PHYSICAL REVIEW B VOLUME 46, NUMBER 6 1 AUGUST 1992-II

Theoretical study of the enhanced paramagnetism in CeNi$_x$ ($x=1$, 2, and 5)

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(Received 13 November 1991; revised manuscript received 24 March 1992)

Theoretical investigations of the paramagnetic compounds CeNi, CeNi$_2$, and CeNi$_5$ have been performed by means of electronic-structure calculations. It is shown that an itinerant picture of the $4f$ states of cerium can explain the enhanced susceptibilities of CeNi and CeNi$_2$. The experimental observations that the induced magnetization in a magnetic field is well localized on the nickel atoms in CeNi$_5$ and well localized on the cerium atoms in CeNi and CeNi$_2$ can be easily understood from the calculated results. An overall good agreement with experiments is achieved for the magnetic properties for all three compounds. From a comparison with specific-heat measurements, a large mass enhancement due to heavy quasiparticles has to be inferred for both CeNi$_2$ and CeNi.

I. INTRODUCTION

The intermetallic compounds CeNi, CeNi$_2$ and CeNi$_5$ all show the so-called intermediate-valence behavior.[1-5] This is, for instance, manifested (Fig. 1) in pronounced anomalies in the experimental equilibrium volumes[6] for $R=$Ce in the RNi$_x$ ($x=1$, 2, or 5) series of systems (R is a rare-earth element). Intermediate valence is, however, a term of empirical origin, which is given to a group of systems with a certain kind of anomalous behavior. Several theoretical models have been proposed to describe cerium-based intermediate-valence compounds. There are mixed-valence models,[7] Kondo models,[8] and models with itinerant $4f$ states.[9] In a mixed-valence model the cerium atom is in a state that is a mixture of two localized $4f$ configurations, $4f^1$ and $4f^0$, resulting in a noninteger average $4f$ occupation number. The Kondo model is based on a localized $4f$ electron that interacts via exchange with the surrounding valence electrons, which results in a many-body singlet ground state. In the model of itinerant $4f$ states the $4f$ wave functions are thought to be extended enough to have a substantial overlap with wave functions on the surrounding atoms, and thereby they can become actively involved in the formation of bands. In the last model, which is the one in focus in the present paper, the volume anomalies in Fig. 1 are explained by the extra bonding of the itinerant $4f$ states in Ce in comparison with the nonbonding localized $4f$ states of the normal rare earths.

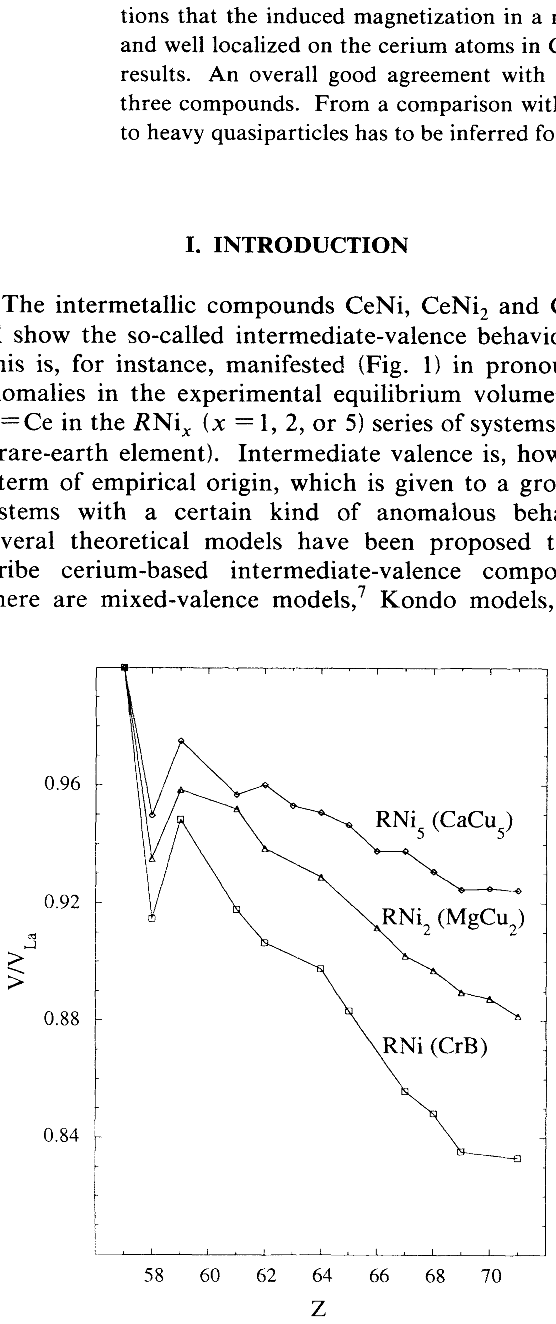

FIG. 1. The experimental equilibrium volumes for the series RNi$_x$ [$R=$La ($Z=57$) to Lu ($Z=71$)] normalized to the volume of LaNi$_x$ (V_{La}) for $x=1$, 2, and 5. Cerium has atomic number $Z=58$.

The three cerium-nickel compounds, which are the subject of this paper, crystallize in the CrB, MgCu$_2$, and CaCu$_5$ structures. These structures are quite different from each other. MgCu$_2$ is based on a face-centered-cubic Bravais lattice with two formula units per unit cell, CaCu$_5$ is hexagonal with six atoms per unit cell, and CrB is more anisotropic with a base centered orthorombic lattice consisting of two formula units per unit cell. Some structural data are collected in Table I. Noteworthy is

TABLE I. Crystallographic data for the compounds CeNi$_x$ ($x=1,2,5$). a, b, and c are the usual lattice constants. The shortest distance between an A atom and a B atom is denoted by d_{AB}.

Compound	CeNi$_5$	CeNi$_2$	CeNi
Crystal structure	CaCu$_5$	MgCu$_2$	CrB
Space group	$P6/mmm$	$Fd\bar{3}m$	$Cmcm$
No. atoms/unit cell	6	6	4
a (Å)	4.875	7.2236	3.783
b (Å)			10.372
c (Å)	4.010		4.286
$d_{\mathrm{Ni-Ni}}$ (Å)	2.44	2.55	2.70
$d_{\mathrm{Ce-Ni}}$ (Å)	2.81	2.99	2.94
$d_{\mathrm{Ce-Ce}}$ (Å)	4.01	3.12	3.62

that, while the $MgCu_2$ and the $CaCu_5$ structures are both close packed the CrB structure is more open, with the atoms ordered in zig-zag chains.

As regards the magnetic properties, all three compounds are known experimentally to be Pauli paramagnets. Both CeNi and $CeNi_5$ show a susceptibility with a maximum at around 140 and 100 K, respectively. Such a temperature dependence is typical for nearly ferromagnetic materials and has also been observed for, e.g., Pd and YCo_2.[10,11] From polarized-neutron-scattering experiments in an applied magnetic field, it has been observed that the induced magnetization density is primarily located on the Ni atoms in the case of $CeNi_5$ but mainly on the Ce atoms in the case of CeNi.[12,13]

Electronic-structure calculations have been reported for CeNi (Ref. 14) and $CeNi_2$ (Ref. 15). For $CeNi_2$ the importance of the hybridization of the $4f$ states with the $3d$ states of Ni was stressed. This effect was, for example, shown to explain why $CeNi_2$ has a larger volume than $CeCo_2$, in contrast to RNi_2 and RCo_2 ($R \neq$Ce) compounds.[16]

In this paper we will show that the so-called intermediate-valence behavior in the $CeNi_x$ compounds can be rather well described with an itinerant $4f$ picture, which emerges naturally from the concepts of electronic-structure calculations within the local spin-density approximation (LSDA) to density functional theory. We also want to show that the magnetic properties of these compounds can be described within the theory of itinerant magnetism. In Sec. II the electronic-structure calculations are described in some detail and Sec. III deals with magnetic properties. The results are discussed in Sec. IV and conclusions are given in Sec. V.

II. THE ELECTRONIC STRUCTURE

To calculate the electronic structure we have employed the linear muffin-tin orbital method.[17] Approximations used in the computations were as follows: (a) the atomic-sphere approximation was used in conjunction with the so-called combined correction,[17] (b) the frozen-core approximation was employed in the generation of the potential, and (c) the LSDA (Ref. 18) for the exchange-correlation potential was used. The basis set included angular momenta up to three on all atomic sites. The Brillouin zones were sampled with a dense mesh of 225, 240, and 560 points in an irreducible part for $CeNi_5$, $CeNi_2$, and CeNi, respectively.

The calculated partial state densities (DOS) for the $3d$ states of Ni and the $4f$ states of Ce are shown in Fig. 2. From these plots it is clear that upon increase of the relative Ce concentration, i.e., when proceeding from $CeNi_5$ to CeNi, the part that consists primarily of Ni $3d$ states becomes filled up. This part may also be considered as the bonding part of a hybridization complex formed by the mixing of the $3d$ states of Ni with the $4f$ and $5d$ states of Ce.

The hybridization complex formed in these compounds is characterized by three parts. Lowest in energy is the part that is mainly of Ni $3d$ character but that due to hybridization, also has some $5d$ and $4f$ character. Higher in energy come first the $4f$ dominated bands and then later the $5d$ dominated bands appear. Both these parts may be regarded as antibonding parts of the hybridization complex. The states of predominately $5d$ character are too high in energy to be seen in Fig. 2. Since the $5d$ admixture is small in the energy range covered by the figure, the $5d$ partial state density is not shown in Fig. 2, although it remains true that the $5d$ states play an important role for the electronic structure of intermetallic compounds of transition elements with rare-earth elements in general. In Table II when the relevant occupation numbers are collected, one can see that the total $5d$ occupation is substantial. A striking result is the constancy of the partial occupation numbers between the compounds. For the Ce $4f$ states the occupation numbers are a little larger than one, which is in strong contradiction to a mixed-valence picture of these compounds, where the $4f$ occupation is expected to be close to zero. As regards the calculated $4f$ occupation numbers, one should distinguish between the contributions from on-site wave functions and from tails of wave functions centered at neighboring atoms. If this is done the occupation of genuinely $4f$ states becomes even closer to one.

The increase in Ce concentration for the three different compounds effectively raises the Fermi level to higher energy. This is so, since the valence electrons of cerium are less bound than those for nickel. For $CeNi_5$ the Ni $3d$ states (i.e., in practice the bonding states dominated by $3d$ character) can contain up to 50 electrons, whereas there are only 45.8 states occupied (of Ni $3d$, Ce $4f$, and Ce $5d$ character, see Table II). Therefore the Fermi level is situated within the bonding part of the energy states, which, as already stressed, is dominated by the Ni $3d$ states. For $CeNi_2$ the corresponding occupation number of 20.2 just fills up the 20 bonding states per formula unit (dominated by Ni $3d$ states). Finally for CeNi there is room for ten states per formula unit in the bonding $3d$-$5d$-$4f$ band complex, but the occupation number is 11.6, which means that antibonding states of mainly Ce $4f$ character have to become partly filled. Hence, the Fermi level moves from a region dominated by Ni $3d$ states ($CeNi_5$) to a region mainly composed of Ce $4f$ states (CeNi), via a situation that is intermediate between the two ($CeNi_2$). However, whereas there is an incipient hybridization gap both for $CeNi_5$ (0.5 eV above E_F) and CeNi (1 eV below E_F) giving rise to a fairly clear separation between the bonding and antibonding states, there is no such a dis-

TABLE II. Occupation numbers n_l for Ce $4f$, Ce $5d$, and Ni $3d$ states. Densities of states per spin at the Fermi energy N and site and angular momentum projected DOS N_l for Ce $4f$ and Ni $3d$.

Compound	$CeNi_5$	$CeNi_2$	CeNi
n_{4f} (atom^{-1})	1.13	1.18	1.15
n_{5d} (atom^{-1})	1.77	1.80	1.77
n_{3d} (atom^{-1})	8.59	8.63	8.69
N [(Ry f.u.)$^{-1}$]	70.8	30.4	34.6
N_{4f} [(Ry f.u.)$^{-1}$]	5.6	17.1	20.4
N_{3d} [(Ry f.u.)$^{-1}$]	56.4	6.7	2.8

tinct separation region for $CeNi_2$. Therefore, the density of states at the Fermi energy is relatively high for the latter compound.

Although the above description in terms of a moving Fermi level usefully describes the gross features of the band structure, there is by no means any rigid band effects visible in the DOS for the different compounds. Rather, the details of the DOS vary a lot between the compounds. For CeNi both the features dominated by the Ni 3*d* and Ce 4*f* states are quite narrow, while the Ni 3*d* bands are relatively broad for $CeNi_5$ and $CeNi_2$. The Ce 4*f* bands are broadest in $CeNi_2$, which reflects the

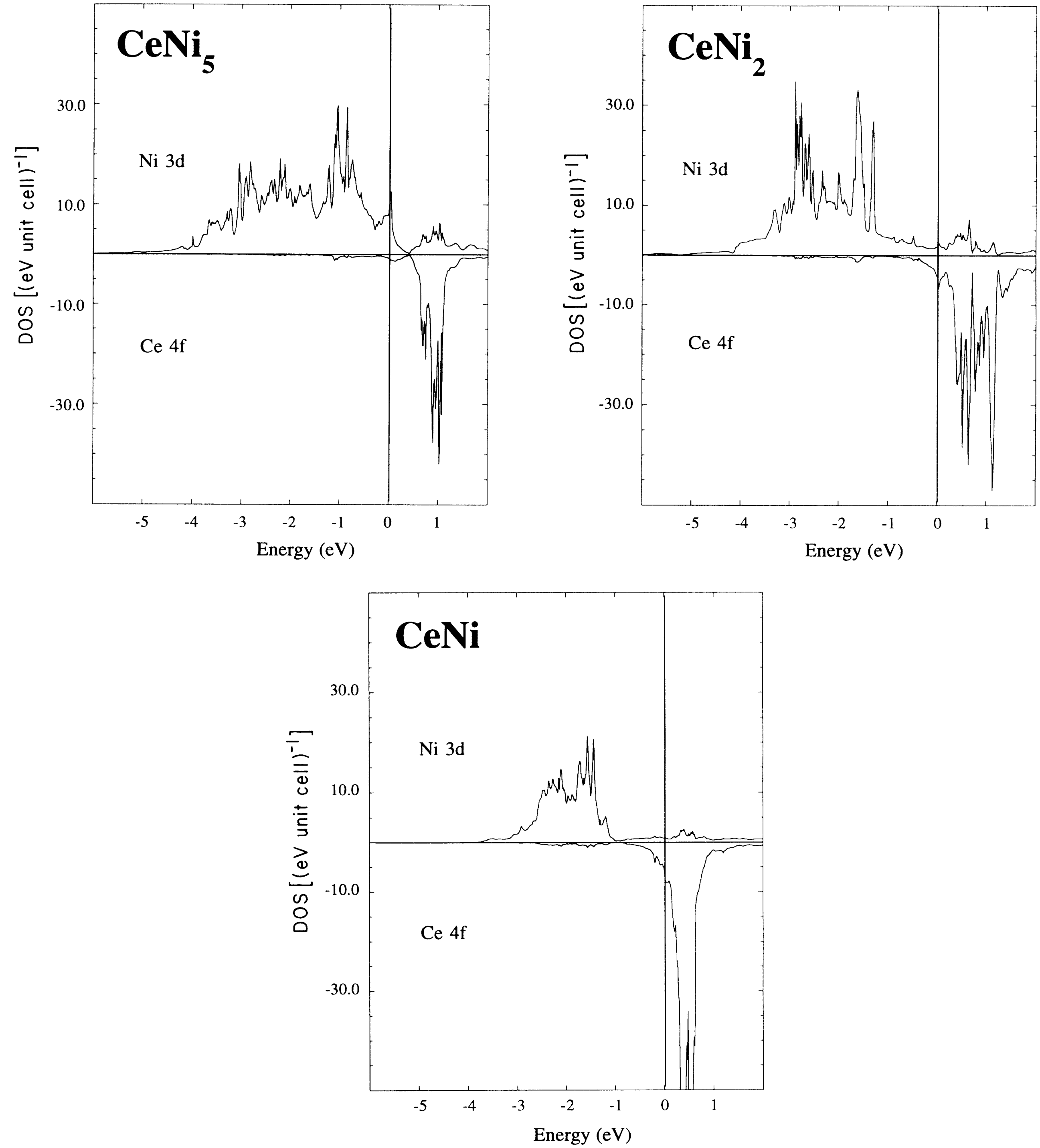

FIG. 2. The site and angular momentum projected density of states (for both spins and per unit cell) for Ni 3*d* (above zero) and Ce 4*f* (below zero) for the compounds (a) $CeNi_5$ (b) $CeNi_2$, and (c) CeNi. The Fermi level is at zero energy and is marked with a vertical line.

comparatively short Ce-Ce distance in this compound (Table I).

III. MAGNETIC PROPERTIES

In the theory of itinerant magnetism[19] the pure Pauli paramagnetic susceptibility, $\chi_0 = 2\mu_0 \mu_B^2 N$, is known to be enhanced by the intra-atomic exchange interaction, which results in the following expression for the susceptibility:

$$\chi = \frac{\chi_0}{1-\alpha} = S\chi_0 \ . \tag{1}$$

Here χ_0 is the susceptibility due to the density of states at the Fermi energy and S is the enhancement factor $S=(1-IN)^{-1}$ containing the Stoner product, $\alpha = IN$. χ is the uniform (i.e., the spatial average) susceptibility of the system. I is the Stoner integral representing the interaction, and N is the DOS per spin at the Fermi energy. It has been shown that in LSDA (Refs. 20–22) I can be calculated as

$$I = \sum_{t,l,l'} n_{tl} I_{tll'} n_{tl'} \ , \tag{2}$$

where $n_{tl} = N_{tl}/N$ and

$$I_{tll'} = \int_0^{S_t} r^2 K(r) \phi_l(\varepsilon_F, r) \phi_{l'}(\varepsilon_F, r) dr \ . \tag{3}$$

In Eq. (3), $K(r)$ is a function of the charge density,[21] $\phi_l(\varepsilon_F r)$ is the wave function of angular momentum l for states at the Fermi energy ε_F, and S_t is the radius of the atomic sphere around site t. In Eq. (2), N_{tl} is the site (t) and angular momentum (l) projected DOS at the Fermi energy.

The quantities entering Eqs. (1)–(3) were calculated self-consistently and are tabulated in Table III. The calculated local Stoner integrals $I_{tll'}$ are found not to vary very much between the compounds, which reflects that the integral is essentially an atomic quantity that does not change much from one crystal to another. As can be seen, the Stoner product is less than one for all three compounds. Hence, the Stoner criterion for an instability towards ferromagnetism is not fulfilled, in agreement with the fact that no magnetic ordering has been observed in these compounds. The calculated enhancement factor S is large for $CeNi_5$ and CeNi but is somewhat smaller for $CeNi_2$.

In general the microscopic response function χ is not uniform in space; the induced magnetization density has a large variation within the unit cell. As the dominant character of the DOS at the Fermi level for $CeNi_5$ originates from the Ni atoms, the largest response will occur on the Ni sites. On the other hand, for CeNi the main response will be located to the Ce atoms. This is in accordance with the results of the above-mentioned neutron experiments[12,13] for CeNi and $CeNi_5$. Especially when looking at the angular momentum projected DOS at the Fermi level (Table II) one can see that it is the Ni $3d$ and Ce $4f$, states, respectively, that are responsible for the large susceptibilities in $CeNi_5$ and CeNi. In the case of CeNi, the itinerant picture of the Ce $4f$ states give a largely enhanced susceptibility located at the cerium sites with the f states mainly responsible. This calculated fact explains very well the experimental observation that the induced magnetization is centered at the cerium sites.

In the derivation of Eq. (1) within LSDA, Vosko and Perdew (Ref. 20) made the ansatz that the magnetization has the same direction in the whole unit cell. This is a valid assumption for an elemental metal. This is however known not to be appropriate for ferromagnetically ordered intermetallic compounds between an early and a late transition element, e.g., $CeFe_2$ and $CeCo_5$ (Refs. 15 and 23), where the direction of the spin magnetization is opposite for the two different atom types.

In order to account for the spatial variation of the induced magnetization density, spin-polarized calculations with a magnetic field (corresponding to 10 T) included in the effective potential have been performed. The results of these calculations will also tell us about the accuracy of the above LSDA-Stoner treatment. The calculated induced local magnetic moments are collected in Table IV.

As can be seen, the so calculated magnetic moments are extremely large for the case of $CeNi_5$. This is however not an induced magnetization, since it turns out that a ferromagnetic state with quite small moments is actually more stable than the paramagnetic solution considered above. This is in contradiction to the calculated Stoner products and with experiment. However, the two states (the ferromagnetic and the paramagnetic state) are found to be very close in energy and this failure of the theory must be regarded as a minor one, since the compound is experimentally known to be close to a ferromagnetic instability. The calculated magnetism in $CeNi_5$ can, however, clearly be attributed to the nickel atoms, especially those with point symmetry *mmm*. We make the plausible assumption that the calculated magnetic moments are essentially proportional to the induced magnetic moments in the true paramagnetic state. Thus, the dominated contribution of the $3d$ electrons to the moments confirms our conclusion above that the magnetic proper-

TABLE III. The local Stoner integrals I_{ll} for l=Ce $4f$ and for l=Ni $3d$. The Stoner products $\alpha = IN$ and the corresponding enhancement $S=1/(1-\alpha)$.

Compound	$CeNi_5$	$CeNi_2$	CeNi
$I_{4f,4f}$ (mRy)	39.4	38.3	39.1
$I_{3d,3d}$ (mRy)	73.6	75.0	74.2
α	0.75	0.52	0.71
S	4.0	2.1	3.4

TABLE IV. Local and total spin magnetic moments induced by an applied magnetic field of 10 T (however, as regards $CeNi_5$ see comments in the text).

Compound	$CeNi_5$	$CeNi_2$	CeNi
m_{Ce} (units of μ_B/atom)	−0.010	0.014	0.022
m_{Ni} (units of μ_B/atom)	0.144	0.002	0.001
m_{tot} (units of μ_B/f.u.)	0.709	0.017	0.022

ties of $CeNi_5$ is governed by the Ni 3*d* states.

For $CeNi_2$ and CeNi there are induced moments mainly on the cerium site, while the nickel sites essentially remain nonmagnetic even in the magnetic field. From the induced magnetizations the susceptibilities can be estimated, assuming a linear dependence in the magnetic field, and these correspond to enhancement factors of 6.9 and 7.6 for $CeNi_2$ and CeNi, respectively.

It now seems clear that the LSDA-Stoner approach to the susceptibility underestimates the exchange enhancement as compared to self-consistent LSDA calculations. This is however in accord with the variational nature of the former method, i.e., it should give a lower bound to the true susceptibility. Our finding of a larger discrepancy between the two approaches than in an earlier investigation[21] is connected to the fact that in the latter case a system with only one atom per unit cell was considered, while for the present systems there are several types of atoms involved.

IV. DISCUSSION

In Table V some experimental data for the low-temperature susceptibility $\chi(0)$ and the linear coefficient of the specific heat γ are collected. These are compared with presently calculated values. Calculated susceptibilities both within the LSDA-Stoner theory and from the self-consistent calculation with a magnetic field included are tabulated. The theoretical value of γ is calculated from the well-known expression

$$\gamma=\frac{2\pi^2}{3}k_B^2 N \ , \tag{4}$$

where k_B is Bolzmann's constant, and N is as before the DOS, per spin and formula unit, at E_F. To make a comparison between the theoretical and experimental values of γ considerations of the enhancement due to the electron-phonon interaction have to be made. This gives typically a factor of about 1.5 to be multiplied to the theoretical values in Table V. In the theoretical susceptibility no consideration of the orbital contribution has been made. It is, however, assumed to be small in comparison with the strongly enhanced spin susceptibility encountered in the present type of systems.

TABLE V. Experimental values of the low-temperature magnetic susceptibility $\chi(0)$ and the coefficient of the linear term in the specific heat γ and the corresponding theoretical values. χ^{Stoner} is calculated with the Stoner-LSDA model and χ^{LSDA} is obtained from a self-consistent spin-polarized calculation. Also given is the enhancement of γ, $\gamma^{\text{expt}}/\gamma^{\text{theory}}$.

Compound	$CeNi_5$	$CeNi_2$	CeNi
$\chi^{\text{expt}}(0)$ (10^{-3} emu/mol)	3.0[a]	1.1[b]	1.8[c]
χ^{Stoner} (10^{-3} emu/mol)	1.4	0.31	0.56
χ^{LSDA} (10^{-3} emu/mol)		1.1	1.3
γ^{expt} [mJ/(mol K^2)]	40.0[d]	27[e]	65[c]
γ^{theory} [mJ/(mol K^2)]	24.8	10.6	12.1
$\gamma^{\text{expt}}/\gamma^{\text{theory}}$	1.6	2.5	5.4

[a] D. Gignoux *et al.*, Ref. 12.

[b] M. A. Sa *et al.*, Ref. 24.

[c] D. Gignoux *et al.*, Ref. 1.

[d] S. Nasu *et al.*, Ref. 25.

[e] A. Andraka, Timlin, and Mihalisin, Ref. 26.

The properties of $CeNi_5$ are very similar to those of YNi_5 and $LaNi_5$, which are both also enhanced Pauli paramagnets.[4] In Fig. 3 the calculated DOS for the three RNi_5 compounds are plotted together for comparison. The occupied part of the DOS is almost identical for the three different compounds with the exception for the states just around the Fermi level. Thus, for $CeNi_5$ the presence of 4*f* states and their hybridization with the Ni 3*d* states changes the detailed structure and produces a peak at the Fermi level, which in turn gives a slightly higher Stoner product for $CeNi_5$ than of the other two compounds. The magnetic properties of these three compounds are mainly governed by the Ni 3*d* states, which are responsible for the substantial enhancement of the susceptibility. The slightly larger DOS at E_F for $CeNi_5$ than for the other two compounds is in agreement with the experimental observation of a 30% larger low-temperature susceptibility for $CeNi_5$ than for YNi_5.[4]

The compounds CeNi and $CeNi_2$ are, on the other hand, known to have somewhat different properties, e.g., larger susceptibility and electronic specific heat, than corresponding compounds without 4*f* electrons (e.g., LaNi and YNi_2) (Refs. 1,26). This can be directly related to the cerium 4*f* states and their contribution to the DOS at the Fermi level found in this investigation (Fig. 2).

As regards the electronic contribution to the specific heat of $CeNi_5$, it can be accounted for (see Table V) by the present calculations, when an electron-phonon enhancement of 1.6 is assumed. For CeNi and $CeNi_2$, however, much larger enhancement factors are needed to account for the experimentally measured values, which

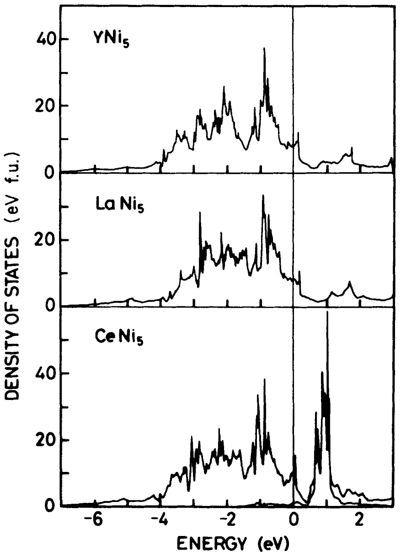

FIG. 3. Total density of states (for both spins) for YNi_5, $LaNi_5$, and $CeNi_5$. Also shown is the 4*f* projected DOS for $CeNi_5$. The Fermi level is at zero energy and is marked with a vertical line.

are actually too large to be ascribed entirely to electron-phonon interactions. Since the compounds are close to a magnetic instability spin fluctuations will be present. These paramagnons may give a substantial contribution to the specific heat,[27] which might explain part of the discrepancy between the presently calculated values and experiments. On the other hand, no large paramagnon effects on γ can be seen for $CeNi_5$, which is as equally close to a magnetic instability as the other two compounds. Hence the large electronic specific heat in CeNi, and the somewhat smaller one in $CeNi_2$, seem to originate from quasiparticles related to the presence of Ce $4f$ states at E_F. There are reports on Fermi surface studies of CeNi, where heavy mass quasiparticles have been observed.[28] The experimental value of γ is, however, somewhat too small for CeNi to be referred to as a heavy fermion system.

CeNi has been reported to undergo a phase transition at an applied pressure of 2 kbar with a large volume discontinuity of 12%.[29] This phase transition has been compared to the α-γ transition in cerium metal and been assumed to have the same origin as in pure cerium. Such an interpretation of the observed volume collapse is in direct conflict with the picture used in the present work for the Ce $4f$ states, since it assumes an essentially localized nature of the $4f$ states in the low pressure phase. However, as mentioned in the introduction, the CrB structure is a relatively open structure and the observed phase transition is known to be accompanied by a structural change, in contrast to the isostructural α-γ transition in Ce. Thus the volume collapse need not be of an electronic origin. Instead, we suggest that the volume change at the phase transition can be understood as a transition to a more close-packed structure, which to our knowledge has not yet been determined. Such a crystal transformation does not necessarily involve any fundamental change in the nature of the cerium $4f$ states.

V. CONCLUSIONS

When the results of *ab initio* electronic-structure calculations for the compounds $CeNi_x$ are compared with experimental data, some quantitative discrepancies can be distinguished. This should not come as a surprise, since the Ce $4f$ states, and also to some extent the Ni $3d$ states, are highly correlated, and such calculations as those reported here stretch the limits of LSDA. However, the qualitative agreement as regards nonmagnetic ground states exhibiting enhanced Pauli paramagnetism for all three compounds is satisfying. Also the experimental identification of the states responsible for this enhancement, namely, that they originate from the nickel atoms in $CeNi_5$, but cross over to originate from the cerium atoms in CeNi, is well accounted for in a model with itinerant Ce $4f$ states.

Even if we refer to heavy quasiparticles in order to explain the relatively large electronic specific heat in CeNi and $CeNi_2$, the magnetic properties are very well described in the calculations as due to itinerant Ce $4f$ states. It is worthwhile pointing out that the induced magnetization in an applied magnetic field (and thereby the spin susceptibility) is a ground-state property and therefore, in principle, is attainable within density functional theory, while the quasiparticle spectrum responsible for the electronic specific heat is not.

Even though no total energy calculations have been performed to determine the theoretical lattice constants (this is a considerable task for an orthorombic structure with three independent lattice constants), one can from the calculated pressures estimate that the calculated volumes are within a few percent of the experimental ones. In case the Ce $4f$ states would not be included in the electronic-structure calculations, but be treated as inert, larger discrepancies for the equilibrium volume would be obtained. In fact such calculations could not explain the dip in the volume for the cerium compounds (Fig. 1). Instead a picture with bonding $4f$ electrons seems to provide the most natural explanation of the so-called intermediate-valence behavior for the present $CeNi_x$ compounds. Recently we have shown that this also holds for the compounds $CeFe_2$, $CeCo_2$, and $CeCo_5$ (Refs. 15 and 23). Therefore, it seems appropriate to start questioning to what extent intermediate valence (in its original formulation) has any relevance at all for cerium systems with anomalous lattice constants, i.e., those systems that traditionally have been referred to as showing intermediate-valence behavior.

ACKNOWLEDGMENT

Lars Nordström and Börje Johansson want to thank the Swedish Natural Science Research Council for financial support.

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