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The magnetic field and spin dependence of quasi-particle mass enhancements in CeB_6

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The field and spin dependence of the quasi-particle mass enhancements are examined in the paramagnetic and ferromagnetic states close to a quantum critical point. The down-spin quasi-particles are found to have heavier masses than the up-spin quasi-particles. It is also found that the spin dependence of the quasi-particles. It is also found that the spin dependence of the quasi-particle mass enhancements is through a factor of the inverse (spin dependent) Fermi wave vector. The mass enhancements drop to the spin independent value of unity at sufficiently high fields, where the magnetization starts to saturate and spin-flip scattering is suppressed. The results are compared with experimental results on CeB_6.

1. Introduction

The subject of the spin dependence of the quasi-particle mass renormalizations has been the subject of recent interest. It has been noticed that in strong magnetic fields, the quasi-particle mass enhancements are spin and field dependent. CeB_6 has been classified as a heavy fermion compound as it shows a large logarithmic temperature variation of the resistivity at high temperatures [1, 2]. The material has a cubic structure and the lowest energy crystal field level has been identified as the Γ_8 quartet [3]. The Γ_8 level has a magnetic moment and an electric quadrupole moment. The material undergoes magnetic and quadrupole transitions at $T_N \approx 2.4$ and $T_Q \approx 3.3$ K [4]. High field de Haas–van Alphen measurements on $Ce_xLa_{1-x}B_6$ for $x < 0.05$, showed that the observed de Hass–van Alphen oscillations originated from two spin components of the Fermi surface, but for $x > 0.05$ the amplitude for one component gradually decreased without any change in topology of the Fermi surface [5]. For $x = 1$, CeB_6 only showed oscillations originating from one spin component of the Fermi surface [6]. An analysis of the amplitude of the harmonics, for $x < 0.05$, suggested that the down-spin sheet of the Fermi surface had the larger mass enhancement and had larger scattering rates [7]. Furthermore for $x > 0.05$, it was concluded that the quasi-particle mass of the spin-down sheet of the Fermi surface became so heavy it could no longer be seen. Similar effects could also be anticipated to occur in

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weak ferromagnets such as $ZrZn_2$ [8, 9]. For the materials under consideration, it is expected that the k dependence of the self-energy is negligible. In fact, the dynamical mean-field approximation (DMFT), where the self-energy is completely k-independent, has often been used to describe the properties of strongly correlated electron systems such as the quasi-particle peak in the electronic excitation spectrum [10]. In the DMFT approximation, the quasi-particle mass renormalization is identical to the wave function renormalization [11].

In this note we shall display the field dependence and spin dependence of the quasi-particle mass renormalization, calculated for the single-band Hubbard model within the Random Phase Approximation (RPA) for both weak-ferromagnetic and paramagnetic phases. The use of the RPA near the quantum critical point is justified in terms of the results obtained by Hertz [12] using a renormalization group analysis. We find the Goldstone modes of the ferromagnet do not appreciably contribute to the electronic self-energy. This finding implies that the physics of the ferromagnetic side of the quantum critical point should be extremely similar to that of the paramagnetic side. It is found that the self-energy near the Fermi energy is only slightly dependent on k, and the quasi-particle mass renormalization is spin dependent and is governed by the frequency dependence of the real part of the self-energy. This suggests that the region of applicability of the DMFT approximation might extend into the weakly ferromagnetic phase.

2. Quasi-particle mass enhancements

The system is described by the Hamiltonian

$$\hat{H} = \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{1}$$

where ε_k describes the dispersion relation of the Bloch states of non-interacting electrons, and U represents the strength of a short-ranged repulsive Coulomb interaction between pairs of electrons. Unlike the work of Edwards and Green [13] or of Wassermann *et al.* [14], the model we use does not invoke two types of electronic states (albeit hybridized) and does not assume strong spin–orbit scattering. Therefore, unlike their work, we do not expect to find a metamagnetic transition caused by a large Zeeman field splitting which removes states with local character from the Fermi energy.

We apply a magnetic field H parallel to the z-axis, so a magnetization $M(H)$ develops along this direction and the continuous spin-rotational symmetry of the Hamiltonian is broken. In the mean-field theory developed by Stoner [15–17] and applied by Wohlfarth and coworker [18, 19], the Coulomb interaction is expressed as

$$\begin{aligned} U\hat{n}_\uparrow \hat{n}_\downarrow = {} & U(\hat{n}_\uparrow - \bar{n}_\uparrow)(\hat{n}_\downarrow - \bar{n}_\downarrow) \\ & + U\hat{n}_\uparrow \bar{n}_\downarrow + U\bar{n}_\uparrow \hat{n}_\downarrow - U\bar{n}_\uparrow \bar{n}_\downarrow \end{aligned} \tag{2}$$

The first term on the right hand side is the fluctuation term which is to be subsequently neglected. The linearization of the interaction has the effect of producing a rigid spin dependent shift of the electronic bands. The electronic sub-band of spin σ is shifted by an energy of $U\bar{n}_{-\sigma} - \mu_B H\sigma$, which depends on the magnetic field H and the total occupation number, per site, of electrons with spin $-\sigma$. This shift produces an exchange splitting, Δ, between the sub-bands. The exchange splitting is defined by

$$\Delta = UM(H) = U(\bar{n}_\uparrow - \bar{n}_\downarrow) \tag{3}$$

The spontaneous magnetization is obtained from the self-consistent solution of the mean-field equations

$$\bar{n}_\uparrow - \bar{n}_\downarrow = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\left[\rho\left(\varepsilon + \frac{\Delta}{2} + \mu_B H\right) - \rho\left(\varepsilon - \frac{\Delta}{2} - \mu_B H\right)\right] \tag{4}$$

and

$$\bar{n}_\uparrow + \bar{n}_\downarrow = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\left[\rho\left(\varepsilon + \frac{\Delta}{2} + \mu_B H\right) + \rho\left(\varepsilon - \frac{\Delta}{2} - \mu_B H\right)\right] \tag{5}$$

in which $\rho(\varepsilon)$ is the one-electron density of states, per spin, per site. At $T=0$ and $H=0$, these equations only have a paramagnetic solution $M(0)=0$ for values of U less than the critical value U_c. For U greater than U_c, the ferromagnetic state with $M(0)\neq 0$ has lower energy than the paramagnetic state. As shown by Stoner [15–17], the critical value U_c is determined by

$$U_c \rho(\mu) = 1 \tag{6}$$

This critical value of $U=U_c$ determines the quantum critical point, at which the paramagnetic state becomes unstable to the ferromagnetic state at $T=0$. The non-trivial ferromagnetic solution of the self-consistency equations are found for $U > U_c$. In the ferromagnetic state, the up-spin sub-band is depressed by an energy of $-(\Delta/2)$, while the down-spin sub-band is raised by an energy of $\Delta/2$. Thus, in zero-field, ferromagnetism produces a spontaneous splitting between the up-spin and down-spin Fermi surfaces. The dependence of the magnetization $M(H)$ on the applied field is shown in figure 1. In the ferromagnetic state, $M(H)$ is reasonably well described by the $T\to 0$ limit of the Edwards–Wohlfarth equation [19]

$$\left(\frac{M(H)}{M(0)}\right)^2 = 1 + \frac{2\rho(\mu)}{U\rho(\mu) - 1}\frac{\mu_B H}{M(H)} \tag{7}$$

where $M(0)$ is the value of the spontaneous magnetization, and the coefficient of $\mu_B H/M(H)$ is twice the uniform static longitudinal susceptibility $\chi^{z,z}(0,0)$ of the magnetically ordered state.

The self-energy due to the emission and absorption of transverse spin fluctuations is calculated within RPA [20–22]. The RPA approach is justified by appealing to the renormalization group approach of Hertz [12]. Hertz showed that, near the quantum critical point, since the system is above its upper critical dimension, it is governed by a mean-field fixed point, with the Gaussian fluctuations about the

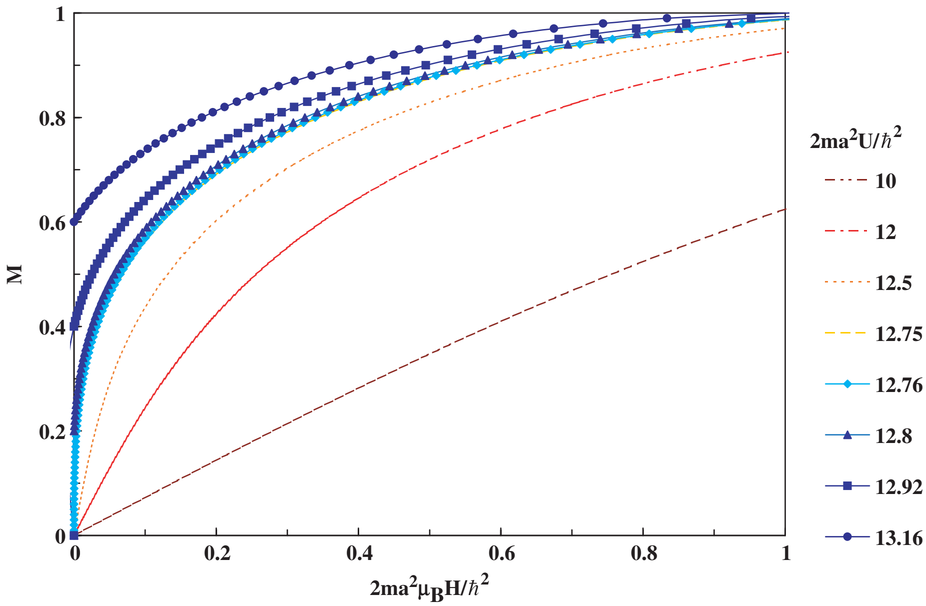

Figure 1. The magnetic field dependence of the magnetization $M(H)$ (in units of the Bohr magneton μ_B), for various values of U. The critical value of U_c is given by 12.761, so the largest value of the applied field shown corresponds to a Zeeman energy of the order of one-tenth of the width of the occupied band. The $M(H)$ curves corresponding to ferromagnetic states in applied fields are denoted by (decorated) solid lines.

fixed point. The Gaussian fluctuations about the mean-field fixed point are in a one to one correspondence with the paramagnon excitations found in the RPA around the Hartree–Fock fixed point. Thus, the recently developed understanding of quantum critical points shows that the RPA approach has the correct functional form to describe the physics close to the magnetic instability. It shall be noted that for a weak-ferromagnet [23], the Goldstone modes connected with the broken spin-rotational invariance [24, 25] do not appreciably contribute to the mass enhancements. It is found that the self-energy is dominated by the resonance in the continuum of Stoner spin-flip excitations. As a result of the diffuse and damped nature of the excitations, the resulting self-energy is a smooth function of k near the spin-split Fermi surfaces. However, the self-energy is rapidly varying as a function of frequency. The spin dependent wave function renormalizations are defined by

$$Z_\sigma(H) = 1 - \frac{\partial}{\partial\omega}\sum_\sigma(\omega, k_{F\sigma})\bigg|_{\omega=0} \tag{8}$$

Since the self-energy is roughly independent of k near the Fermi surface, the quasi-particle mass enhancements are given by $Z_\sigma(H)$. The mass enhancements are calculated from the expression

$$\frac{\partial}{\partial\omega}\sum_{\sigma}(\omega,k_{F\sigma})\bigg|_{\omega=0} = -\frac{U^2a^3}{(2\pi)^2}\frac{m}{\hbar^2 k_{F\sigma}}\int_{k_{F\uparrow}-k_F}^{k_{F\uparrow}+k_{F\downarrow}} dq\,q\int_{-\infty}^{\infty}\frac{d\nu}{\pi}\frac{\mathrm{Im}\,\chi^{\sigma,-\sigma}(\nu+i\eta,q)}{\nu}$$
$$-\frac{U^2a^3}{(2\pi)^2}\frac{m}{\hbar^2 k_{F\sigma}}\int_0^{\infty} dq\,q\int_0^{\infty}\frac{d\nu}{\pi}\mathrm{Im}\,\chi^{\sigma,-\sigma}(\nu+i\eta,q)$$
$$\times\left[\frac{\Theta\left(e_{k_{F-\sigma}}-e_{k_{F\sigma-q}}\right)}{e_{k_{F\sigma-q}}-e_{k_{F-\sigma}}-\nu}-\frac{\Theta\left(e_{k_{F-\sigma}}-e_{k_{F\sigma+q}}\right)}{e_{k_{F\sigma+q}}-e_{k_{F-\sigma}}-\nu}\right]$$
$$+\frac{U^2a^3}{(2\pi)^2}\frac{m}{\hbar^2 k_{F\sigma}}\int_0^{\infty} dq\,q\int_{-\infty}^{0}\frac{d\nu}{\pi}\mathrm{Im}\,\chi^{\sigma,-\sigma}(\nu+i\eta,q)$$
$$\times\left[\frac{\Theta\left(e_{k_{F\sigma-q}}-e_{k_{F-\sigma}}\right)}{e_{k_{F\sigma-q}}-e_{k_{F-\sigma}}-\nu}-\frac{\Theta\left(e_{k_{F\sigma+q}}-e_{k_{F-\sigma}}\right)}{e_{k_{F\sigma+q}}-e_{k_{F-\sigma}}-\nu}\right] \tag{9}$$

where $\chi^{\sigma,-\sigma}(\nu,q)$ is the transverse dynamic susceptibility. Within RPA, in the magnetically ordered phase at zero field, the imaginary part of the transverse susceptibility contains a delta function contribution with strength M at positive energies corresponding to the spin wave pole

$$\hbar\nu_q = Dq^2 \tag{10}$$

where D is the spin-wave stiffness constant [24] and is given by

$$D = \frac{U}{3N\Delta}\sum_k\left[\left(\frac{f_{k\uparrow}+f_{k\downarrow}}{2}\right)\nabla^2\varepsilon_k - \left(\frac{f_{k\uparrow}-f_{k\downarrow}}{\Delta}\right)|\nabla\varepsilon_k|^2\right]. \tag{11}$$

This branch of modes are the Goldstone excitations which dynamically restore the spontaneously broken spin-rotational invariance. This branch of excitations only exists for a range of small q and positive frequencies, where

$$e_{k_{F\uparrow-q}} - e_{k_{F\downarrow}} > 0. \tag{12}$$

It is seen that, due to the above kinematic restriction, the Goldstone modes do not contribute to the mass enhancements. The first term of equation (9) contains the singular part of the mass enhancement and it can be written in the form

$$-\frac{U^2a^3}{(2\pi)^2}\frac{m}{\hbar^2 k_{F\sigma}}\int_{k_{F\uparrow}-k_{f\downarrow}}^{k_{F\uparrow}+k_{F\downarrow}} dq\,q\,\mathrm{Re}\,\chi^{\sigma,-\sigma}(0+i\eta,q). \tag{13}$$

This expression also holds for paramagnetic materials close to the quantum critical point. If a magnetic field is applied, it induces a magnetization and, thereby, introduces a total spin-splitting of magnitude

$$\Delta + 2\mu_B H = \frac{2\mu_B H}{1 - U\rho(\mu)} \tag{14}$$

is the Stoner continuum. The exchange splitting acts to enhance the spin-splitting above the Zeeman splitting expected for non-interacting electrons. Therefore, for both paramagnetic and ferromagnetic phases, an applied magnetic field creates a sharp dispersive branch of massive spin waves that start at $q = 0$ with a frequency given by $\hbar\nu = 2\mu_B H$. That is, the spectrum contains a delta function branch at the spin wave pole $\hbar\nu_q = 2\mu_B H + Dq^2$. This branch of massive collective modes enters the Stoner continuum at a finite value of q, and for larger q values it exists as a broadened resonance. Therefore, in the presence of an applied magnetic field, one has

$$\mathrm{Re}\chi^{\sigma,\,\sigma}(0 + i\eta,\, q) \approx \frac{M}{2\mu_B H + Dq^2}. \tag{15}$$

This equation holds quite generally for small q and is independent of the type of model used, in that it can also be derived by a Landau–Ginzberg analysis for the case of a conserved vector order parameter. The above equation shows that the applied field magnetic suppresses spin-flip excitations. Using this result, one finds

$$\begin{aligned} Z_\sigma &\approx 1 - \frac{3k_F}{k_{F\sigma}} \ln\left(\frac{2\mu_B H + D(k_{F\uparrow} - k_{F\downarrow})^2}{2\mu_B H + D(k_{F\uparrow} + k_{F\downarrow})^2}\right) \\ &\approx 1 - \frac{3}{(1+\sigma M)^{1/3}} \ln\left(\frac{2\mu_B H_\rho(\mu) + (M/3)^3}{2\mu_B H_\rho(\mu) + (M/3)}\right) \end{aligned} \tag{16}$$

where k_F is the value of the Fermi wave vector for $M = 0$. The spin dependence of the singular part of the quasi-particle mass enhancements is entirely contained in a factor of the spin dependent Fermi momentum. The boundary terms in equation (9) are only important close to the fully polarized state where $M \sim 1$, in which case they have the effect of cancelling the singular part of the mass enhancement. This cancellation results in the quasi-particle masses for both spin-directions in becoming unrenormalized.

3. Discussion

The field dependence of Z_σ is shown in figure 2, for various values of U. The largest value of the field roughly corresponds to a tenth of the width of the occupied portion of the band. It is seen that for $M = 0$ the quasi-particle mass enhancements are spin independent. For the case where there is a finite value of the magnetization, the spin-rotational symmetry of the system is broken and, therefore, the physical properties become spin dependent. The dependence of the contribution of the correlations on the inverse of the spin dependent Fermi wave vector implies that the although the spin dependent quasi-particle masses may be observed directly

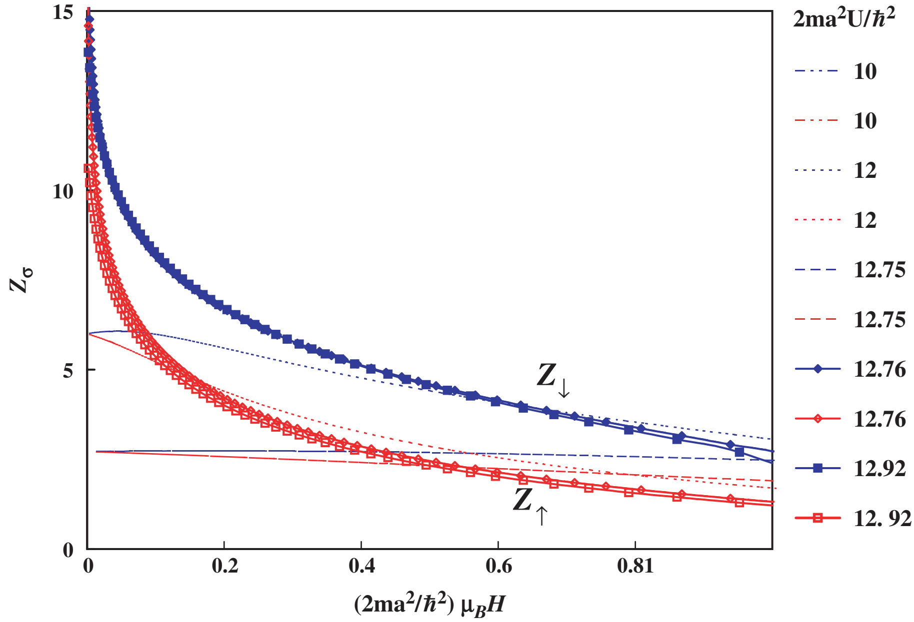

Figure 2. The spin dependent quasi-particle mass enhancements Z_σ as a function of the applied field. In the unpolarized state, the quasi-particle masses are spin independent, whereas they are spin dependent in spin-polarized states. In the ferromagnetic stats, the down-spin enhancements are denoted by the filled symbols, and the up-spin enhancement by the open symbols.

in de Haas–van Alphen experiments, the spin dependence of the correlations will not have any remnant effects on the low-temperature electronic specific heat.

The form of the field-dependence, shown in figure 2, depends strongly on the proximity to the critical point. For example, for a ferromagnet in zero field, the mass enhancement in equation (16) contains a singular term that diverges logarithmically as M approaches zero.

$$\begin{aligned} Z_\sigma &\approx 1 - \frac{6k_F}{k_{F\sigma}} \ln\left(\frac{k_{F\uparrow} - k_{F\downarrow}}{k_{F\uparrow} - k_{F\downarrow}}\right) \\ &\approx 1 - \frac{6}{(1+\sigma M)^{(1/3)}} \ln\left(\frac{M}{3}\right) \end{aligned} \tag{17}$$

as was previously derived by Brinkman and Engelseberg [22]. Whereas in the paramagnetic state where the terms of higher order in M can be neglected, the transverse fluctuations produce a contribution to the enhancement of the form

$$\approx +3 \ln\left(1 + \frac{1}{3(1 - U_\rho(\mu))}\right). \tag{18}$$

Due to the spin-rotational invariance of the paramagnetic phase, the longitudinal fluctuations also provide a contribution to the mass enhancement which differs from the above result only by a multiplicative factor of (1/2). Therefore, in the paramagnetic phase, one recovers the result of Doniach and Engelsberg [20] or Berk and Schrieffer [21]

$$Z = 1 + \frac{9}{2}\ln\left(1 + \frac{1}{3(1 + U_\rho(\mu))}\right). \tag{19}$$

Therefore, in zero field, the effective mass diverges as the quantum critical point is approached from both sides.

The effect of the applied magnetic field is that of increasing the magnetization which also suppresses the spin-flip excitations and thereby tends to reduce the mass enhancements. For a paramagnet in weak applied fields, the positive term linear in M in the expansion for the down-spin mass enhancement due to the spin-split Fermi surface, has the effect of producing a slight initial increase in the down-spin mass enhancement after which it goes through a maximum and then decreases as the spin-flip scattering is suppressed. For sufficiently strong fields, the mass enhancements of the enhanced paramagnetic almost show the same scaling with the magnetization as the ferromagnets, as can be seen in figure 3. The mass enhancements do not follow the singular contribution of equation (9) as $M \to 1$, since as the magnetization approaches saturation, the boundary terms in equation (16) become important.

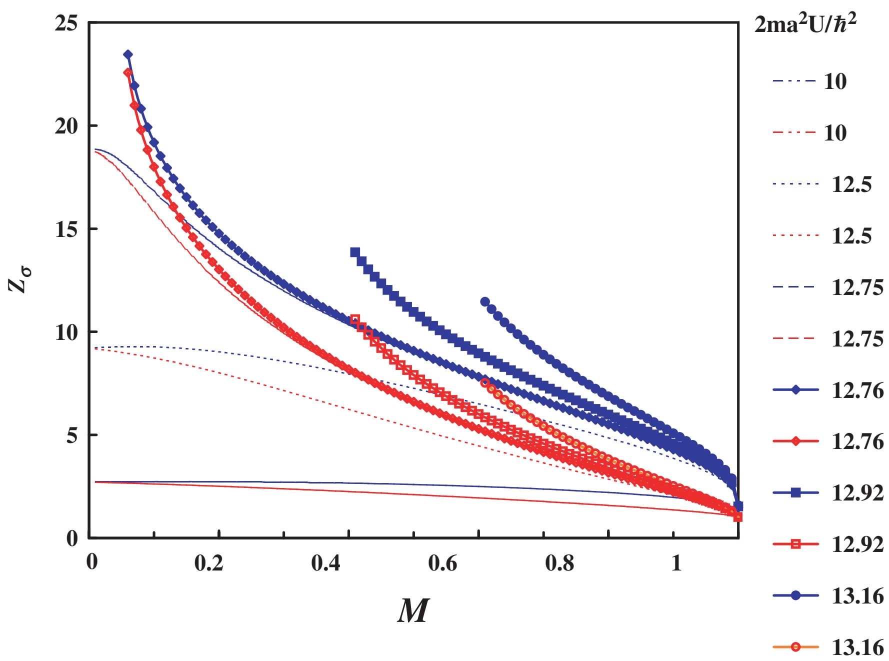

Figure 3. The mass enhancements as a function of magnetization. The legend is the same as in figures 1 and 2. It is seen that, in the ferromagnetic state, Z_σ almost scales with the magnetization. For sufficiently large magnetization, the spin-flip scattering and the effective masses are suppressed.

In this limit, the boundary terms cancel with the singular term causing the mass enhancements to drop to unity. Near the fully polarized limit, the effects of vertex corrections are anticipated to be large [26, 27]. However, the cancellation of the mass enhancements is expected from general arguments. The vanishing of the up-spin mass enhancements is expected since the fully polarized Stoner state is an exact eigenstate of the Hamiltonian, albeit not the groundstate, and remains an exact eigenstate even if the system has any number of up-spin electron excitations. Hence, the up-spin quasi-particle has a mass enhancement of unity for the fully polarized state. The case of down-spin excitations is more subtle, but also produces a down-spin quasi-particle mass enhancement of unity for the fully polarized state. In all cases, the mass enhancements are found to obey the inequality

$$Z_{\downarrow} \geq Z_{\uparrow} \tag{20}$$

showing that the down-spin quasi-particles are heavier than the up-spin quasi-particles.

The inequality between the up-spin and down-spin quasi-particle masses can be explained by using the ideas of Reynolds *et al*. [28] and of Klenjberg and Spalek [29] on the large U limit of the model. Using a Gutzwiller-like approximation, the effective tight-binding matrix element for an electron for spin σ to hop from site I to site j is given by

$$t_{\sigma,\,i\to j} = t_{i,j}\left(\frac{1-\bar{n}_j}{1-\bar{n}_{j,\sigma}}\right) \tag{21}$$

since the large value of the Coulomb interaction U prevents an electron from hopping onto the site j if it is already occupied. The factor in the denominator explicitly excludes double counting of the correlations due to the Pauli exclusion principle. Therefore, for a spatially homogeneous system, one finds that the dispersion of the quasi-particle bands is narrowed by a spin dependent factor and that

$$Z_{\sigma}(M) \approx \frac{1}{1-\bar{n}}\left[1-\frac{\bar{n}}{2}-\sigma\frac{M}{2}\right] \tag{22}$$

where $\bar{n}$ is the average number of electrons per site. Hence, the down-spin quasi-particles have higher effective masses than do the up-spin quasi-particles. Also, the down-spin mass may be expected to show an increase with increasing magnetization. These are in agreement with our findings and also with measurements of the de Haas–van Alphen oscillations in $Ce_xLa_{1-x}B_6$ [7]. However, as seen in figure 3, the magnetization dependence of the wave function renormalization found in our results is nonlinear and depends strongly on the proximity to either the ferromagnetic phase or to the fully polarized state, in contrast to the slave boson result.

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