Magnetic susceptibility of γ-Mn alloys

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This paper provides theoretical results for the magnetic susceptibility in the single (S), double (D), and triple (T) spin-density wave (SDW) states of γ-Mn alloys. Whereas the S SDW state is collinear, the D and T SDW states are noncollinear phases which are stabilized at higher impurity concentrations. As expected, the susceptibility along any spin direction is suppressed below the Néel temperature. Averaged over all possible domains, the magnetic susceptibility of each SDW phase approaches the same limit near the Néel temperature. At low temperatures, however, the average susceptibility depends on the relative sizes of the electron and hole Fermi surfaces. For Fermi surfaces of approximately the same size, the average susceptibility is largest in the S SDW state and smallest in the T SDW state. But when one Fermi surface is sufficiently larger than the other, the relative magnitudes of the average susceptibilities are reversed. As a consequence, the transition between different SDW phases with temperature or doping concentration should be marked by a sudden change in the magnetic susceptibility. [S0163-1829(99)03213-0]

I. INTRODUCTION

Although the magnetic susceptibility of rare-earth[1] and transition-metal[2–4] antiferromagnets with collinear moments has been well known for many years, little is known about the magnetic susceptibility of transition-metal antiferromagnets with noncollinear moments. The fcc phase of doped Mn alloys is believed[5] to support three different magnetic phases, two of which are noncollinear. These spin configurations are stable in distinct ranges of doping and temperature.[6–9] In this paper, we provide theoretical results for the susceptibility of each magnetic phase. Even when averaged over all possible domains, the susceptibilities of the three spin configurations are found to be different. The predictions of this paper can be tested in a γ-Mn alloy which transforms from one phase to another as a function of temperature.

The three magnetic phases of γ-Mn alloys are sketched in Fig. 1 for a single unit cell of the fcc lattice. Whereas the magnetic susceptibility of the collinear phase in Fig. 1(a) may be conjectured to be quite similar to that of a fcc rare-earth antiferromagnet, intuition fails for the two noncollinear phases. We certainly expect the susceptibility to be suppressed below the Néel transition along any spin direction for each magnetic configuration. But a formal calculation is required to determine the relative magnitudes of the susceptibilities in the collinear and noncollinear spin states.

All three magnetic phases of γ-Mn are produced by the Coulomb attraction between electrons and holes on Fermi surfaces centered at the Γ and X points in reciprocal space. Those Fermi surfaces are roughly nested[10] by the three wave vectors $\mathbf{Q}_x=(2\pi/a)\hat{x}$, $\mathbf{Q}_y=(2\pi/a)\hat{y}$, and $\mathbf{Q}_z=(2\pi/a)\hat{z}$. In the single (S), double (D), and triple (T) spin-density wave (SDW) phases[11] sketched in Fig. 1, either one, two, or all three of the nesting wave vectors modulate the spin order. Formally, the SDW phases may be written as

$$\mathbf{S}_i=M\hat{z}\cos(\mathbf{Q}_z\cdot\mathbf{R}_i) \quad \text{S SDW}, \tag{1}$$

$$\mathbf{S}_i=\frac{1}{\sqrt{2}}M[\hat{x}\cos(\mathbf{Q}_x\cdot\mathbf{R}_i)+\hat{y}\cos(\mathbf{Q}_y\cdot\mathbf{R}_i)] \quad \text{D SDW}, \tag{2}$$

$$\mathbf{S}_i=\frac{1}{\sqrt{3}}M[\hat{x}\cos(\mathbf{Q}_x\cdot\mathbf{R}_i)+\hat{y}\cos(\mathbf{Q}_y\cdot\mathbf{R}_i)+\hat{z}\cos(\mathbf{Q}_z\cdot\mathbf{R}_i)] \quad \text{T SDW}. \tag{3}$$

These relations are obtained by replacing the sharply peaked Bloch wave functions of the d-band electrons by δ functions in the spin density. In the remainder of this paper, $\mathbf{Q}_\gamma$ will refer to the one, two, or three ordering wave vectors of the SDW phases defined above. For the T SDW of Eq. (3), the spin points along the $(1,1,1)$, $(1,1,\bar{1})$, $(1,\bar{1},1)$, and $(\bar{1},1,1)$ directions. Consequently, a single domain of the T SDW phase does not violate cubic symmetry and is consistent with the cubic phase of FeMn (Refs. 6–8) and MnNi alloys.[9]

Because the fcc phase of pure Mn is only stable between 1079 and 1140 K, γ-Mn is commonly produced[12] by doping with Fe, Ni, or Cu. For low dopant concentrations, γ-Mn

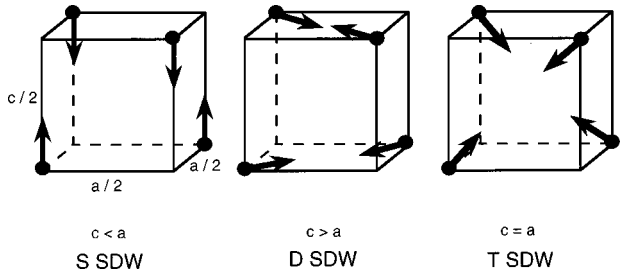

FIG. 1. The single, double, and triple SDW phases which are stabilized in different crystal structures.

alloys have Néel temperatures close to 470 K and magnetic moments of about $2.3\mu_B$.[7] When $x<15\%$, both Fe_xMn_{1-x} (Refs. 6,7) and $Mn_{1-x}Ni_x$ alloys[9] undergo transitions into a S SDW state. More heavily doped Fe_xMn_{1-x} [$x>45\%$ (Ref. 6)] and $Mn_{1-x}Ni_x$ [$x>22\%$ (Ref. 9)] alloys support a T SDW phase and remain cubic for all temperatures below T_N. In a narrow impurity range between 18 and 22%, MnNi alloys are believed[5] to support a D SDW phase.

Magnetoelastic energies are crucial to the stability of these different magnetic phases. The formation of the S SDW phase in FeMn and MnNi alloys coincides with a tetragonal lattice distortion[7] of between 3 and 5% with $c<a$. In MnNi alloys, the appearance of a D SDW phase coincides with a tetragonal distortion with $c>a$.[9] By contrast, the formation of a T SDW with cubic symmetry results in a uniform volume contraction with $c=a$.[7,8]

For some time, the existence of noncollinear states was questioned[13] because multiple S SDW domains have the same neutron-scattering fingerprint as a single T SDW domain.[6] Subsequently, Mössbauer transmission spectra[14] and γ-ray emission[15] studies have largely confirmed the presence of a T SDW phase in FeMn and MnNi alloys. The predictions of this paper can be used to provide additional evidence for the existence of noncollinear phases since, even when averaged over all possible spin domains, the magnetic susceptibilities of the S, D, and T SDW phases remain different.

Unlike the magnetic susceptibility of the noncollinear SDW phases of γ-Mn alloys, the susceptibility of the collinear, commensurate SDW phase of bcc Cr alloys has been studied extensively, both experimentally[3,4] and theoretically.[2,4] Assuming that the electron and hole Fermi surfaces are the same size, Maki and Sakurai[2] concluded that the susceptibility parallel to the spins vanishes at $T=0$ while the perpendicular susceptibility is unchanged below T_N, precisely as expected for a local-moment system. A few years latter, Kelly, Moyer, and Arajs[4] considered the more general case of Fermi surfaces with different sizes and also included the effects of impurity and electron-phonon scattering. Their results are in good agreement with measurements on CrRu (Ref. 3) and CrRe (Ref. 4) alloys.

For the sake of simplicity, we ignore impurity and electron-phonon scattering corrections to the magnetic susceptibility of γ-Mn alloys. But we consider the electron and hole Fermi surfaces to have different sizes. Linear response theory is used to confirm the results obtained by explicitly expanding the Green's functions in a magnetic field. Our final results for the susceptibility are surprisingly simple. As expected, the magnetic susceptibility along any spin direction is suppressed by the antiferromagnetic order. Once averaged over possible spin domains, the magnetic susceptibility near the Néel temperature is identical in all three possible magnetic phases. But the relative magnitudes of the average susceptibilities at low temperatures depend on the relative sizes of the electron and hole Fermi surfaces.

To streamline the following discussion, the magnetic susceptibility is derived in two appendices: Appendix A explicitly expands the Green's functions in powers of H while Appendix B develops a linear-response theory. Section II outlines the basic formalism, Sec. III summarizes our previous results[16] for the SDW ordering in zero field, Sec. IV discusses our results for the magnetic susceptibility, and Sec. V contains a conclusion and summary.

II. HAMILTONIAN AND GREEN'S FUNCTIONS

Our starting Hamiltonian contains four terms: the kinetic energy of the electrons, the Coulomb attraction U between electrons and holes, the magnetoelastic interaction[17] between the N spins and the lattice, and the interaction with the external magnetic field:

$$H=H_0+H_{\rm Coul}+H_{\rm me}+H_{\rm ext}, \tag{4}$$

$$H_0=\sum_{\mathbf{k},\alpha}\{\epsilon_a(\mathbf{k})a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}+\epsilon_b(\mathbf{k})b^\dagger_{\mathbf{k}\alpha}b_{\mathbf{k}\alpha}\}, \tag{5}$$

$$H_{\rm Coul}=\frac{U}{V}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}',\alpha,\beta}a^\dagger_{\mathbf{k}\alpha}b^\dagger_{\mathbf{k}'\beta}b_{\mathbf{k}'+\mathbf{q}\beta}a_{\mathbf{k}-\mathbf{q}\alpha}, \tag{6}$$

$$\begin{aligned}H_{\rm me}=V\Big\{&\frac{1}{2}c_{11}(\epsilon_{xx}^2+\epsilon_{yy}^2+\epsilon_{zz}^2)+c_{12}(\epsilon_{xx}\epsilon_{yy}+\epsilon_{yy}\epsilon_{zz}+\epsilon_{zz}\epsilon_{xx})\\&+\frac{g_1}{N}\sum_i(S_{ix}^2\epsilon_{xx}+S_{iy}^2\epsilon_{yy}+S_{iz}^2\epsilon_{zz})\\&+\frac{g_2}{N}(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz})\sum_i(S_{ix}^2+S_{iy}^2+S_{iz}^2)\Big\},\end{aligned} \tag{7}$$

$$H_{\rm ext}=-2\mu_B\mathbf{H}\cdot\sum_i\mathbf{S}_i, \tag{8}$$

where $a^\dagger_{\mathbf{k}\alpha}$ and $b^\dagger_{\mathbf{k}\alpha}$ are the creation operators for quasiparticles on the a (electron) and b (hole) bands. The strain components are given by ϵ_{ii}, c_{11}, and c_{12} are the elastic constants, and g_i are the magnetoelastic coupling strengths.

With terms up to order $S_{i\alpha}^2$, $H_{\rm me}$ is the most general Hamiltonian consistent with the cubic symmetry of the paramagnetic phase. After minimizing $H_{\rm me}$ with respect to the strain components, it is easy to obtain the average strain components for each SDW configuration.[16] In agreement with experiments,[17] the strain components and tetragonality (for the S and D SDW states) are proportional to $M(T)^2$.

In Ref. 16, we used mean-field theory to replace the magnetoelastic energy $H_{\rm me}$ with

$$H'_{\rm me}=-2\mu_B\sum_i\mathbf{B}_i\cdot\mathbf{S}_i+\text{const}, \tag{9}$$

$$B_{i\alpha}=-\frac{V}{\mu_B N}\{g_1\epsilon_{\alpha\alpha}+g_2(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz})\}\langle S_{i\alpha}\rangle. \tag{10}$$

Within this approximation, every electron and hole independently experiences the effective field $\mathbf{B}_i$ exerted by the magnetoelastic interaction. The interaction constant κ is defined in terms of c_{11}, c_{12}, and g_i through the relation $\langle H_{\rm me}\rangle=-N\kappa M^4$.

In previous work[16] on the spin dynamics of γ-Mn alloys, we predicted that the gap in the spin-wave spectrum is proportional to $\sqrt{\kappa T_N/\rho_{eh}U}M(T)^{3/2}$, where ρ_{eh} is the density-of-states of the electron and hole Fermi surfaces. Fitting this

result to the observed spin-wave gap[18] of roughly 10 meV, we found that κ is of order 1 μeV.

Despite the small size of κ, the strain field $\mathbf{B}_i \sim \kappa M^3/2\mu_B$ has a magnitude of roughly 200 G. This field stabilizes one or the other of the SDW phases. Qualitatively, the magnetoelastic interaction alters the magnetic susceptibility by distorting the crystal along the direction of the external field. Nevertheless, as shown by the following argument, the magnetoelastic interaction is largely irrelevant to our calculation of the magnetic susceptibility for a given SDW phase. In the presence of an applied field $\mathbf{H}$ in the z direction, the magnetoelastic energy generates the additional interaction $8\kappa M_z^2 \Delta M_z \Sigma_i \mathbf{S}_{iz}$, where $2\mu_B \Delta M_z = \chi H$ is the change in the average z moment. Hence, the magnetoelastic interaction enhances the external field by the factor $1 + 2\kappa\chi M^2/\mu_B^2$. Using the paramagnetic susceptibility $\chi_p = \mu_B^2 V \rho_{eh}/N$ as an upper limit on χ, we find that $\kappa\chi M^2/\mu_B^2 < 10^{-6}$. Therefore, the magnetoelastic interaction can be safely neglected in the remaining calculations.

Using the standard notation, the imaginary time Green's functions may be written as

$$G(\mathbf{k},\tau)_{\alpha\beta,aa} = -\langle T_\tau a_{\mathbf{k}\alpha}(\tau) a^\dagger_{\mathbf{k}\beta}(0)\rangle, \tag{11}$$

$$G(\mathbf{k},\tau)^\gamma_{\alpha\beta,ab} = -\langle T_\tau a_{\mathbf{k}\alpha}(\tau) b^\dagger_{\mathbf{k}+\mathbf{Q}_\gamma\beta}(0)\rangle, \tag{12}$$

$$G(\mathbf{k},\tau)^\gamma_{\alpha\beta,ba} = -\langle T_\tau b_{\mathbf{k}+\mathbf{Q}_\gamma\alpha}(\tau) a^\dagger_{\mathbf{k}\beta}(0)\rangle, \tag{13}$$

$$G(\mathbf{k},\tau)^\gamma_{\alpha\beta,bb} = -\langle T_\tau b_{\mathbf{k}+\mathbf{Q}_\gamma\alpha}(\tau) b^\dagger_{\mathbf{k}+\mathbf{Q}_\gamma\beta}(0)\rangle, \tag{14}$$

$$G(\mathbf{k},\tau)^{\gamma\gamma'}_{\alpha\beta,bb'} = -\langle T_\tau b_{\mathbf{k}+\mathbf{Q}_\gamma\alpha}(\tau) b^\dagger_{\mathbf{k}+\mathbf{Q}_{\gamma'}\beta}(0)\rangle, \quad \gamma \neq \gamma'. \tag{15}$$

Note that $G(\mathbf{k},\tau)^{\gamma\gamma'}_{\alpha\beta,bb'}$ is only defined for the D or T SDW states with more than one ordering wave vector. For $\delta \neq \gamma$ (so that $\mathbf{Q}_\delta$ is not an ordering wave vector), the hole Green's function

$$G(\mathbf{k},\tau)^\delta_{\alpha\beta,bb} = -\langle T_\tau b_{\mathbf{k}+\mathbf{Q}_\delta\alpha}(\tau) b^\dagger_{\mathbf{k}+\mathbf{Q}_\delta\beta}(0)\rangle \tag{16}$$

is unaffected by the formation of the SDW.

For future reference, we define the energy-gap tensors

$$\Delta^\gamma_{\alpha\beta} = -\frac{U}{V}\sum_{\mathbf{k}} \langle b^\dagger_{\mathbf{k}+\mathbf{Q}_\gamma\beta}(0) a_{\mathbf{k}\alpha}(0)\rangle = -\frac{U}{V} T\sum_{\mathbf{k},l} G(\mathbf{k}, i\nu_l)^\gamma_{\alpha\beta,ab}, \tag{17}$$

$$\overline{\Delta}^\gamma_{\alpha\beta} = -\frac{U}{V}\sum_{\mathbf{k}} \langle a^\dagger_{\mathbf{k}\beta}(0) b_{\mathbf{k}+\mathbf{Q}_\gamma\alpha}(0)\rangle = -\frac{U}{V} T\sum_{\mathbf{k},l} G(\mathbf{k}, i\nu_l)^\gamma_{\alpha\beta,ba}. \tag{18}$$

The above relation also introduces the Fourier-transformed Green's functions

$$G(\mathbf{k}, i\nu_l)_{\alpha\beta,ij} = \int_0^\beta d\tau e^{i\nu_l\tau} G(\mathbf{k},\tau)_{\alpha\beta,ij}, \tag{19}$$

with Matsubara frequency $\nu_l = (2l+1)\pi T$.

In terms of the Fermi operators for the two bands, the spin operator is defined by

$$S_{i\delta} = \frac{1}{2}(a^\dagger_{i\alpha} + b^\dagger_{i\alpha})\sigma^\delta_{\alpha\beta}(a_{i\beta} + b_{i\beta}), \tag{20}$$

where repeated spin indices are summed and $\sigma^\delta_{\alpha\beta}$ are the Pauli matrices. If the external field lies in the z direction, then the induced moment in this direction is

$$\Delta M_z = \frac{1}{2N} T\sum_{\mathbf{k},l} \sigma^z_{\beta\alpha}\Big\{ G(\mathbf{k}, i\nu_l)_{\alpha\beta,aa} + \sum_{\delta=x,y,z} G(\mathbf{k}, i\nu_l)^\delta_{\alpha\beta,bb}\Big\}. \tag{21}$$

Hence, the magnetic susceptibility χ is given by the zero-field limit of $2\mu_B \Delta M_z/H$. When the external field is perpindicular to all the spins, $\chi = \chi_\perp$. So for the S and D SDW states of Eqs. (1) and (2), $\chi_\perp$ is obtained when $\mathbf{H}$ lies in the xy plane or along the z axis, respectively. When the field is parallel to one of the ordering wave vectors, $\chi = \chi_\parallel$. For a T SDW, $\chi = \chi_\parallel$ regardless of whether the field points along the x, y, or z axis.

III. SDW ORDERING IN ZERO FIELD

In zero field, the spin symmetry of the Green's functions is given by the relations $G(\mathbf{k},\tau)_{\alpha\beta,aa} = \delta_{\alpha\beta} E(\mathbf{k},\tau)_{aa}$, $G(\mathbf{k},\tau)^\gamma_{\alpha\beta,ab} = \sigma^\gamma_{\alpha\beta} E(\mathbf{k},\tau)_{ab}$, $G(\mathbf{k},\tau)^\gamma_{\alpha\beta,ba} = \sigma^\gamma_{\alpha\beta} E(\mathbf{k},\tau)_{ba}$, $G(\mathbf{k},\tau)^\gamma_{\alpha\beta,bb} = \delta_{\alpha\beta} E(\mathbf{k},\tau)_{bb}$, and $G(\mathbf{k},\tau)^{\gamma\gamma'}_{\alpha\beta,bb'} = (\sigma^\gamma \cdot \sigma^{\gamma'})_{\alpha\beta} E(\mathbf{k},\tau)_{bb'}$. Then $E(\mathbf{k},\tau)_{ab}$, $E(\mathbf{k},\tau)_{ba}$, $E(\mathbf{k},\tau)_{bb}$, and $E(\mathbf{k},\tau)_{bb'}$ are independent of γ provided that the hole band b has cubic symmetry about X so that $\epsilon_b(\mathbf{k} + \mathbf{Q}_\gamma) \equiv \epsilon_{b+}(\mathbf{k})$ does not depend on γ. This approximation would be satisfied by spherical or octagonal Fermi surfaces.

Using the random-phase approximation (RPA) to solve the equations-of-motion for the Green's functions in zero field, we previously found[16] that

$$E(\mathbf{k}, i\nu_l)_{aa} = \frac{i\nu_l - \epsilon_{b+}(\mathbf{k})}{D(\mathbf{k}, i\nu_l)}, \tag{22}$$

$$E(\mathbf{k}, i\nu_l)_{ab} = E(\mathbf{k}, i\nu_l)_{ba} = \frac{1}{\sqrt{m}} \frac{\Delta}{D(\mathbf{k}, i\nu_l)}, \tag{23}$$

$$E(\mathbf{k}, i\nu_l)_{bb} = \frac{1}{m} \frac{i\nu_l - \epsilon_a(\mathbf{k})}{D(\mathbf{k}, i\nu_l)} + \frac{m-1}{m} \frac{1}{i\nu_l - \epsilon_{b+}(\mathbf{k})}, \tag{24}$$

$$E(\mathbf{k}, i\nu_l)_{bb'} = \frac{1}{m} \frac{i\nu_l - \epsilon_a(\mathbf{k})}{D(\mathbf{k}, i\nu_l)} - \frac{1}{m} \frac{1}{i\nu_l - \epsilon_{b+}(\mathbf{k})}, \tag{25}$$

where $m = 1$, 2, or 3 for S, D, and T SDW's and

$$D(\mathbf{k}, i\nu_l) = [i\nu_l - \epsilon_a(\mathbf{k})][i\nu_l - \epsilon_{b+}(\mathbf{k})] - \Delta^2. \tag{26}$$

The energy gap

$$\Delta = -\sqrt{m}\frac{U}{V} T\sum_{\mathbf{k},l} E(\mathbf{k}, i\nu_l)_{ab} \tag{27}$$

is obtained from the general spin-dependent gap $\Delta^{\gamma}_{\alpha\beta} = (\Delta/\sqrt{m})\sigma^{\gamma}_{\alpha\beta}$. Below the Néel temperature, the hybridized quasiparticle energies are obtained from the zeroes of $D(\mathbf{k},\epsilon)$. So a gap of 2Δ opens between the upper and lower hybridized bands. Band-structure calculations[19] suggest that $2\Delta(0)$ lies between 1.8 and 2.2 eV.

Using Eq. (12), the sublattice magnetization in zero field may be written

$$M = -\frac{2\sqrt{m}}{N}\sum_{\mathbf{k}} E(\mathbf{k},0^-)_{ab} = -\frac{2\sqrt{m}}{N}T\sum_{\mathbf{k},l} E(\mathbf{k},i\nu_l)_{ab}. \tag{28}$$

Comparing Eqs. (28) and (27), we conclude that the magnetization $M(T) = (2V/NU)\Delta(T)$ is proportional to the energy gap in all three phases.

Physically, Eq. (24) for $E(\mathbf{k},i\nu_l)_{bb}$ implies that only $1/m$ of the holes on each of the m nested hole Fermi surfaces (connected to each electron Fermi surface by the m ordering wave vectors $\mathbf{Q}_\gamma$) participates in the SDW and experiences an energy gap. The remaining fraction $1-1/m$ of holes on these nested Fermi surfaces are unaffected by the formation of the SDW. Of course, holes on the $m-1$ non-nested hole Fermi surfaces are also unaffected by the SDW. So for any SDW state, two thirds of the holes with density of states $\rho_{eh}/2$ do not contribute to the electron-hole condensate.

Because of the size difference between the electron and hole Fermi surfaces, there is an energy mismatch $\epsilon_{b+}(\mathbf{k}) - \epsilon_a(\mathbf{k}) = z_0/2$ at the Fermi momentum $\mathbf{k}_F$ of the a Fermi surface. Consequently, we may write $\epsilon_a(\mathbf{k}) \equiv z$ and $\epsilon_{b+}(\mathbf{k}) \equiv z_0/2 - z$. When the electron Fermi surface is larger (smaller) than the hole Fermi surface, z_0 is negative (positive). This mismatch is assumed to be the same for all points on the a Fermi surface. As described in Appendix A, a summation over $\mathbf{k}$ is evaluated by performing an integral over z with the linearized energies given above.

Solving Eq. (27) with $z_0 = 0$ as $\Delta \to 0$, we find that the Néel temperature of a perfectly nested alloy is given by

$$T_N^{\star} = \frac{2\gamma}{\pi}\epsilon_0 e^{-8/U\rho_{eh}}, \tag{29}$$

where $\ln\gamma \approx 0.577$ is Euler's constant. Here, ϵ_0 is the cutoff in the quasiparticle energy spectrum. Since the Fermi surface nesting is imperfect with $z_0 \neq 0$, the actual Néel temperature T_N will be much less than $T_N^{\star}$. When $T=0$, Eq. (27) yields the quasiparticle gap $\Delta(0) = \pi T_N^{\star}/\gamma$, which is identical to the familiar BCS relation for the energy gap of a superconductor. Hence, we estimate that $T_N^{\star} \approx 500$ meV.

IV. MAGNETIC SUSCEPTIBILITY

Our results for the parallel susceptibilities of S, D, and T SDW's are summarized in Eqs. (A47), (A46), and (A48), respectively. For S and D SDW's, the perpendicular susceptibility is unchanged below T_N with $\chi_\perp = \mu_B^2\rho_{eh}V/N$. The magnetizations of the S, D, and T SDW's defined by Eqs. (1)–(3) are generally given by

$$\Delta\mathbf{M} = \chi_\parallel \hat{z}\mathbf{H}\cdot\hat{z} + \chi_\perp(\hat{x}\mathbf{H}\cdot\hat{x} + \hat{y}\mathbf{H}\cdot\hat{y}) \quad \text{S SDW}, \tag{30}$$

$$\Delta\mathbf{M} = \chi_\perp \hat{z}\mathbf{H}\cdot\hat{z} + \chi_\parallel(\hat{x}\mathbf{H}\cdot\hat{x} + \hat{y}\mathbf{H}\cdot\hat{y}) \quad \text{D SDW}, \tag{31}$$

$$\Delta\mathbf{M} = \chi_\parallel \mathbf{H} \quad \text{T SDW}. \tag{32}$$

These results follow from the absence of off-diagonal terms such as $\partial\Delta M_z/\partial H_x$ in the linear-response theory developed in Appendix B.

At $T=0$, the parallel susceptibilities are given by Eqs. (A49)–(A51), which imply that for any Fermi surface mismatch z_0, $\chi_\parallel$ is always largest for the T SDW state and smallest for the S SDW. This means that the induced magnetization along one of the ordering wave vectors is smallest in the collinear state. Even in this state, however, the susceptibility does not vanish at $T=0$ as it would for a local-moment antiferromagnet. This is easy to understand. For the S SDW state of γ-Mn, only one of the three hole Fermi surfaces (displaced from the electron Fermi surface by $\mathbf{Q}_z$) contributes to the condensate of electron-hole pairs. The remaining susceptibility $\mu_B^2\rho_{eh}V/2N$ at $T=0$ is produced by the two hole Fermi surfaces which do not participate in the formation of the SDW.

For either noncollinear state, the moments of the SDW can be rotated by an external field even at $T=0$. So the susceptibility at $T=0$ contains two contributions: one from the density-of-states $\rho_{eh}/2$ of holes not involved in the SDW and the other from the SDW itself. This latter part is responsible for the dependence of $\chi_\parallel$ on the mismatch z_0 between the electron and hole Fermi surfaces.

As mentioned in the Introduction, neutron scattering is unable to distinguish multiple domains of a S SDW from a T SDW: both possibilities produce the same neutron-scattering intensity at every Γ in reciprocal space.[6] Other probes[14,15] have been used to confirm the presence of a noncollinear T SDW in FeMn and MnNi alloys. Averaged over all possible domains, the susceptibilities are given by $\chi_{\rm av} = \chi_\parallel/3 + 2\chi_\perp/3$ (S SDW), $2\chi_\parallel/3 + \chi_\perp/3$ (D SDW), or $\chi_\parallel$ (T SDW). As $T \to 0$,

$$\chi_{\rm av} \to \frac{5}{6}\mu_B^2\frac{V}{N}\rho_{eh} \quad \text{S SDW}, \tag{33}$$

$$\chi_{\rm av} \to \mu_B^2\frac{V}{N}\rho_{eh}\left\{\frac{3}{4} + \frac{1}{48}\left(\frac{z_0}{\Delta}\right)^2\right\} \quad \text{D SDW}, \tag{34}$$

$$\chi_{\rm av} \to \mu_B^2\frac{V}{N}\rho_{eh}\left\{\frac{13}{18} + \frac{1}{36}\left(\frac{z_0}{\Delta}\right)^2\right\} \quad \text{T SDW}. \tag{35}$$

Now the relative magnitudes of the average susceptibilities depend on the size of the Fermi surface mismatch. For $z_0 = 0$, the S SDW susceptibility is the largest and the T SDW susceptibility is the smallest. For $|z_0| > 2\Delta(0) = 3.53T_N^{\star}$, the relative sizes are reversed with the T SDW susceptibility the largest and the S SDW susceptibility the smallest. Most importantly, the average susceptibilities are different even when multiple domains are present.

Close to the Néel temperature, however, the average susceptibilities converge. As $T \to T_N$, the parallel susceptibilities approach the limit

$$\chi_\parallel \to \mu_B^2\rho_{eh}\frac{V}{N}\left\{1 - \frac{1}{8m\pi^2}\left(\frac{\Delta}{T_N}\right)^2\sum_{n=0}^{\infty}\mathrm{Re}\left(\frac{1}{X_n^3}\right)\right\}, \tag{36}$$

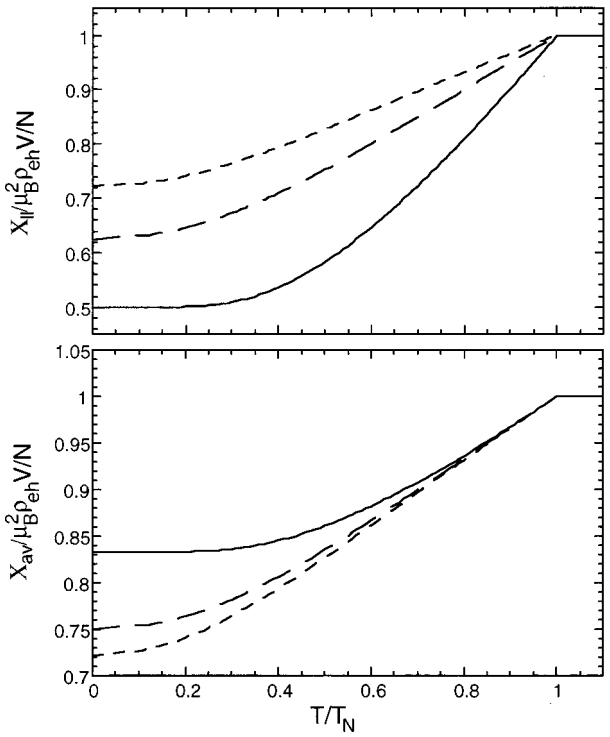

FIG. 2. The parallel and average susceptibilities versus T/T_N for a S (solid), D (long dash), and T (short dash) SDW with $z_0=0$.

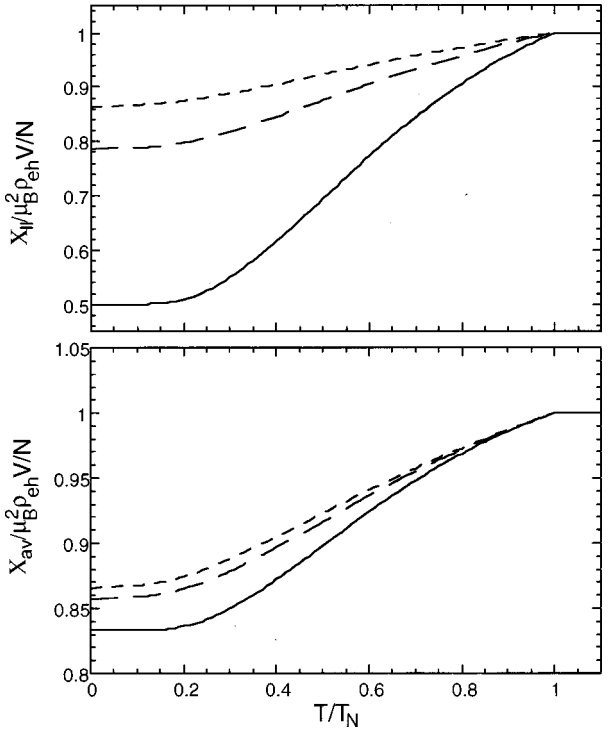

FIG. 3. The parallel and average susceptibilities versus T/T_N for a S (solid), D (long dash), and T (short dash) SDW with $z_0=4T_N^\star$.

where $X_n=n+1/2+iz_0/8\pi T_N$. Therefore, the average susceptibilities approach the same limit for all three SDW's:

$$\chi_{\rm av}\rightarrow\mu_B^2\rho_{eh}\frac{V}{N}\left\{1-\frac{1}{24\pi^2}\left(\frac{\Delta}{T_N}\right)^2\sum_{n=0}^{\infty}{\rm Re}\left(\frac{1}{X_n^3}\right)\right\}. \quad (37)$$

Since $\Delta(T)^2\propto 1-T/T_N$ near T_N, these results also imply that the parallel and average suceptibilities are linear functions of temperature just below the Néel transition. But the condition for the triple point $|z_0|\approx 4.29T_N^\star$, above which the commensurate SDW configurations considered so far become unstable to an incommensurate SDW at T_N, is given by $\Sigma_{n=0}^{\infty}{\rm Re}(1/X_n^3)=0$. Therefore, the linear terms in the parallel and average susceptibilities dominate in a smaller range of temperatures as the mismatch energy increases in magnitude.

Our numerical results for the parallel and average susceptibilities are plotted in Figs. 2 and 3 for $z_0=0$ and $4T_N^\star$, respectively. For the larger Fermi surface mismatch, the relative magnitudes of the average suceptibilities are reversed compared to Fig. 2, as expected from the above discussion. Unlike the parallel susceptibilties, the average susceptibilities merge into one curve close to the Néel temperature, corresponding to the limit of Eq. (37). As expected, the temperature range over which the average susceptibility is approximately linear near T_N is smaller for $z_0=4T_N^\star$ than for $z_0=0$.

V. DISCUSSION AND CONCLUSION

This paper has evaluated the magnetic susceptibility of the collinear and noncollinear SDW states of γ-Mn alloys. While the susceptibility parallel to any of the ordering wave vectors is always smallest in the collinear S SDW state, the relative magnitudes of the susceptibilites averaged over all possible domains depends on the relative sizes of the electron and hole Fermi surfaces. For a small mismatch between the Fermi surfaces, the average susceptibility is largest in the collinear state of Fig. 1(a).

Perhaps the most important result of this work is that the average susceptibilities are different in the three possible SDW states. An experiment which cuts across different SDW states by varying temperature or doping should observe a sudden change in the average susceptibility. For example, $Mn_{1-x}Ni_x$ alloys with x between 18 and 22 % transform from a high-temperature T SDW phase to a low-temperature D SDW phase.[9] According to Figs. 2 and 3, the average suceptibility can jump by a few percent across such a transition.

To simplify our calculations, we ignored scattering effects which were found[4] to play important roles in the susceptibility of bcc Cr alloys. Based on linear-response theory, Kelly, Moyer, and Arajs[4] concluded that impurity and electron-phonon scattering are required to obtain quantitative agreement with susceptibility measurements[3,4] on CrRe and CrRu alloys.

Unfortunately, we are aware of only one set of susceptibility measurements on γ-Mn alloys. Those early measurements were performed by Endoh and Ishikawa[7] on a group of FeMn alloys. Within the T SDW phase, the low-temperature susceptibility is suppressed by about 10% from its value at T_N. For comparison, Fig. 3 suggests that the susceptibility may be depressed by about 16%. The contribution of extraneous electron or hole pockets to the background susceptibility can easily account for this difference. In agreement with our predictions, the susceptibility is linear

just below the Néel temperature.

The difference between the parallel and perpendicular susceptibilities can be used to selectively eliminate spin domains by cooling the sample in a magnetic field. If the appropriate MnNi alloy is field cooled through the T SDW phase, then the D SDW domain with ordering wave vectors and spins perpendicular to **H** will be selected. For a S SDW, the domain with $\mathbf{S}\|\mathbf{H}$ will be eliminated by field cooling.

Since the internal strain field $\mathbf{B}_i$ responsible for selecting the SDW phase is only about 200 G, it might be naively expected that an applied field of more than 200 G can induce a transformation between SDW phases. However, the applied field will have a significant effect on the SDW configuration only when $2\mu_B\Delta MH$ is of order $2\mu_B MB_i$. Using the paramagnetic susceptibility to find an upper bound on $2\mu_B\Delta M \leqslant \chi_p H$, we conclude that a field of at least 30 T is required to eliminate one SDW phase in favor of another.

Simliar to Cr alloys, γ-Mn alloys provide a testing ground for our ideas about itinerant antiferromagnetism. Because they support noncollinear SDW states, γ-Mn alloys may allow even more stringent tests of theoretical models than Cr alloys. We hope that the present work motivates experimentalists to revisit this important system and to perform updated susceptibility measurements on MnNi and FeMn alloys.

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APPENDIX A: RANDOM-PHASE APPROXIMATION

In this appendix, we provide a detailed calculation for the field-dependence of the Green's functions. Rather than repeat essentially the same steps for all three magnetic phases, we shall provide the important details of this calculation for the D SDW phase only. It is quite straightforward to extend this calculation to the S and T SDW phases.

The RPA equations for the Green's functions of the D SDW phase with the field **H** along an arbitrary direction are given by

$$(i\nu_l-\epsilon_a)G_{\alpha\beta,aa}-\Delta^x_{\alpha\nu}G^x_{\nu\beta,ba}-\Delta^y_{\alpha\nu}G^y_{\nu\beta,ba}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G_{\nu\beta,aa}=\delta_{\alpha\beta}, \tag{A1}$$

$$(i\nu_l-\epsilon_{b+})G^\gamma_{\alpha\beta,ba}-\overline{\Delta}^\gamma_{\alpha\nu}G_{\nu\beta,aa}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^\gamma_{\nu\beta,ba}=0, \tag{A2}$$

$$(i\nu_l-\epsilon_a)G^x_{\alpha\beta,ab}-\Delta^x_{\alpha\nu}G^x_{\nu\beta,bb}-\Delta^y_{\alpha\nu}G^{yx}_{\nu\beta,bb'}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^x_{\nu\beta,ab}=0, \tag{A3}$$

$$(i\nu_l-\epsilon_a)G^y_{\alpha\beta,ab}-\Delta^y_{\alpha\nu}G^y_{\nu\beta,bb}-\Delta^x_{\alpha\nu}G^{xy}_{\nu\beta,bb'}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^y_{\nu\beta,ab}=0, \tag{A4}$$

$$(i\nu_l-\epsilon_{b+})G^\gamma_{\alpha\beta,bb}-\overline{\Delta}^\gamma_{\alpha\nu}G^\gamma_{\nu\beta,ab}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^\gamma_{\nu\beta,bb}=\delta_{\alpha\beta}, \tag{A5}$$

$$(i\nu_l-\epsilon_{b+})G^{xy}_{\alpha\beta,bb'}-\overline{\Delta}^x_{\alpha\nu}G^y_{\nu\beta,ab}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^{xy}_{\nu\beta,bb'}=0, \tag{A6}$$

$$(i\nu_l-\epsilon_{b+})G^{yx}_{\alpha\beta,bb'}-\overline{\Delta}^y_{\alpha\nu}G^x_{\nu\beta,bb}+\mu_B\mathbf{H}\cdot\sigma_{\alpha\nu}G^{yx}_{\nu\beta,bb'}=0, \tag{A7}$$

where we suppress the $(\mathbf{k},i\nu_l)$ dependence of each Green's function and repeated spin indices are summed. Since a D SDW has ordering wave vectors $\mathbf{Q}_x$ and $\mathbf{Q}_y$, $\gamma=x$ or y.

1. Perpendicular susceptibility

When **H** is along the *perpendicular* or z axis, the Green's functions obey the following spin symmetries:

$$G_{\alpha\beta,aa}=\delta_{\alpha\beta}E_{aa}+\sigma^z_{\alpha\beta}F_{aa}, \tag{A8}$$

$$G^x_{\alpha\beta,ab}=\sigma^x_{\alpha\beta}E^x_{ab}-i\sigma^y_{\alpha\beta}F^x_{ab}, \tag{A9}$$

$$G^y_{\alpha\beta,ab}=\sigma^y_{\alpha\beta}E^y_{ab}-i\sigma^x_{\alpha\beta}F^y_{ab}, \tag{A10}$$

$$G^x_{\alpha\beta,ba}=\sigma^x_{\alpha\beta}E^x_{ab}+i\sigma^y_{\alpha\beta}F^x_{ab}, \tag{A11}$$

$$G^y_{\alpha\beta,ba}=\sigma^y_{\alpha\beta}E^y_{ab}+i\sigma^x_{\alpha\beta}F^y_{ab}, \tag{A12}$$

$$G^\gamma_{\alpha\beta,bb}=\delta_{\alpha\beta}E_{bb}+\sigma^z_{\alpha\beta}F_{bb}, \tag{A13}$$

$$G^{xy}_{\alpha\beta,bb'}=i\sigma^z_{\alpha\beta}E^{xy}_{bb'}+i\delta_{\alpha\beta}F^{xy}_{bb'}, \tag{A14}$$

$$G^{yx}_{\alpha\beta,bb'}=-i\sigma^z_{\alpha\beta}E^{xy}_{bb'}-i\delta_{\alpha\beta}F^{xy}_{bb'}. \tag{A15}$$

As verified in the next section using linear-response theory, the change in the energy gap $\Delta^\gamma_{\alpha\beta}$ due to an external field is of order $\Delta\mu_B H(NU/V)/\epsilon_F T^\star_N$. Because this correction is so small, $\Delta^\gamma_{\alpha\beta}=\overline{\Delta}^\gamma_{\alpha\beta}=(\Delta/\sqrt{2})\sigma^\gamma_{\alpha\beta}$ is taken to be unchanged by the external field.

Using the Green's functions defined above to solve the equations-of-motion, we find

$$E_{aa}\pm F_{aa}=\frac{i\nu_l-\epsilon_{b+}\mp\mu_B H}{D_2(\mp H)}, \tag{A16}$$

$$E^x_{ab}\pm F^x_{ab}=\frac{1}{\sqrt{2}}\frac{\Delta}{D_2(\pm H)}, \tag{A17}$$

$$E^y_{ab}\pm F^y_{ab}=\frac{1}{\sqrt{2}}\frac{\Delta}{D_2(\mp H)}, \tag{A18}$$

$$E_{bb}\pm F_{bb}=\frac{1}{2}\frac{1}{i\nu_l-\epsilon_{b+}\pm\mu_B H}+\frac{1}{2}\frac{i\nu_l-\epsilon_a\mp\mu_B H}{D_2(\pm H)}, \tag{A19}$$

$$E^{xy}_{bb'}\pm F^{xy}_{bb'}=-\frac{1}{2}\frac{1}{i\nu_l-\epsilon_{b+}\pm\mu_B H}+\frac{1}{2}\frac{i\nu_l-\epsilon_a\mp\mu_B H}{D_2(\pm H)}, \tag{A20}$$

where

$$D_2(H)=(i\nu_l-\epsilon_a-\mu_B H)(i\nu_l-\epsilon_{b+}+\mu_B H)-\Delta^2 \tag{A21}$$

generalizes the zero-field denominator of Eq. (26).

It follows that

$$\Delta M_z=\frac{T}{N}\sum_{\mathbf{k},l}\{F(\mathbf{k},i\nu_l)_{aa}+F(\mathbf{k},i\nu_l)^x_{bb}+F(\mathbf{k},i\nu_l)^y_{bb}\}+\frac{T}{2N}\sum_{\mathbf{k},l}\left\{\frac{1}{i\nu_l-\epsilon_{b+}+\mu_BH}-\frac{1}{i\nu_l-\epsilon_{b+}-\mu_BH}\right\}. \tag{A22}$$

For both sets of terms in brackets, the summations over ν_l and $\mathbf{k}$ do not commute. Based on the definition of the spin, the summation over ν_l must come first. Once the normal-state contribution is subtracted from the first set of terms, the summations over ν_l and $\mathbf{k}$ can be interchanged:

$$\Delta M_z=\frac{T}{N}\sum_{l,\mathbf{k}}\left\{F(\mathbf{k},i\nu_l)_{aa}+F(\mathbf{k},i\nu_l)^x_{bb}+F(\mathbf{k},i\nu_l)^y_{bb}-\frac{1}{2}\frac{1}{i\nu_l-\epsilon_a+\mu_BH}+\frac{1}{2}\frac{1}{i\nu_l-\epsilon_a-\mu_BH}-\frac{1}{i\nu_l-\epsilon_{b+}+\mu_BH}+\frac{1}{i\nu_l-\epsilon_{b+}-\mu_BH}\right\}+\frac{T}{2N}\sum_{\mathbf{k},l}\left\{\frac{1}{i\nu_l-\epsilon_a+\mu_BH}-\frac{1}{i\nu_l-\epsilon_a-\mu_BH}+\frac{3}{i\nu_l-\epsilon_{b+}+\mu_BH}-\frac{3}{i\nu_l-\epsilon_{b+}-\mu_BH}\right\}. \tag{A23}$$

The summation over $\mathbf{k}$ is made using

$$\frac{1}{V}\sum_{\mathbf{k}}F(\mathbf{k})=\frac{\rho_{eh}}{8}\int_{-\epsilon_0}^{\epsilon_0}dzF(z), \tag{A24}$$

where $\epsilon_a=z$ and $\epsilon_{b+}=z_0/2-z$ are the linearized quasiparticle energies and $\rho_{eh}/8$ is the density-of-states for a single spin on a single electron or hole Fermi surface. But for the field in the perpendicular direction, each Green's function depends on H only through one of the combinations $z-\mu_BH$ or $z+\mu_BH$. So the integration over z wipes out the field dependence of the first set of terms. It follows that $\Delta M_z=(V/2N)\rho_{eh}\mu_BH$ and

$$\chi_\perp=\mu_B^2\frac{V}{N}\rho_{eh}, \tag{A25}$$

which is unchanged by the spin ordering. The same result may be obtained for a S SDW when the field is in the xy plane.

2. Parallel susceptibility

For the field along the x axis, *parallel* to the ordering wave vector $\mathbf{Q}_x$ and in the plane of the spins of the D SDW, the Green's functions obey the spin symmetries

$$G_{\alpha\beta,aa}=\delta_{\alpha\beta}E_{aa}+\sigma^x_{\alpha\beta}F_{aa}, \tag{A26}$$

$$G^x_{\alpha\beta,ab}=\sigma^x_{\alpha\beta}E^x_{ab}+\delta_{\alpha\beta}F^x_{ab}, \tag{A27}$$

$$G^y_{\alpha\beta,ab}=\sigma^y_{\alpha\beta}E^y_{ab}-i\sigma^z_{\alpha\beta}F^y_{ab}, \tag{A28}$$

$$G^x_{\alpha\beta,ba}=\sigma^x_{\alpha\beta}E^x_{ab}+\delta_{\alpha\beta}F^x_{ab}, \tag{A29}$$

$$G^y_{\alpha\beta,ba}=\sigma^y_{\alpha\beta}E^y_{ab}+i\sigma^z_{\alpha\beta}F^y_{ab}, \tag{A30}$$

$$G^\gamma_{\alpha\beta,bb}=\delta_{\alpha\beta}E^\gamma_{bb}+\sigma^x_{\alpha\beta}F^\gamma_{bb}, \tag{A31}$$

$$G^{xy}_{\alpha\beta,bb'}=i\sigma^z_{\alpha\beta}E^{xy}_{bb'}+\sigma^y_{\alpha\beta}F^{xy}_{bb'}, \tag{A32}$$

$$G^{yx}_{\alpha\beta,bb'}=i\sigma^z_{\alpha\beta}E^{yx}_{bb'}+\sigma^y_{\alpha\beta}F^{yx}_{bb'}. \tag{A33}$$

Upon solving the equations of motion, we find

$$E_{aa}\pm F_{aa}=\frac{(i\nu_l-\epsilon_{b+})^2-(\mu_BH)^2}{D_3(\mp H)}, \tag{A34}$$

$$E^x_{ab}\pm F^x_{ab}=\frac{1}{\sqrt{2}}\frac{\Delta(i\nu_l-\epsilon_{b+}\mp\mu_BH)}{D_3(\mp H)}, \tag{A35}$$

$$E^y_{ab}\pm F^y_{ab}=\frac{1}{\sqrt{2}}\frac{\Delta(i\nu_l-\epsilon_{b+}\mp\mu_BH)}{D_3(\pm H)}, \tag{A36}$$

$$E^x_{bb}\pm F^x_{bb}=\frac{1}{2}\frac{1}{i\nu_l-\epsilon_{b+}\pm\mu_BH}+\frac{1}{2}\frac{(i\nu_l-\epsilon_a\pm\mu_BH)(i\nu_l-\epsilon_{b+}\mp\mu_BH)}{D_3(\mp H)}\mp\frac{\mu_BH}{2}\frac{\Delta^2}{(i\nu_l-\epsilon_{b+}\pm\mu_BH)D_3(\mp H)}, \tag{A37}$$

$$E^y_{bb}\pm F^y_{bb}=\frac{1}{2}\frac{1}{i\nu_l-\epsilon_{b+}\pm\mu_BH}+\frac{1}{2}\frac{(i\nu_l-\epsilon_a\mp\mu_BH)(i\nu_l-\epsilon_{b+}\mp\mu_BH)}{D_3(\pm H)}\mp\frac{\mu_BH}{2}\frac{\Delta^2}{(i\nu_l-\epsilon_{b+}\pm\mu_BH)D_3(\pm H)}, \tag{A38}$$

$$E^{xy}_{bb'}\pm F^{xy}_{bb'}=\frac{1}{2}\frac{\Delta^2}{D_3(\mp H)}, \tag{A39}$$

$$E^{yx}_{bb'}\pm F^{yx}_{bb'}=-\frac{1}{2}\frac{\Delta^2}{D_3(\pm H)}, \tag{A40}$$

where

$$D_3(H)=(i\nu_l-\epsilon_a-\mu_BH)[(i\nu_l-\epsilon_{b+})^2-(\mu_BH)^2]-\Delta^2(i\nu_l-\epsilon_{b+}). \tag{A41}$$

It follows that

$$\Delta M_x=\frac{T}{N}\sum_{l,\mathbf{k}}\left\{F(\mathbf{k},i\nu_l)_{aa}+F(\mathbf{k},i\nu_l)^x_{bb}+F(\mathbf{k},i\nu_l)^y_{bb}\right.$$
$$-\frac{1}{2}\frac{1}{i\nu_l-\epsilon_a+\mu_BH}+\frac{1}{2}\frac{1}{i\nu_l-\epsilon_a-\mu_BH}$$
$$\left.-\frac{1}{i\nu_l-\epsilon_{b+}+\mu_BH}+\frac{1}{i\nu_l-\epsilon_{b+}-\mu_BH}\right)$$
$$+\frac{T}{2N}\sum_{\mathbf{k},l}\left\{\frac{1}{i\nu_l-\epsilon_a+\mu_BH}-\frac{1}{i\nu_l-\epsilon_a-\mu_BH}\right.$$
$$\left.+\frac{3}{i\nu_l-\epsilon_{b+}+\mu_BH}-\frac{3}{i\nu_l-\epsilon_{b+}-\mu_BH}\right\}. \quad \text{(A42)}$$

The first summation may be evaluated to linear order in the magnetic field using

$$D_3(H=0)=(i\nu_l-\epsilon_{b+})D_2(H=0)$$
$$=-(i\nu_l-z_0/2+z)(z-z_{1l})(z-z_{2l}), \quad \text{(A43)}$$

$$z_{1l}=\frac{z_0}{4}+\sqrt{(i\nu_l-z_0/4+\mu_BH)^2-\Delta^2}, \quad \text{(A44)}$$

$$z_{2l}=\frac{z_0}{4}-\sqrt{(i\nu_l-z_0/4+\mu_BH)^2-\Delta^2}. \quad \text{(A45)}$$

The square root is defined so that $\mathrm{sgn}\,(\mathrm{Im}z_{1l})=\mathrm{sgn}(\nu_l)$. After performing the z integral, we find for a D SDW

$$\chi_\parallel=\mu_B^2\frac{V}{N}\rho_{eh}\left\{1+\frac{\pi i}{8}T\sum_l\ \mathrm{sgn}(\nu_l)\left[\frac{\Delta^2}{(-\tilde{\nu}_l^2-\Delta^2)^{3/2}}\right.\right.$$
$$\left.\left.+\frac{4}{\sqrt{-\tilde{\nu}_l^2-\Delta^2}}+\frac{8}{\Delta^2}(\sqrt{-\tilde{\nu}_l^2-\Delta^2}-i\tilde{\nu}_l)\right]\right\}, \quad \text{(A46)}$$

where $i\tilde{\nu}_l=i\nu_l-z_0/4$.

The analogous result for a S SDW is

$$\chi_\parallel=\mu_B^2\frac{V}{N}\rho_{eh}\left\{1+\frac{\pi i}{2}\Delta^2T\sum_l\ \frac{\mathrm{sgn}(\nu_l)}{(-\tilde{\nu}_l^2-\Delta^2)^{3/2}}\right\}. \quad \text{(A47)}$$

By comparison, the parallel susceptibility for a commensurate, bcc Cr alloy[2] is given by the same result without the factor of 1/2 in front of the Matsubara sum. For a T SDW, we obtain

$$\chi_\parallel=\mu_B^2\frac{V}{N}\rho_{eh}\left\{1+\frac{\pi i}{18}T\sum_l\ \mathrm{sgn}(\nu_l)\left[\frac{\Delta^2}{(-\tilde{\nu}_l^2-\Delta^2)^{3/2}}\right.\right.$$
$$\left.\left.+\frac{8}{\sqrt{-\tilde{\nu}_l^2-\Delta^2}}+\frac{16}{\Delta^2}(\sqrt{-\tilde{\nu}_l^2-\Delta^2}-i\tilde{\nu}_l)\right]\right\}. \quad \text{(A48)}$$

In the limit of zero temperature, the parallel susceptibilities can be explicitly evaluated:

$$\chi_\parallel\to\frac{1}{2}\mu_B^2\frac{V}{N}\rho_{eh} \quad \text{S SDW}, \quad \text{(A49)}$$

$$\chi_\parallel\to\mu_B^2\frac{V}{N}\rho_{eh}\left\{\frac{5}{8}+\frac{1}{32}\left(\frac{z_0}{\Delta}\right)^2\right\} \quad \text{D SDW}, \quad \text{(A50)}$$

$$\chi_\parallel\to\mu_B^2\frac{V}{N}\rho_{eh}\left\{\frac{13}{18}+\frac{1}{36}\left(\frac{z_0}{\Delta}\right)^2\right\} \quad \text{T SDW}. \quad \text{(A51)}$$

For commensurate Cr alloys, the absence of the factor of 1/2 in Eq. (A47) implies that $\chi_\parallel\to0$ as $T\to0$.

APPENDIX B: LINEAR-RESPONSE THEORY

We now confirm the results of the previous appendix for $\chi_\perp$ and $\chi_\parallel$ of the D SDW state using linear-response theory.

1. Perpendicular susceptibility

Starting with the definition $\Delta M_z=(1/N)\Sigma_i\langle S_{iz}\rangle$, we find

$$\chi_\perp=2\mu_B\left.\frac{\partial\Delta M_z}{\partial H_z}\right|_{\mathbf{H}=0}=\frac{4\mu_B^2}{N}\int_0^\beta d\tau\sum_{i,j}\ \langle T_\tau S_{iz}(\tau)S_{jz}(0)\rangle. \quad \text{(B1)}$$

Employing Eq. (20) for the spin operator, applying Wick's theorem, and substituting the spin-dependent Green's functions, we obtain

$$\chi_\perp=-\frac{2\mu_B^2}{N}T\sum_{\mathbf{k},l}\{E(\mathbf{k},i\nu_l)^2_{aa}+E(\mathbf{k},i\nu_l)^{x2}_{bb}+E(\mathbf{k},i\nu_l)^{y2}_{bb}$$
$$+E(\mathbf{k},i\nu_l)^{z2}_{bb}-2E(\mathbf{k},i\nu_l)^{x2}_{ab}-2E(\mathbf{k},i\nu_l)^{y2}_{ab}$$
$$-2E(\mathbf{k},i\nu_l)^{xy}_{bb'}E(\mathbf{k},i\nu_l)^{yx}_{bb'}\}$$
$$=-\frac{2\mu_B^2}{N}T\sum_{\mathbf{k},l}\left\{\frac{1}{(i\nu_l-\epsilon_a)^2}+\frac{3}{(i\nu_l-\epsilon_{b+})^2}\right\}$$
$$-\frac{2\mu_B^2}{N}T\sum_{l,\mathbf{k}}\left\{\frac{(i\nu_l-\epsilon_{b+})^2}{{D_2}^2}+\frac{1}{2}\left(\frac{1}{i\nu_l-\epsilon_{b+}}+\frac{i\nu_l-\epsilon_a}{D_2}\right)^2\right.$$
$$-\frac{2\Delta^2}{{D_2}^2}+\frac{\Delta^4}{2}\frac{1}{{D_2}^2}\frac{1}{(i\nu_l-\epsilon_{b+})^2}-\frac{1}{(i\nu_l-\epsilon_a)^2}$$
$$\left.-\frac{2}{(i\nu_l-\epsilon_{b+})^2}\right\}, \quad \text{(B2)}$$

where the order of the $\mathbf{k}$ and ν_l summations has been reversed in the last set of terms. After performing the complex integral over z, we find that the last set of terms vanishes and $\chi_\perp=\mu_B^2\rho_{eh}V/N$, as expected.

2. Parallel susceptibility

For the parallel susceptibility, we use

$$\chi_\parallel=2\mu_B\left.\frac{\partial\Delta M_x}{\partial H_x}\right|_{\mathbf{H}=0}=\frac{4\mu_B^2}{N}\int_0^\beta d\tau\sum_{i,j}\ \langle T_\tau S_{ix}(\tau)S_{jx}(0)\rangle. \quad \text{(B3)}$$

Applying the same manipulations as above, we find that

$$\chi_{\|}=-\frac{2\mu_B^2}{N}T\sum_{\mathbf{k},l}\{E(\mathbf{k},i\nu_l)^2_{aa}+E(\mathbf{k},i\nu_l)^{x2}_{bb}+E(\mathbf{k},i\nu_l)^{y2}_{bb}$$
$$+E(\mathbf{k},i\nu_l)^{z2}_{bb}+2E(\mathbf{k},i\nu_l)^{x2}_{ab}-2E(\mathbf{k},i\nu_l)^{y2}_{ab}$$
$$+2E(\mathbf{k},i\nu_l)^{xy}_{bb'}E(\mathbf{k},i\nu_l)^{yx}_{bb'}\}$$
$$=-\frac{2\mu_B^2}{N}T\sum_{\mathbf{k},l}\left\{\frac{1}{(i\nu_l-\epsilon_a)^2}+\frac{3}{(i\nu_l-\epsilon_{b+})^2}\right\}$$
$$-\frac{2\mu_B^2}{N}T\sum_{l,\mathbf{k}}\left\{\frac{(i\nu_l-\epsilon_{b+})^2}{{D_2}^2}+\frac{1}{2}\left(\frac{1}{i\nu_l-\epsilon_{b+}}+\frac{i\nu_l-\epsilon_a}{D_2}\right)^2\right.$$
$$\left.-\frac{\Delta^4}{2}\frac{1}{{D_2}^2}\frac{1}{(i\nu_l-\epsilon_{b+})^2}-\frac{1}{(i\nu_l-\epsilon_a)^2}-\frac{2}{(i\nu_l-\epsilon_{b+})^2}\right\}. \tag{B4}$$

After performing the complex integral over z, we obtain precisely the same result as in Eq. (A46). Considering the general susceptibility $\partial\Delta M_i/\partial H_j$, off-diagonal terms with $i\neq j$ vanish because $\mathrm{Tr}(\underline{\sigma}^i\underline{\sigma}^k\underline{\sigma}^j\underline{\sigma}^k)=2\delta_{ij}(2\delta_{jk}-1)$.

3. Energy gap

Linear-response theory can also be used to verify that the energy gap is unaffected by the magnetic field. Starting with the definition of the gap tensor

$$\Delta^{\gamma}_{\alpha\beta}=-\frac{U}{V}\sum_{\mathbf{k}}\langle b^{\dagger}_{\mathbf{k}+\mathbf{Q}_\gamma,\beta}a_{\mathbf{k}\alpha}\rangle, \tag{B5}$$

we find that

$$\left.\frac{\partial\Delta^{\gamma}_{\alpha\beta}}{\partial H_x}\right|_{\mathbf{H}=0}=-\frac{\mu_B U}{V}\sum_{\mathbf{k},\mathbf{k}'}\int_0^{\beta}d\tau\langle T_\tau[a^{\dagger}_{\mathbf{k}'\delta}(\tau)$$
$$+b^{\dagger}_{\mathbf{k}'\delta}(\tau)]\sigma^x_{\delta\nu}[a_{\mathbf{k}'\nu}(\tau)$$
$$+b_{\mathbf{k}'\nu}(\tau)]b^{\dagger}_{\mathbf{k}+\mathbf{Q}_\gamma,\beta}(0)a_{\mathbf{k}\alpha}(0)\rangle. \tag{B6}$$

So for a D SDW,

$$\left.\frac{\partial\Delta^{x}_{\alpha\beta}}{\partial H_x}\right|_{\mathbf{H}=0}=\delta_{\alpha\beta}\frac{\mu_B U}{V}T\sum_{\mathbf{k},l}\{E(\mathbf{k},i\nu_l)_{bb}E(\mathbf{k},i\nu_l)_{ab}$$
$$+E(\mathbf{k},i\nu_l)_{ab}E(\mathbf{k},i\nu_l)_{aa}$$
$$-E(\mathbf{k},i\nu_l)^{xy}_{bb'}E(\mathbf{k},i\nu_l)_{ab}\}, \tag{B7}$$

$$\left.\frac{\partial\Delta^{y}_{\alpha\beta}}{\partial H_x}\right|_{\mathbf{H}=0}=i\sigma^z_{\alpha\beta}\frac{\mu_B U}{V}T\sum_{\mathbf{k},l}\{-E(\mathbf{k},i\nu_l)_{bb}E(\mathbf{k},i\nu_l)_{ab}$$
$$+E(\mathbf{k},i\nu_l)_{ab}E(\mathbf{k},i\nu_l)_{aa}$$
$$+E(\mathbf{k},i\nu_l)^{xy}_{bb'}E(\mathbf{k},i\nu_l)_{ab}\}, \tag{B8}$$

whereas $\partial\Delta^z_{\alpha\beta}/\partial H_x|_{\mathbf{H}=0}=0$. Since both summations are well-defined in the limit $\epsilon_0\to\infty$, both derivatives are of order $\Delta\mu_B U\rho_{eh}/T_N^{\star}\sim\Delta\mu_B(NU/V)/\epsilon_F T_N^{\star}$. Formally, the $\epsilon_0\to\infty$ limit corresponds to the $U\to 0$ limit with a fixed $T_N^{\star}$ in Eq. (29). So the field dependence of the energy-gap tensor can be ignored.

Surprisingly, a direct application of Eq. (17) for the gap tensor, together with Eqs. (A27), (A28), (A35), and (A36) for $G(\mathbf{k},i\nu_l)^{\gamma}_{\alpha\beta,ab}$, would lead to an entirely different conclusion: that an external field changes the gap by a term of order $\Delta\mu_B H/T_N^{\star}$ rather than of order $\Delta\mu_B H(NU/V)/T_N^{\star}\epsilon_F$. This erroneous result comes applying the RPA too soon. Within linear-response theory, it would arise from using the RPA rather than the exact Hamiltonian in the expectation value $\langle A\rangle=\mathrm{Tr}[A\exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)]$ of Eq. (B5) prior to differentiating with respect to $\mathbf{H}$.

[1] See, for example, Kei Yosida, *Theory of Magnetism* (Springer-Verlag, Berlin, 1996).
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