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1990 J. Phys.: Condens. Matter 2 969

(http://iopscience.iop.org/0953-8984/2/4/016)

J. Phys.: Condens. Matter 2 (1990) 969–981. Printed in the UK

Temperature-dependent magnetic susceptibilities and magnetic moments of Ce heavy-fermion systems

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Received 7 November 1988, in final form 5 September 1989

Abstract. As a low-temperature model for Ce heavy-fermion systems with strong spin–orbit coupling ($J = \frac{5}{2}$), quasiparticle states are derived at low temperature across a crossover transition from the high-temperature regime using a finite-temperature Green-function decoupling method for the spin–orbit Anderson lattice Hamiltonian. In order to compare these quasiparticle states with those of the Zou–Anderson mean-field model, the low-temperature magnetic susceptibilities $\chi_q(T)$ ($q = 0$ and $q = Q$) and the effective magnetic moments of quasiparticles are calculated for the simple cubic lattice using these two approaches, and then compared with the experimental results.

1. Introduction

Recent experimental results indicate that an antiferromagnetic correlation is a characteristic phenomenon commonly observed in many heavy-fermion systems between the Kondo temperature T_K and the coherence temperature T_0. While an antiferromagnetic phase transition often takes place in uranium heavy-fermion compounds (URu_2Si_2 T_N = 17.5 K (Palstra *et al* 1985), UPt_3 T_N = 5 K (Aeppli *et al* 1988), UBe_{13} (Neumann *et al* 1986), U_2Zn_{17} T_N = 9.7 K (Broholm *et al* 1987a), etc.), only antiferomagnetic correlations are observed in the cerium compounds ($CeAl_3$ (Barth *et al* 1989), $CeCu_2Si_2$ (Uemura *et al* 1989), $CeCu_6$ (Gangopadhyay *et al* 1988), etc., except for $CeAl_2$ T_N = 3.58 K (Barbara *et al* 1977)) which remain normal heavy-fermion systems down to very low temperatures. It is known that the former heavy-fermion compounds generally have higher T_K values (30–70 K), whereas the latter ones have lower T_K values (~5 K). Therefore, to understand the low-temperature properties of a prototype heavy-fermion system it is important to study the temperature-dependent magnetic susceptibilities and magnetic moments of the Ce heavy-fermion compounds in comparison with those of the U compounds.

A theoretical model to describe the low-temperature quasiparticle states of Ce heavy-fermion systems is the spin–orbit-coupling Zou–Anderson (ZA) model. This model, which was derived as a mean-field model from a band-theory treatment of the Kondo-resonance phase shift by Zou and Anderson (1986), can also be obtained using the mean-field slave-boson approach in the spirit of the Gutzwiller approximation. Beyond the mean-field level one can, in principle, incorporate into this model the various quasiparticle interactions through the fluctuations of the slave-bosons and the constraint field (Auerbach *et al* 1988, Kaga and Yoshida 1989). However, in this approach it is extremely

0953-8984/90/040969 + 13 $03.50

hard to take properly into account finite-temperature effects as well as these fluctuations. Therefore, we adopt the finite-temperature Green-function approach of the spin–orbit-coupling Anderson lattice Hamiltonian for Ce heavy-fermion systems, which was earlier employed for the non-spin–orbit Anderson lattice model (Kaga *et al* 1988). Though the treatment of Coulomb interaction in this approach is still quite limited, the characteristic lattice self-energies can be obtained as a function of temperature and the heavy-fermion quasiparticle states can be derived after the crossover transition from the high-temperature regime (Kaga and Kubo 1987). Using the resulting quasiparticle Green functions of this approach and of the ZA model we calculate the temperature-dependent uniform and antiferromagnetic (staggered) susceptibilities at low temperatures and compare them with experiment.

An important question that has been posed regarding the ZA model (Zhang and Lee 1987, Aeppli and Varma 1987, Cox 1987) is whether or not the four non-hybridised linear combinations of the six f orbitals ($M = -\frac{5}{2}$–$\frac{5}{2}$, $J = \frac{5}{2}$) other than the hybridised quasiparticle doublets with pseudo-spins $\alpha = \pm 1$ can be raised to the renormalised f-level $\varepsilon_f = \mu_F + T_K$ close to the Fermi level μ_F after the renormalisation. This is because these non-hybridised levels could contribute to the non-negligible Van Vleck term in the magnetic susceptibility. Since the ZA model was derived essentially in the Gutzwiller approximation using the mean-field approach, whose renormalisation effect simply squashes the hybridisation matrix element and lifts the bare atomic f-level ε_f^0 to the Kondo-resonance level ε_f, this point was not clear, or rather the non-hybridised levels as well could have been taken to be similarly renormalised at low temperatures. It is therefore necessary to go one step beyond the mean-field approximation. We shall show that our finite-temperature approach sheds some light on this problem.

In this connection, we will demonstrate that the effective magnetic moments obtained for the Ce spin–orbit-coupling quasiparticle states are severely reduced from the free-ion values $\mu_{\rm eff} \simeq 2.54\ \mu_B$, which are observed at high temperatures. The calculated values are smaller for the antiferromagnetic moment than for the ferromagnetic one, and come close to the observed antiferromagnetically ordered moment ($CeAl_2$) and ordering moment ($CeAl_3$) of some Ce heavy-fermion compounds.

2. Two spin–orbit coupling models

Two quasiparticle models with spin–orbit coupling for the Ce heavy-fermion compounds are studied in order to calculate the temperature dependences of the magnetic susceptibilities $\chi_q(T)$ and magnetic moments for $\boldsymbol{q} = \boldsymbol{0}$ and $\boldsymbol{q} = \boldsymbol{Q} \equiv (\pi/a, \pi/a, \pi/a)$ of the simple cubic lattice. The first is the mean-field effective Hamiltonian for quasiparticles proposed by Zou and Anderson (1986) (ZA model), and the second is the $U = \infty$ spin–orbit Anderson lattice model (SA model), whose non-spin–orbit version has been studied in the Green-function-decoupling approach by Kaga *et al* (1988), Kaga and Kubo (1988) and others (Fedro and Sinha 1982, Baumgartel and Muller-Hartmann 1982, Costi 1985, Czycholl 1985), and is adapted here for spin–orbit coupling.

2.1. *The Zou–Anderson quasiparticle (ZA) model*

The Zou–Anderson (ZA) model can be considered as the slave-boson, mean-field Hamiltonian for quasiparticles with spin–orbit coupling, and is given by

$$H_{\rm ZA} = \sum_{k\sigma} \varepsilon(\boldsymbol{k}) c_{k\sigma}^{+} c_{k\sigma} + \varepsilon_f \sum_{iM} f_{iM}^{+} f_{iM} + (\mathrm{i}^3 \bar{b}_0/\sqrt{N_i}) \sum_{ikM\sigma} \{\alpha_{M\sigma}(\boldsymbol{k}) f_{iM}^{+} c_{k\sigma} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i] + \mathrm{HC}\} \qquad (1)$$

with the renormalised anisotropic hybridisation $i^3 b_0 \alpha_{M\sigma}(\boldsymbol{k})/\sqrt{N}$ at site R_i, where $i = \sqrt{-1}$ and b_0 is the mean-field slave-boson amplitude of order $b_0^2 \sim T_K D$ (D is half the conduction band width measured from its centre at energy zero), and the anisotropy coefficient $\alpha_{M\sigma}(\boldsymbol{k})$ is given by

$$\alpha_{M\sigma}(\boldsymbol{k}) = -(4\pi/3)^{1/2}\sigma[(7 - 2M\sigma)/14]^{1/2} Y_3^{M-\sigma/2}(\boldsymbol{k}). \tag{2}$$

Here, N_i is the number of lattice sites, M the z component of the spin-orbit angular momentum $\boldsymbol{J} = \boldsymbol{l} + \boldsymbol{s}$ ($J = \frac{5}{2}$), and $\sigma(= \pm 1)$ is the eigenvalue of the z component of the Pauli spin matrix σ. In the ZA model the quasiparticle states are formed around the renormalised f-level ε_f close to the Fermi level μ_F with the opening of a hybridisation gap for temperatures below the mean-field transition temperature T_K (the Kondo temperature); $\varepsilon_f = \mu_F + T_K$ at $T = 0$. The eigenstate $|\psi_\nu^\alpha(\boldsymbol{k})\rangle_{ZA}$ and the eigenvalue $E_\nu^{ZA}(\boldsymbol{k})$ of the Hamiltonian (1) are expressed as

$$|\psi_\nu^\alpha(\boldsymbol{k})\rangle_{ZA} = A_\nu^{ZA}(\boldsymbol{k})\left(|\boldsymbol{k}, \sigma\rangle + C_\nu^{ZA}(\boldsymbol{k}) \sum_{M=-5/2}^{M=5/2} \alpha_{M\sigma}^*(\boldsymbol{k})|\boldsymbol{k}, \tfrac{5}{2}, M\rangle\right) \tag{3}$$

$$E_\nu^{ZA}(\boldsymbol{k}) = \tfrac{1}{2}\{\varepsilon(\boldsymbol{k}) + \varepsilon_f + \nu[(\varepsilon(\boldsymbol{k}) - \varepsilon_f)^2 + 4b_0^2]^{1/2}\} \tag{4}$$

for the hybridised quasiparticle band with index $\nu (= \pm 1)$. The quasiparticle carries a pseudo-spin α ($= \pm 1$), which is comprised of the real conduction spin $\boldsymbol{s} = \frac{1}{2}\boldsymbol{\sigma}$ ($\sigma = \pm 1$ correspond to $\alpha = \pm 1$) in the intersite region and the f-orbital magnetic moment on Ce atoms; the latter, which must be compatible with the conduction spin $\boldsymbol{s}$ ($\boldsymbol{J} = \boldsymbol{l} + \boldsymbol{s}$), is given by the particular linear combination of the z components $M(= -\frac{5}{2}\text{–}\frac{5}{2})$ at each $\boldsymbol{k}$. Therefore, in this model the quasiparticle states of Ce heavy-fermion systems are represented by only the two-fold degenerate (with pseudo-spin $\alpha = \pm 1$) hybridised wavefunctions, corresponding to the Kramers doublets, with coherence factors $A_\nu^{ZA}(\boldsymbol{k})$ and $A_\nu^{ZA}(\boldsymbol{k})C_\nu^{ZA}(\boldsymbol{k})$, where $A_\nu^{ZA}(\boldsymbol{k}) = [1 + C_\nu^{ZA}]^{-1/2}$ and $C_\nu^{ZA}(\boldsymbol{k}) = b_0/[E_\nu^{ZA}(\boldsymbol{k}) - \varepsilon_f]$.

We consider the heavy-fermion states in which the Fermi level μ_F is situated near the top of the lower ($\nu = -$) hybridised band, i.e., $\mu_F = E_-(\boldsymbol{k}_F)$; $\mu_F = E_-(\varepsilon(\boldsymbol{k}_F))$ gives the conduction band energy as $\varepsilon(\boldsymbol{k}_F) = \mu_F + b_0^2/T_K$ ($T_K = \varepsilon_f - \mu_F$) which conveniently defines the Fermi surface. The hybridisation gap $E_g = E_+(0) - E_-(\boldsymbol{Q})$ is obtained as $E_g = 2T_K[\varepsilon(\boldsymbol{k}) - \mu_F]/(D - \mu_F) = 2b_0^2/(D - \mu_F)$.

The quasiparticle Green function for the ZA model is represented as the sum of the f- and conduction-electron components

$$\begin{aligned}\sum_{\nu=\pm} G_{\nu\alpha}^{ZA}(\boldsymbol{k}, \omega) &= \frac{1}{\omega - \varepsilon_f - b_0^2[\omega - \varepsilon(\boldsymbol{k})]^{-1}} + \frac{1}{\omega - \varepsilon(\boldsymbol{k}) - b_0^2[\omega - \varepsilon_f]^{-1}} \\ &= \sum_{\nu=\pm} \{[A_\nu^{ZA}(\boldsymbol{k})C_\nu^{ZA}(\boldsymbol{k})]^2/[\omega - E_\nu^{ZA}(\boldsymbol{k})] + (A_\nu^{ZA}(\boldsymbol{k}))^2/[\omega - E_\nu^{ZA}(\boldsymbol{k})]\} \\ &= \sum_{\nu=\pm} \frac{1}{\omega - E_\nu^{ZA}(\boldsymbol{k})}\end{aligned} \tag{5}$$

where the second-order effect of the anisotropic hybridisation $i^3 b_0 \alpha_{M\sigma}(\boldsymbol{k})$ leads to only the squared hybridisation strength b_0^2 in the denominator after taking the sum over M. The Green function in the spin–orbit ZA model is therefore of the same form as that of the non-spin–orbit isotropic hybridisation model. However, the expression for the magnetic susceptibility in the ZA model becomes different from that in the latter in terms of the effective magnetic moment, as we shall see later.

2.2. Quasiparticle states derived from the spin–orbit Anderson lattice (SA) model

In this section we show a derivation of quasiparticle Green functions from the bare particle spin–orbit-coupling Anderson lattice (SA) model for Ce heavy-fermion systems. For this purpose the same Green function decoupling scheme can be used as was employed for the non-spin–orbit model (Kaga *et al* 1988). Here, an important issue arises as to the heavy-fermion states formed under spin–orbit coupling; whether or not only the two degenerate hybridised f orbitals are renormalised and raised near the Fermi level μ_F to act as the quasiparticle states and contribute to the low-temperature properties of the heavy-fermion systems (Anderson and Zou 1987). There are other assertions (Zhang and Lee 1987, Aeppli and Varma 1987, Cox 1987) that the other four non-hybridised combinations of f orbitals are also renormalised contributing to the low-energy, heavy-fermion excitations. Our derivation of quasiparticle states in this section will shed some light on this issue.

The bare particle SA model is written as

$$H_{SA} = \sum_{k,\sigma} \varepsilon(k) c^{0+}_{k\sigma} c^{0}_{k\sigma} + \varepsilon^0_f \sum_{i,M} f^{0+}_{iM} f^{0}_{iM} + U \sum_{i,M=M'} f^{0+}_{iM} f^{0+}_{iM'} f^{0}_{iM'} f^{0}_{iM}$$
$$+ (i^3 V_0/\sqrt{N_i}) \sum_{ikM\sigma} [\alpha_{M\sigma}(\boldsymbol{k}) f^{0+}_{iM} c^0_{k\sigma} \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}_i) + \text{HC}], \tag{6}$$

where ε^0_f and V_0 are the deep bare f-electron level and the bare hybridisation, and f^0_{iM} and $c^0_{k\sigma}$ are the bare annihilation operators. The Coulomb repulsion U is taken here as infinitely large ($U = \infty$) for comparison with the Zou–Anderson model derived in the $U = \infty$ slave-boson approach. The eigenstates and eigenvalues of this Hamiltonian without the Coulomb term are written as

$$|\psi^\alpha_\nu(\boldsymbol{k})\rangle_0 = A^0_\nu(\boldsymbol{k})[\,|\boldsymbol{k}, \sigma\rangle_0 + C^0_\nu(\boldsymbol{k})|\boldsymbol{k}, \tfrac{5}{2}, \alpha\rangle_0] \tag{7}$$

$$|\boldsymbol{k}, \tfrac{5}{2}, \alpha\rangle_0 \sum_{M=-5/2}^{M=5/2} \alpha^*_{M\sigma}(\boldsymbol{k})|\boldsymbol{k}, \tfrac{5}{2}, M\rangle_0 \tag{8}$$

$$E^0_\nu(\boldsymbol{k}) = \tfrac{1}{2}[\![\varepsilon(\boldsymbol{k}) + \varepsilon^0_f + \nu\{[\varepsilon(\boldsymbol{k}) - \varepsilon^0_f]^2 + 4V^2_0\}^{1/2}]\!]. \tag{9}$$

There are four more non-hybridised linear combinations of f orbitals with energy ε^0_f. Let us consider how these states and energies are renormalised with the introduction of the Coulomb interaction U. Instead of deriving these quantities, we will obtain the bare-particle Green functions in the higher-order decoupling scheme, from which we construct the quasiparticle Green functions for heavy-fermion states corresponding to that (5) of the ZA model. We assume the anisotropy coefficients $\alpha^*_{M\sigma}(\boldsymbol{k})$ which come from the spin–orbit coupling of f orbitals are invariant in the SA model without the Coulomb term and in the ZA model. $|\boldsymbol{k}, \tfrac{5}{2}, \alpha\rangle_0$ in (8) is the Bloch state with pseudo-spin α made up of a linear combination of the spin–orbit-coupled bare f orbitals, which hybridises with a conduction state $|\boldsymbol{k}, \boldsymbol{\sigma}\rangle_0$ with spin $s = \tfrac{1}{2}\boldsymbol{\sigma}$.

The bare f electron Green function with spin–orbit coupling can be derived by using the decoupling procedure in the hierarchy of the equations of motion (Kaga *et al* 1988). We assume that the spin–orbit splitting is much larger than the bare hybridisation energy V_0, a condition that is satisfied in heavy-fermion compounds. Then one can readily show that in the decoupling approximation the pseudo-spin α is conserved even under the influence of the Coulomb interaction U. The bare-particle Green function $G^0_{\nu\alpha}(\boldsymbol{k}, \omega)$ at finite temperature is the sum of the f and conduction components, $G^0_{f\alpha}(\boldsymbol{k}, \omega)$ and $G^0_{c\alpha}(\boldsymbol{k}, \omega)$, being given, using the temperature-dependent self-energy $\Sigma^0_{f\alpha}(\omega) = \mathrm{Re}\,\Sigma^0_{f\alpha}(\omega) + \mathrm{i}\,\mathrm{Im}\,\Sigma^0_{f\alpha}(\omega)$, as

$$\sum_{\nu=\pm} G^0_{\nu\alpha}(\boldsymbol{k}, \omega) = G^0_{f\alpha}(\boldsymbol{k}, \omega) + G^0_{c\alpha}(\boldsymbol{k}, \omega) \tag{10}$$

$$G^0_{f\alpha}(\boldsymbol{k}, \omega) = 1/\{\omega - \varepsilon^0_f - \Sigma^0_{f\alpha}(\omega) - V_0^2/[\omega - \varepsilon(\boldsymbol{k})]\} \tag{11}$$

$$G^0_{c\alpha}(\boldsymbol{k}, \omega) = 1/\{\omega - \varepsilon(\boldsymbol{k}) - V_0^2/[\omega - \varepsilon^0_f - \Sigma^0_{f\alpha}(\omega)]\}. \tag{12}$$

Though this self-energy is independent of momentum $\boldsymbol{k}$, it has the characteristics of a periodic lattice and is different from the single-site impurity self-energy, which was verified in the detailed analysis of the two self-energies (Kaga and Kubo 1987).

At low temperature there is a large self-energy renormalisation—$\partial\,\mathrm{Re}\,\Sigma^0_{f\alpha}(\omega)/\partial\omega \sim \Delta/T_K$, ($T_K \sim D\exp(-\pi\varepsilon^0_f/\Delta)$, $\Delta \equiv \pi N_0(\mu_F)V_0^2$)—for $G^0_{f\alpha}(\boldsymbol{k}, \omega)$ in the energy range $\omega \sim \mu_F$ (the Fermi level), where $\mathrm{Im}\,\Sigma^0_{f\alpha}(\omega)$ is vanishingly small, and the quasiparticle picture becomes valid. Now, in this regime the spin–orbit-coupled quasiparticle states are formed having the quasiparticle bands $E^q_{\nu\alpha}(\boldsymbol{k})$, ($\nu = \pm$), where $E^q_{\nu\alpha}(\boldsymbol{k})$ is obtained from the poles of $G^0_{f\alpha}(\boldsymbol{k}, \omega)$, as $\omega = E^q_{\nu\alpha}(\boldsymbol{k})$. The quasiparticle Green function $G^q_{\nu\alpha}(\boldsymbol{k}, \omega)$ is constructed by employing the standard procedure; the energy-denominator of $G^0_{f\alpha}(\boldsymbol{k}, \omega)$ is expanded to first order in power-series of $\omega - E^q_{\nu\alpha}(\boldsymbol{k})$ in the energies ω close to μ_F which is assumed to be in the $E^q_{-\alpha}(\boldsymbol{k})$ band. The quasiparticle Green function $G^q_{\nu\alpha}(\boldsymbol{k}, \omega)$ is then formed so as to satisfy the spectral sum-rule at each $\boldsymbol{k}$-vector with the Lorentzian broadening for a small imaginary part $\mathrm{Im}\,\Sigma^0_{f\alpha}(E^q_{-\alpha}(\boldsymbol{k}))$. First, the renormalised bare-particle Green functions are written as

$$G^0_{f\alpha}(\boldsymbol{k}, \omega) = z_f(\boldsymbol{k})/[\omega - \tilde{E}^q_{-\alpha}(\boldsymbol{k})] \tag{13}$$

$$G^0_{c\alpha}(\boldsymbol{k}, \omega) = z_c(\boldsymbol{k})/[\omega - \tilde{E}^q_{-\alpha}(\boldsymbol{k})] \tag{14}$$

using the renormalisation factors

$$z(\boldsymbol{k}) = \left(1 - \partial\,\mathrm{Re}\,\Sigma^0_{f\alpha}(\omega)/\partial\omega\,|_{\omega = E^q_{-\alpha}(\boldsymbol{k})}\right)^{-1} \tag{15}$$

$$z_f(\boldsymbol{k}) = \{z(\boldsymbol{k})^{-1} + V_0^2/[E^q_{-\alpha}(\boldsymbol{k}) - \varepsilon(\boldsymbol{k})]^2\}^{-1} \tag{16}$$

$$z_c(\boldsymbol{k}) = V_0^2 z_f(\boldsymbol{k})/[E^q_{-\alpha}(\boldsymbol{k}) - \varepsilon(\boldsymbol{k})]^2 \tag{17}$$

and the complex quasiparticle energy $\tilde{E}^q_{\nu\alpha}(\boldsymbol{k})$ with the small imaginary part

$$\tilde{E}^q_{-\alpha}(\boldsymbol{k}) \equiv E^q_{-\alpha}(\boldsymbol{k}) + \mathrm{i}z_f(\boldsymbol{k})\,\mathrm{Im}\,\Sigma^0_{f\alpha}(E^q_{-\alpha}(\boldsymbol{k})). \tag{18}$$

Here, the quasiparticle band $E^q_{-\alpha}(\boldsymbol{k})$ defined as the zeros of the denominator $P(\boldsymbol{k}, \omega)$ of $G^0_{f\alpha}(\boldsymbol{k}, \omega)$, (11), is also given approximately by the solution of

$$\begin{aligned} P(\boldsymbol{k}, \omega) &= \omega - \varepsilon^0_f - \mathrm{Re}\,\Sigma^0_{f\alpha}(\omega) - V_0^2/[\omega - \varepsilon(\boldsymbol{k})] \\ &= z(\boldsymbol{k})^{-1}\{\omega - \varepsilon^q_f - z(\boldsymbol{k})V_0^2/[\omega - \varepsilon(\boldsymbol{k})]\} = 0 \end{aligned} \tag{19}$$

because $z_f(\boldsymbol{k})^{-1} \sim z(\boldsymbol{k})^{-1} \gg V_0^2/[E^q_{-\alpha}(\boldsymbol{k}) - \varepsilon(\boldsymbol{k})]^2$, where $\varepsilon^q_f \equiv \varepsilon^0_f + \mathrm{Re}\,\Sigma^0_{f\alpha}(E^q_{-\alpha}(\boldsymbol{k}))$. The quasiparticle band $E^q_{-\alpha}(\boldsymbol{k})$ thus obtained coincides with that of the Zou–Anderson model (4) only when $z(\boldsymbol{k})V_0^2$ is independent of $\boldsymbol{k}$ and is equal to b_0^2 of the latter. In contrast to the ZA model, the quasiparticle bands $E^q_{\nu\alpha}(\boldsymbol{k})$ and the imaginary part $z_f(\boldsymbol{k})\,\mathrm{Im}\,\Sigma^0_{f\alpha}(E^q_{-\alpha}(\boldsymbol{k}))$ are given only numerically in the SA model. The quasiparticle

Green function $G^{q}_{-\alpha}(\boldsymbol{k}, \omega)$ is obtained by multiplying $G^{0}_{f\alpha}(\boldsymbol{k}, \omega)$ by the self-energy renormalisation factor $z(\boldsymbol{k})^{-1}$ as

$$G^{q}_{-\alpha}(\boldsymbol{k}, \omega) = z_{f}(\boldsymbol{k})z(\boldsymbol{k})^{-1}/[\omega - \tilde{E}^{q}_{-\alpha}(\boldsymbol{k})] + z_{c}(\boldsymbol{k})/[\omega - \tilde{E}^{q}_{-\alpha}(\boldsymbol{k})]$$
$$= 1/[\omega - \tilde{E}^{q}_{-\alpha}(\boldsymbol{k})]. \qquad (20)$$

Here, we assume that the quasiparticle renormalisation comes from the large ω dependence of Re $\Sigma^{0}_{f\alpha}(\omega)$ term only. The first and second terms of the first right-hand side of (20) represent the quasiparticle Green functions of f and conduction components, respectively.

2.3. Roles of the non-hybridised spin–orbit orbitals

Soon after Zou and Anderson proposed the ZA model without the non-hybridised linear combinations of f orbitals, a question was raised by a number of workers (Zhang and Lee 1987, Aeppli and Varma 1987, Cox 1987) about its validity for the evaluation of the magnetic moment; non-inclusion of these orbitals leads to the Van Vleck term in the magnetic susceptibility for quasiparticles being neglected, whose contribution was estimated to be of the same order as the Pauli term. The important point is then whether or not the non-hybridised f orbitals are also renormalised to become quasiparticle states near the Fermi level at low temperature (Anderson and Zou 1987).

According to the bare f Green function obtained in the decoupling scheme in (11) under the assumption that the spin–orbit energy is much larger than the bare hybridisation matrix V_0, it follows also for the bare states at high temperature that hybridisation with conduction state of spin index $\boldsymbol{\sigma}(= \pm 1)$ is possible only for the particular linear combination of f orbitals with pseudo-spin $\alpha(= \pm 1)$ compatible with its spin $\sigma(= \pm 1)$. The self-energy renormalisation $\Sigma^{0}_{f\alpha}(\omega)$ due to the Coulomb interaction U, which comes into play through this anisotropic hybridisation $(V_0 \alpha_{M\sigma}(\boldsymbol{k}))$, also becomes effective only for the $\alpha = \pm 1$ pseudo-spin f combinations $|\boldsymbol{k}, \frac{5}{2}, \alpha\rangle_0$, (8). Therefore, within the present decoupling scheme approximation the two degenerate hybridised orbitals $|\psi^{\alpha}_{-}(\boldsymbol{k})\rangle_0$ $(\alpha = \pm)$ at high temperature, (7), are carried over to the degenerate heavy-fermion quasiparticle states $|\psi^{\alpha}_{-}(\boldsymbol{k})\rangle$ at low temperatures. These heavy-fermion states correspond to the two degenerate $(\alpha = \pm 1)$ quasiparticle states obtained by Zou and Anderson (1986) in (3).

Since only the two degenerate quasiparticle states with pseudo-spins $\alpha = \pm 1$ near the Fermi level μ_F in both the models of sections 2.1 and 2.2 arise, we leave out the Van Vleck contributions from the non-hybridised, spin–orbit f orbitals in our expressions for the magnetic susceptibility of the low-temperature quasiparticle states. There are, however, different types of Van Vleck contributions that arise between the lower $(\nu = -)$ and upper $(\nu = +)$ hybridised bands $E^{q}_{\nu\alpha}(\boldsymbol{k})$. These are discussed in the following sections.

3. Magnetic moment and magnetic susceptibility

Under a small external magnetic field $\boldsymbol{h}$ applied along the z direction the Hamiltonian H_{ZA} in (1) and H_{SA} in (6) acquire an additional perturbation $H' = -\boldsymbol{\mu} \cdot \boldsymbol{h}$, where $\boldsymbol{\mu}$ is the total magnetic moment operator $\boldsymbol{\mu} = -(\boldsymbol{l} + 2\boldsymbol{s})\mu_B$. Now, consider the magnetic moment for quasiparticles states under strong spin–orbit coupling which is much larger than the effective quasiparticle band width ($\sim T_K$). While the conduction-electron component has only spin magnetic moment $-2s\mu_B$, the f-electron component decomposes its magnetic moment $\boldsymbol{\mu} = -(\boldsymbol{l} + 2\boldsymbol{s})\mu_B$ into $\mu = -(g_j \boldsymbol{J} + \boldsymbol{J}')\mu_B$ for the $J = \frac{5}{2}$ multiplet states $|\boldsymbol{k}, \frac{5}{2}, M\rangle$, ($M = -\frac{5}{2}$–$\frac{5}{2}$). Here, $-\boldsymbol{J}'\mu_B$ is the component orthogonal to the magnetic moment operator $\mu_j = -g_j \boldsymbol{J}\mu_B$ being diagonalised in the spin–orbit multiplets, and is neglected for the large spin–orbit splitting assumed in the present model. Hence, the magnetic moment in the quasiparticle state is not conserved between the two components of conduction and f electrons. The matrix element of the spatially varying external perturbation $H' = -\boldsymbol{\mu} \cdot \boldsymbol{h}_q = -h(\mu_z \exp(i\boldsymbol{q} \cdot \boldsymbol{r})) = -h\mu_{zq}$, where $\boldsymbol{h}_q = \boldsymbol{h} \exp(i\boldsymbol{q} \cdot \boldsymbol{r})$ with wavevector $\boldsymbol{q}$, or rather that of μ_{zq} between $|\psi_\nu^\alpha(\boldsymbol{k} + \boldsymbol{q})\rangle$ and $|\psi_{\nu'}^{\alpha'}(\boldsymbol{k})\rangle$ is written as

$$\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k} + \boldsymbol{q}, \boldsymbol{k}) \equiv \langle \psi_\nu^\alpha(\boldsymbol{k} + \boldsymbol{q}) | \mu_{zq} | \psi_{\nu'}^{\alpha'}(\boldsymbol{k}) \rangle = \mu_B A_\nu(\boldsymbol{k} + \boldsymbol{q}) A_{\nu'}(\boldsymbol{k})$$

$$\times \left[\alpha\delta_{\alpha\alpha'} + g_j C_\nu(\boldsymbol{k} + \boldsymbol{q}) C_{\nu'}(\boldsymbol{k}) \sum_M \alpha_{M\sigma}(\boldsymbol{k} + \boldsymbol{q}) \alpha^*_{M\sigma}(\boldsymbol{k}) M\right] \qquad (21)$$

for the two (ZA and SA) quasiparticle models. Here, the $C_\nu(\boldsymbol{k})$ and $C_{\nu'}(\boldsymbol{k})$ are the $C_\nu^{\mathrm{ZA}}(\boldsymbol{k})$ and $C_{\nu'}^{\mathrm{ZA}}(\boldsymbol{k})$ in the former model, and $(A_\nu(\boldsymbol{k}))^2 = z_c(\boldsymbol{k})$, $(A_\nu(\boldsymbol{k}) C_\nu(\boldsymbol{k}))^2 = z_f(\boldsymbol{k}) z(\boldsymbol{k})^{-1}$, $E_\nu(\boldsymbol{k}) = \tilde{E}^{\mathrm{q}}_{-\alpha}(\boldsymbol{k})$, and $b_0^2 = z(\boldsymbol{k}) V_0^2$ in the latter model. In equation (21) the values of the pseudo-spins α, $\alpha'(= \pm 1)$ and the conduction-electron spins σ, $\sigma'(= \pm 1)$ correspond to each other, and $g_j = \frac{6}{7}$.

Magnetic susceptibility is given in linear response theory as the linear coefficient in the expansion of the magnetisation in an applied magnetic field $\boldsymbol{h}$. This linear coefficient is the spin–spin correlation function which is the retarded electron-hole two-particle propagator. In order to represent magnetic susceptibilities at finite temperature in terms of the electron-hole propagators, we convert the Green functions $G_{\nu\alpha}^{\mathrm{ZA}}(\boldsymbol{k}, \omega)$ in (5) and $G^{\mathrm{q}}_{-\alpha}(\boldsymbol{k}, \omega)$ in (20) into the temperature Green functions $G^{\mathrm{ZA}}_{-\alpha}(\boldsymbol{k}, i\omega_n)$ and $G^{\mathrm{q}}_{-\alpha}(\boldsymbol{k}, i\omega_n)$ by analytical continuation, $\omega \to i\omega_n$. Then, the temperature-dependent magnetic susceptibility $\chi_q(T)$ for the two models is expressed, using the magnetic moment $\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k} + \boldsymbol{q}, \boldsymbol{k})$ of (21), in terms of the static retarded function $\Pi^{\mathrm{R}}(\boldsymbol{q}, 0)$ of the finite-temperature two-particle propagator $\Pi(\boldsymbol{q}, i\omega_n)$, which represents the magnetic response function

$$\Pi(\boldsymbol{q}, i\omega_n) = -T \sum_{\boldsymbol{k}\omega_n'} \sum_{\substack{\nu\nu' \\ \alpha\alpha'}} |\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k} + \boldsymbol{q}, \boldsymbol{k})|^2 G_{\nu\alpha}(\boldsymbol{k} + \boldsymbol{q}, i\omega_n + i\omega_n') G_{\nu'\alpha'}(\boldsymbol{k}, i\omega_n') \qquad (22)$$

where the respective expressions are to be used for the two models. In the expression (22) the inclusion of the interband as well as the intraband contributions are important because the former becomes dominant for large $\boldsymbol{q}$. Writing the product of the two Green functions in (22) as their difference and performing the sum over ω_n' under the assumption that the imaginary part of $\tilde{E}^{\mathrm{q}}_{-\alpha}(\boldsymbol{k})$ in (18) for the SA model is negligibly small, one obtains the expression for magnetic susceptibility $\chi_q(T)$

$$\chi_q(T) = \sum_{\nu\nu'} \sum_{\boldsymbol{k}} \frac{f(E_{\nu'}(\boldsymbol{k})) - f(E_\nu(\boldsymbol{k} + \boldsymbol{q}))}{E_\nu(\boldsymbol{k} + \boldsymbol{q}) - E_{\nu'}(\boldsymbol{k})} \sum_{\alpha\alpha'} |\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k} + \boldsymbol{q}, \boldsymbol{k})|^2 \qquad (23)$$

where the $E_\nu(\boldsymbol{k})$, $E_{\nu'}(\boldsymbol{k})$ and $E_\nu(\boldsymbol{k} + \boldsymbol{q})$ refer to the $E_\nu^{\mathrm{ZA}}(\boldsymbol{k})$, $E_{\nu'}^{\mathrm{ZA}}$ and $E_\nu^{\mathrm{ZA}}(\boldsymbol{k} + \boldsymbol{q})$ of the ZA model and $\tilde{E}^{\mathrm{q}}_{-}(\boldsymbol{k})$, etc. for the SA model. In the latter model the numerically given quasiparticle bands $E_\nu^{\mathrm{q}}(\boldsymbol{k})$ and the imaginary parts (18) are dependent on temperature.

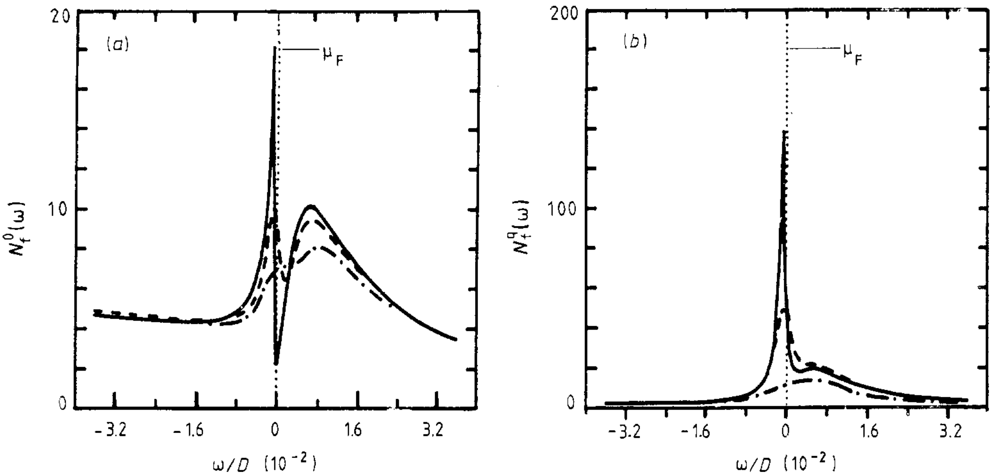

Figure 1. (*a*) Temperature-dependent bare f-electron density of states $N_f^0(\omega)$, and (*b*) the corresponding quasiparticle density of states $N^q(\omega)$ around the Fermi level μ_F in the spin–orbit Anderson lattice (SA) model with $T_K = 10$ K. The pseudo-gap is considerably reduced on the $N^q(\omega)$ curve. ——, $T = 1$ K; - - -, $T = 10$ K; -·-·-, $T = 40$ K.

4. Temperature dependences of $\chi_0(T)$ and $\chi_Q(T)$

In this section we study the temperature dependences of uniform $\chi_0(T)$ and antiferromagnetic $\chi_Q(T)$ susceptibilities for the quasiparticle states by explicit numerical calculations using the expression (23) in the two different models: the ZA model and the SA model. We use the tight-binding conduction band in a simple cubic lattice with half the band width D given by $D \equiv 6t$;

$$\varepsilon(\boldsymbol{k}) = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]. \tag{24}$$

In the SA model the quasiparticle quantities such as the bands $\tilde{E}_\nu^q(\boldsymbol{k})$, the renormalisation factors $z_f(\boldsymbol{k})$, $z_c(\boldsymbol{k})$, $z(\boldsymbol{k})$, the magnetic moments $\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k}+\boldsymbol{q}, \boldsymbol{k})$ and the densities of states $N^*(\omega)$ are only given numerically. While in the ZA model we can assume the insulating and metallic cases by putting the Fermi level μ_F either in the hybridisation gap E_g or near the top of the $E_-^{ZA}(\boldsymbol{k})$ band, in the SA model the Fermi level cannot be controlled and is fixed once the bare parameters such as ε_f^0, V_0, and the number of bare f electrons are given (Kaga *et al* 1988); ε_f^q appears again about T_K above μ_F. It is now well known that the Kondo resonance gives rise to a pseudo-gap on the bare-particle density of states at the Fermi level μ_F when the Anderson-lattice model is renormalised at low temperature (Grewe 1984, Kaga *et al* 1988). The relative position of the Fermi level μ_F with respect to that of the pseudo-gap is uniquely determined and is almost the same in the well defined Kondo-lattice states. In figure 1(*a*) and 1(*b*) we show the typical temperature dependences of bare f-electron density-of-states curves $N_f^0(\omega)$ (figure 1(*a*)) and of quasiparticle density-of-states curves $N^q(\omega)$ (figure 1(*b*)) near the Fermi level μ_F in the SA model for $T_K = 10$ K. The $N^q(\omega)$ is enhanced by a factor of over 10 times $N_f^0(\omega)$ and has a less pronounced pseudo-gap near the Fermi level. These quasiparticle states derived in the SA model are different from the mean-field quasiparticle states

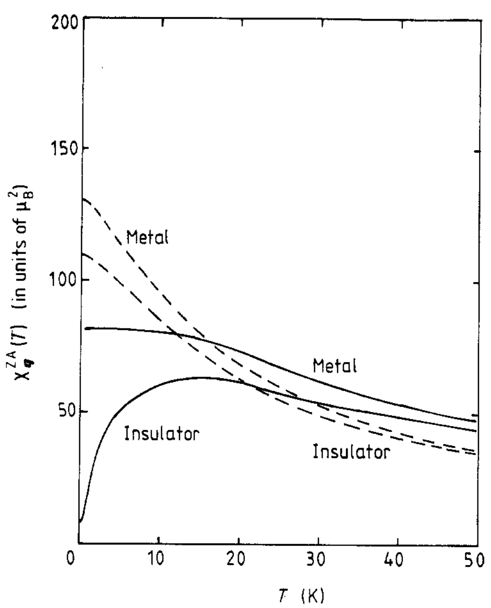

Figure 2. The temperature-dependent uniform and antiferromagnetic (staggered) magnetic susceptibilities of the Zou–Anderson (ZA) model, $\chi_0^{ZA}(T)$ and $\chi_Q^{ZA}(T)$, with $T_K = 10$ K for the two cases of large quasiparticle fillings, $\varepsilon(k_F) = 0.5$ and $\varepsilon(k_F) = 0.475$, which represent the insulating case (lower curve of each pair) and the typical metallic case (upper curve of each pair), respectively. ——, $\chi_0^{ZA}(T)$; – – –, $\chi_Q^{ZA}(T)$. $\chi_0^{ZA}(T)$ in the metallic case of this model shows no maximum.

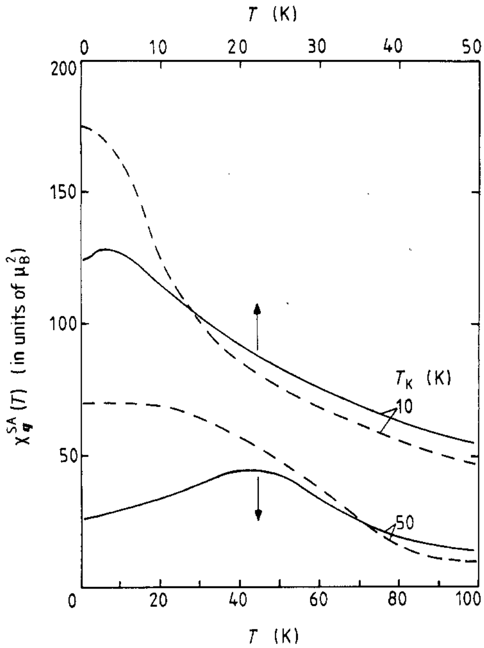

Figure 3. The temperature-dependent uniform and antiferromagnetic magnetic susceptibilities ——, $\chi_0^{SA}(T)$; – – –, $\chi_Q^{SA}(T)$ of the SA model for the two Kondo temperatures; the upper two curves for $T_K = 10$ K and the lower two curves for $T_K = 50$ K. In contrast to the metallic $\chi_0^{ZA}(T)$, the $\chi_0^{SA}(T)$ exhibits a maximum near T_K for large T_K and shows a small bump well below T_K for small T_K, while the behaviour of $\chi_Q^{SA}(T)$ is similar to $\chi_Q^{ZA}(T)$.

obtained in the ZA spin–orbit model. Therefore, we investigate the temperature dependences of the magnetic susceptibilities in these two models and compare the results with experiment.

The mean-field hybridisation gap which is given as $E_g = 2b_0^2/(D - \mu_F) = 2T_K[\varepsilon(k_F) - \mu_F]/(D - \mu_F)$ at $T = 0$ K should actually depend on temperature T because b_0^2 is obtained as a function of T and vanishes at $T \simeq T_K$ in the mean-field theory. Although it is suggested that the mean-field theory with this temperature-dependent gap is valid for $T \leqslant \frac{1}{2}T_K$ (Auerbach *et al* 1988), we mainly investigate here the constant $T = 0$ gap for the reasons explained below.

Figure 2 illustrates the uniform $\chi_0^{ZA}(T)$ and antiferromagnetic (staggered) $\chi_Q^{ZA}(T)$ susceptibilities calculated in the ZA model for the insulating ($\varepsilon(k_F) = 0.5$) and metallic ($\varepsilon(k_F) = 0.475$) large quasiparticle-filling parameters (large k_F) with $T_K = 10$ K. While the uniform susceptibility $\chi_0^{ZA}(T)$ in this model shows a plateau below $T \simeq T_K$ in the metallic case, representing a typical heavy-fermion system and a broad maximum at $T \simeq T_K$ in the insulating case with a finite hybridisation gap at μ_F, the antiferromagnetic one $\chi_Q^{ZA}(T)$ is always a monotonically decreasing function of temperature. The high-temperature behaviours of both the susceptibilities are of the Curie–Weiss form with

$\chi_0^{ZA}(T) > \chi_Q^{ZA}(T)$. Lower quasiparticle filling (smaller $\varepsilon(k_F)$) gives these susceptibilities larger values reflecting an increase in the tight-binding conduction density of states at $\varepsilon(k_F)$. These temperature-dependent behaviours do not change for different Kondo temperatures in contrast to those in the SA model described below. Owing to the non-conservation of magnetic moment between the two components (f and conduction) in the spin–orbit-coupling model, the zero-temperature $\chi_0^{ZA}(T)$ for the insulating case does not vanish ($\chi_0^{ZA}(0) \simeq 2N_0(D)\mu_B^2$).

Figures 3 plots the $\chi_0^{SA}(T)$ and $\chi_Q^{SA}(T)$ versus temperature curves for the SA model for two different values of T_K; the upper two curves for $T_K = 10$ K and the lower two curves for $T_K = 50$ K. Quasiparticle filling for a fixed T_K cannot be controlled in this model, and the absolute magnitudes of $\chi_0^{SA}(T)$ and $\chi_Q^{SA}(T)$ cannot be directly compared with those of the ZA model. Because of the absence of a real hybridisation gap at finite temperature in the quasiparticle spectrum of this model (with only the very weak pseudo-gap), no insulating-like behaviour is found. The most remarkable feature in this model is that the temperature dependence of the uniform susceptibility $\chi_0^{SA}(T)$ always exhibits a small maximum, which appears at a temperature much lower than T_K for a low-T_K system ($T_K \lesssim 10$ K) and at about T_K for a high-T_K system ($T_K \gtrsim 20$ K). The anti-ferromagnetic susceptibility $\chi_Q^{SA}(T)$ curves look rather similar to those of the ZA model.

On the other hand, if in the ZA model we take into account the temperature dependence of the hybridisation gap $E_g(T) = 2b(T)^2/(D - \mu_F)$ by solving for $b(T)^2$ from the gap equation at finite temperatures, we find that the decrease in the gap with increasing temperature causes increasingly larger quasiparticle densities of states at the Fermi level and leads to the unreasonably large uniform susceptibilities.

5. Discussion

The ZA model (Zou and Anderson 1986) is the mean-field theory for describing the quasiparticle states in the spin–orbit-coupling, heavy-fermion systems at low temperatures, $T \ll T_K$. It is therefore not straightforwardly applicable to the finite-temperature properties of the heavy-fermion systems. On the other hand, the SA (spin–orbit Anderson lattice) model, being treated in the Green-function decoupling approach, can produce the quasiparticle states at low temperatures, $T \ll T_K$, and with inclusion of the temperature-dependent renormalisation it can also describe the crossover behaviours from the quasiparticle regime to the bare-particle regime. This has been already demonstrated in the calculations of the low-temperature specific heat coefficients $\gamma(T)$ of heavy-fermion systems (Kaga and Kubo 1988). Hence, the approach in the SA model leads more naturally to the quasiparticle states by renormalisations from the high-temperature regime. With these limitations in mind for the two models, we have investigated the low-temperature magnetic susceptibilities.

From a comparison of figures 2(*a*) and 3(*a*) we notice that while the uniform susceptibility of the ZA model, $\chi_0^{ZA}(T)$, scales well with T_K and always forms a plateau, whose height depends upon filling factor $\varepsilon(k_F)$, for $T \lesssim T_K$ (except for the insulating case), that of the SA model, $\chi_0^{SA}(T)$, exhibits a small bump at a temperature (T_{max}) below T_K and a decrease at lower temperatures. This maximum-$\chi_0^{SA}(T)$ temperature, T_{max}, is much smaller than T_K for low-T_K systems and tends to approach T_K for high-T_K systems. Moreover, this maximum is more pronounced for higher T_K. The reasons for these behaviours are the following. When a Kondo resonance evolves at $T \simeq T_K$, a pseudo-gap begins to form in the bare-particle density of states. Here, while the imaginary parts of the self-energies, Im $\Sigma^{0}_{f\alpha}(\omega)$, for the high- and low-$T_K$ systems are comparable at each temperature T_K, for temperatures $T > T_K$ it becomes smaller for the high-T_K systems (Kaga and Kubo 1987). Therefore, although these states at $T \simeq T_K$ are different from the so-called quasiparticle states, a wider energy range with a relatively smaller imaginary part for the high-T_K systems leads to a large hybridisation splitting and a large $\chi_0(T)$ peak even at $T \simeq T_K$. This is impossible for the low-T_K systems because at $T = T_K$ the imaginary part is larger than the T_K value. Only at temperatures low enough for Im $\Sigma^{0}_{f\alpha}(\omega)$ to become near vanishing the pseudo-gap grows and a weak $\chi_0(T)$ maximum can appear. The high-temperature behaviours of both the $\chi_0^{ZA}(T)$ and the $\chi_0^{SA}(T)$ are of the Curie-like form, $\chi_0(T) \sim T^{-1}$, as expected.

Although the magnetic moment discussed in this paper is applicable only to Ce heavy-fermion compounds with the $J = \frac{5}{2}$ spin–orbit state, the general temperature-dependent behaviours of the uniform susceptibility $\chi_0(T)$ calculated here can be compared with the experimental results of other heavy-fermion compounds as well. These observed susceptibilities of the uranium heavy-fermion systems URu_2Si_2 (Palstra *et al* 1985, Maple *et al* 1986, Schlabitz *et al* 1986) and UPt_3 (Frings *et al* 1983, Ramirez *et al* 1986) clearly exhibit a peak around their conceivable Kondo temperatures of 70 K and 30 K, respectively, before they undergo an antiferromagnetic phase transition at a lower temperature. On the other hand, the low-temperature susceptibilities of the cerium compounds $CeAl_3$ (Edelstein *et al* 1974, Andres *et al* 1975) and $CeCu_6$ (Gangopadhyay *et al* 1988) show only a very weak maximum at a temperature, $\simeq$0.7 K for $CeAl_3$ and $\simeq$0.3 K for $CeCu_6$, much lower than their Kondo temperatures, $\simeq$3 K and $\simeq$4 K, respectively. These observed maximum-$\chi_0(T)$ temperatures are close to their coherence temperatures $T_0 = 0.3$–0.5 K and 0.5 K, respectively, which were estimated from the resistivity measurements (Andres *et al* 1975, Ott *et al* 1984, Lieke *et al* 1982, Stewart 1984, Sumiyama *et al* 1985) and the observed specific-heat coefficients $\gamma(T)$ (Flouquet *et al* 1982, Bredl *et al* 1984, Fujita *et al* 1985, Brodale *et al* 1986; the origin of a weak maximum in $CeCu_6$ is still unclear and could be due to either to a magnetic transition or to a coherence effect). The above experimental trends for the high-T_K U compounds and the low-T_K Ce compounds are consistent with the present results obtained for $T_K =$ 10 K and 50 K in the SA model. In fact, it has also been shown in the same decoupling treatment of the non-spin–orbit Anderson lattice model (Kaga and Kubo 1988) that a maximum appears on the specific-heat-coefficient $(\gamma(T))$ curve not around T_K but around the coherence temperature T_0.

From these experimental facts one can conclude that the quasiparticle states and the temperature-dependent magnetic susceptibilities obtained in the SA model are more appropriate for the real heavy-fermion systems, and that those obtained in the mean-field ZA model are rather artificial and quite unphysical at finite temperatures. This is because the former model takes into account the temperature-dependent imaginary part of the self-energy which starts to appear from right above $T = 0$ or the Fermi energy. It falls with decreasing temperature and leads to an incoherent–coherent crossover transition across the temperature T_K, forming a pseudo-gap, whereas the latter model gives rise to a phase transition, opening a real gap. The most important effect in the SA model is the large temperature dependence of the quasiparticle density of states for temperatures across T_K. The self-energy correction made in the SA model however is still quite limited and a better self-energy correction is desirable in future.

We have calculated the effective magnetic moments $\mu_{eff}(\boldsymbol{q})$ per Ce atom for $\boldsymbol{q} = 0$ and $\boldsymbol{q} = \boldsymbol{Q}$, corresponding to the uniform and antiferromagnetic susceptibilities in the two models. Here, $\mu_{eff}(\boldsymbol{q})^2$ is defined as the value of $\chi_{\boldsymbol{q}}(0)$, (23), divided by that of the expression (23) without the factor $\Sigma_{\alpha,\alpha'=\pm1}|\mu_{\nu\nu'}^{\alpha\alpha'}(\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k})|^2$. Approximately the same values were obtained for both models; $\mu_{\rm eff}^{\rm ZA}(0)^2 = 1.20\,\mu_{\rm B}^2$/atom, $\mu_{\rm eff}^{\rm SA}(0)^2 = 1.16\,\mu_{\rm B}^2$/atom and $\mu_{\rm eff}^{\rm ZA}(\boldsymbol{Q})^2 = 0.73\,\mu_{\rm B}^2$/atom, $\mu_{\rm eff}^{\rm SA}(\boldsymbol{Q})^2 = 0.65\,\mu_{\rm B}^2$/atom. These agreements are to be expected because the effects of the different quasiparticle states obtained in the two models are largely cancelled out for the derivation of $\mu_{\rm eff}(\boldsymbol{q})$. A model-independent effective magnetic moment is also seen in the agreement between the uniform moments obtained in the present tight-binding models and the Zou–Anderson value $\mu_{\rm eff}(0)^2 = 1.16\,\mu_{\rm B}^2$/atom (Zou and Anderson 1986) obtained in the spherical conduction-band model. The above antiferromagnetic moments $\mu_{\rm eff}^{\rm ZA}(\boldsymbol{Q}) = 0.81\,\mu_{\rm B}$/atom and $\mu_{\rm eff}^{\rm SA}(\boldsymbol{Q}) = 0.85\,\mu_{\rm B}$/atom can be roughly compared with the observed magnetic moments having antiferromagnetic correlations found in the Ce compounds at low temperatures; $\simeq 0.89\,\mu_{\rm B}$/Ce for $CeAl_2$ (Barbara *et al* 1977, Lawrence *et al* 1981) and $\simeq 0.5\,\mu_{\rm B}$/Ce for $CeAl_3$ (Barth *et al* 1989). Such a reduced ordered moment from the free-ion value is not limited to Ce compounds and has been found in U compounds as well; for example, in U_2Zn_{17} the ordered moment ($0.8\,\mu_{\rm B}$/U) is observed as opposed to the high-temperature effective moment (2.2–$3.3\mu_{\rm B}$/U) (Broholm *et al* 1987a). However, the antiferromagnetic moment observed in the static short-range order of the heavy-fermion superconductor $CeCu_2Si_2$ is $\simeq 0.1\,\mu_{\rm B}$/Ce (Uemura *et al* 1989), being considerably smaller than the above values. These small antiferromagnetic moments are rather common to the other heavy-fermion superconductors URu_2Si_2 ($\simeq 0.03\,\mu_{\rm B}$/U) (Broholm *et al* 1987b), UPt_3 ($\simeq 0.02\,\mu_{\rm B}$/U) (Aeppli *et al* 1988) and UBe_{13} ($\simeq 0.001\,\mu_{\rm B}$/U) (Neumann *et al* 1986). However, it is interesting to notice that, when the superconductivity or these systems is broken by doping, these small moments are enhanced and an antiferromagnetic moment of roughly the calculated magnitude is observed, e.g., $U_{1-x}Th_xPt_3$ ($\simeq 0.7\,\mu_{\rm B}$/U) and $U(Pt_{1-x}Pd_x)_3$ (Fisk *et al* 1987). The superconductivity in all these systems takes place in an antiferromagnetically (long or short-range) ordered state, and its effect must be suppressing a further growth of the antiferromagnetic correlations and ordered moments. This seems to indicate that there are two competing quasiparticle interactions in the heavy-fermion states for superconducting pairing and antiferromagnetic correlation (Kaga and Yoshida 1988, 1989). The high-temperature effective moment of the bare particles ($T \gg T_{\rm K}$) can be evaluated using the same approach in the SA model. In this case the four non-hybridised, f-orbital combinations in addition to the two-fold degenerate hybridised ones have their energies at or around the same bare f-level $\varepsilon_{\rm f}^0$. Thus, there are the Van Vleck-term as well as the Pauli-term contributions to the susceptibility, giving the effective magnetic moment at the free-ion value $\mu_{\rm eff} = 2.54\,\mu_{\rm B}$. This is in agreement with the high-temperature moments observed for the various Ce compounds ($2.61\,\mu_{\rm B}$/Ce for $CeCu_2Si_2$, $2.63\,\mu_{\rm B}$/Ce for $CeAl_3$, $2.56\,\mu_{\rm B}$/Ce for $CeCu_6$).

Figures 2 and 3 show that the high-temperature Curie-like uniform susceptibility is larger than that of the antiferromagnetic susceptibility. This is explained by the relative magnitudes of the effective magnetic moments $\mu_{\rm eff}(0)^2$ and $\mu_{\rm eff}(\boldsymbol{Q})^2$ that we have seen above. On the other hand, the origin for this difference between $\mu_{\rm eff}(0)^2$ and $\mu_{\rm eff}(\boldsymbol{Q})^2$ is due to the quasiparticle coherence factor $A_\nu(\boldsymbol{k}+\boldsymbol{q})A_{\nu'}(\boldsymbol{k})C_\nu(\boldsymbol{k}+\boldsymbol{q})C_{\nu'}(\boldsymbol{k})$ rather than the hybridisation anisotropy factor $\Sigma_M \alpha(\boldsymbol{k}+\boldsymbol{q})\alpha^*(\boldsymbol{k})M$.

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