1}{4},\frac{1}{2}$, and $P(\chi_u)$'s obtained from ~ 1200 realizations each yielding stable $S_z^{\text{tot}}=0$ Ising-like UHF solutions. For $\tilde{\Delta}=\frac{1}{8}$, Fig. 3 inset, χ_u is sharply distributed about its most probable value χ_{mp}. With increasing disorder, however, $P(\chi_u)$ broadens considerably, and by $\tilde{\Delta}=\frac{1}{2}$ (Fig. 3) some 15% of realizations yield χ_u's in excess of $2\chi_{mp}$. A Gaussian fit to the distribution is wholly untenable. A log-normal fit is shown in Fig. 3, with $\delta=0.29$ the rms fluctuation in $\ln\chi_u$; this is tolerable for the bulk of the distribution, although $P(\chi_u)$ decays more slowly at large χ_u. The disorder-induced fluctuations in $P(\chi_u)$ do not appear to be trivial finite-size effects, at least on the length scales we can adequately probe in practice: vary-

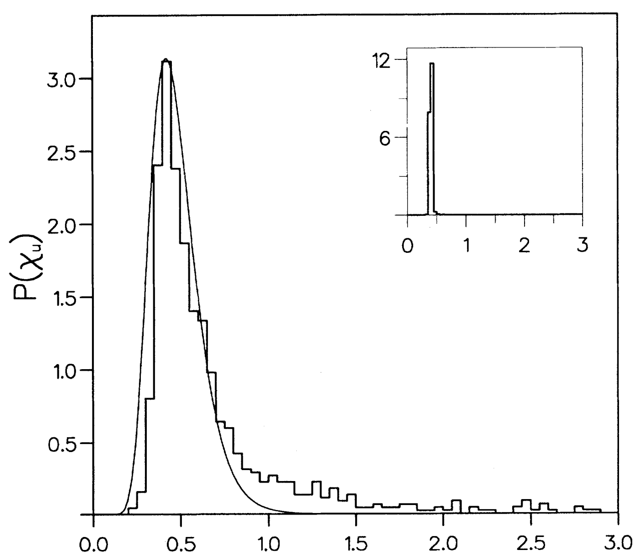

FIG. 3. Probability density $P(\chi_u)$ of the total uniform susceptibility χ_u for $\tilde{U}=\frac{1}{2}$ and $\tilde{\Delta}=\frac{1}{2}$, obtained by sampling approximately 1200 disorder realizations. A log-normal fit to the distribution is shown by the solid line. Inset: $P(\chi_u)$ for $\tilde{U}=\frac{1}{2}$ and $\tilde{\Delta}=\frac{1}{8}$ is shown for comparison.

ing N from 64 to 216 produces no significant change in the form or moments of the distribution (for $\tilde{U}=\frac{1}{2}$, even $N=64$ reproduces the $N\to\infty$ RPA χ_u for $\tilde{\Delta}=0$); and while $P(\chi_u)$ shows strong fluctuations, the corresponding $P(\chi_u^0)$ for the UHF χ_u^0 is an extremely sharp, essentially Gaussian distribution.

Fluctuations in $P(\chi_u)$ cannot occur in either the pure Hubbard ($\tilde{\Delta}=0$) or Anderson ($\tilde{U}=0$) limits: they clearly require both disorder and interactions. This is further apparent from the deconvolution of χ_u in terms of $\chi(\epsilon)$, Eq. (4). Figure 2 shows typical $\chi(\epsilon)$ profiles (for $\chi_u \sim \chi_{mp}$), and the same deconvolution may be performed for realizations yielding large χ_u's in the tail of $P(\chi_u)$. From such, we find consistently that large fluctuations in χ_u arise from large fluctuations occurring quite uniformly in $\chi(\epsilon)$ for the strong local moment sites with $|\tilde{\epsilon}| \lesssim \frac{1}{2}\tilde{U}$; while fluctuations in $\chi(\epsilon)$ for nonmagnetic (Pauli) sites outside this range are by contrast minor. Fluctuations in the total χ_u are thus dominated by large disorder-induced fluctuations in the local susceptibilities of the strong local moment sites, and clearly reflect a fluctuation-induced softening of the transverse-spin excitation spectrum.[10] The fluctuations in $P(\chi_u)$ are at least reminiscent of conductance fluctuations,[11,12] occurring on mesoscopic length scales in the pure localization problem; and, relatedly, to fluctuations in the spin-stiffness constant of the classical Heisenberg model,[13] wherein thermal fluctuations are closely analogous to those due to disorder. Work on these problems tends naturally to focus on the scale (N or L) dependence of the problem, a feature we cannot reasonably address in the present context; but while much remains to be understood, we speculate on the possibility of a connection.

In summary, and via study of a site-disordered Anderson-Hubbard model, we have given a microscopic description of the magnetic response of a disordered, interacting system. Disorder, in producing a range of local environments and thus local moment formation on an inhomogeneous scale,[1,5] leads further to a strong site-differential enhancement of the local susceptibilities for moment carrying sites, whose evolution with increasing disorder controls both the total susceptibility and observable Knight shifts of the system; and we have shown that a careful treatment of disorder, even when weak, is necessary to describe moment formation, the resultant inhomogeneous magnetic response of the system, and even the total susceptibilities on submacroscopic length scales.

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