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LETTER TO THE EDITOR

The self-consistent quasiparticle density of states of paramagnetic transition metals

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A widely accepted point of view is that a satellite structure in the nickel local density of states (LDOS) about 6 eV below the Fermi level arises from many-body effects within unfilled d bands (see, for example, Kisker 1983, Davis 1986, Liebsch 1979, Penn 1979). The problem of electron correlation is usually treated within the degenerate Hubbard Hamiltonian, either in the T-matrix approximation (Liebsch 1979, Drchal and Kudrnovsky 1980) or using non-self-consistent (NSC) second-order perturbation theory (SOPT) (Treglia *et al* 1980, 1982, Drchal and Kudrnovsky 1983). In particular, the NSC SOPT methods are frequently used to study Coulomb correlation effects in metals or their compounds (Bisi *et al* 1984, Calandra and Bisi 1985, Kulikov *et al* 1987).

In previous papers (Taranko *et al* 1987, 1988a, b) we have reported on self-consistent (SC) SOPT calculations of one-particle spectra of metals described by a simple model (rectangular and semielliptic) uncorrelated band local density of states. We have found that any additional (satellite) structure in one-particle spectra appearing in the NSC approach is smoothed out by the SC process. However, real metals reveal rather complicated structure of the density of states so we feel it to be necessary to verify again to what extent a more complex (d-band BCC canonical (Andersen *et al* 1985) and d-band nickel realistic (Riedinger and Nauciel-Bloch 1975)) band LDOS is modified by correlation effects. This Letter is organised as follows: firstly we present a short recapitulation of the SOPT approach developed by Treglia *et al* (1980) and describe the SC procedure; secondly we report on numerical results and give a short discussion.

We start with the Hamiltonian

$$H = H_0 + \frac{U}{2} \sum_{i\nu\nu'\sigma\sigma'} (1 - \delta_{\nu\nu'}\delta_{\sigma\sigma'}) n_{i\nu\sigma} n_{i\nu'\sigma'} \tag{1}$$

where H_0 is the band Hamiltonian, U is the average on-site Coulomb interaction, which is the same for each of the five d bands (label ν), σ denotes a spin variable and $n_{i\nu\sigma}$ is the particle number operator on the ith site. The one-particle spectrum is obtained by summing the imaginary part of the perturbed retarded Green function $G(\boldsymbol{k}, E)$ over wavevector $\boldsymbol{k}$:

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$$D(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\frac{1}{N}\sum_{\boldsymbol{k}} G(\boldsymbol{k}, E) = -\frac{1}{\pi}\,\mathrm{Im}\,\frac{1}{N}\sum_{\boldsymbol{k}} (E^{+} - \varepsilon(\boldsymbol{k}) - \Sigma(\boldsymbol{k}, E))^{-1} \tag{2}$$

where $\varepsilon(\boldsymbol{k})$ denotes a band energy and $\Sigma(\boldsymbol{k}, E)$ stands for the self-energy. If μ is the chemical potential of quasiparticles then at the absolute zero of temperature we have ($\mu = E_{\mathrm{F}}$)

$$n = \int_{-\infty}^{E_{\mathrm{F}}} D(E)\,\mathrm{d}E = N_{\mathrm{e}}/10 \tag{3}$$

where N_{e} is the number of electrons per site. We note that the quasiparticle Fermi energy E_{F} may differ from a one-electron Fermi level found in a band calculation.

The local approximation for the self-energy written in the first and second order in U/W (W denotes the one-electron band width) reads as (Treglia *et al* 1980)

$$\Sigma(E) = -\tfrac{9}{10}N_{\mathrm{e}}U + 9U^{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega_1\,\mathrm{d}\omega_2\,\mathrm{d}\omega_3}{E^{+} + \omega_1 - \omega_2 - \omega_3}$$
$$\times N(\omega_1\omega_2\omega_3)D(\omega_1)D(\omega_2)D(\omega_3) \tag{4}$$

where $D(\omega)$ is the quasiparticle local density of states,

$$N(\omega_1\omega_2\omega_3) = f(\omega_1)(1 - f(\omega_2))(1 - f(\omega_3)) + (1 - f(\omega_1))f(\omega_2)f(\omega_3)$$

and $f(\omega)$ stands for the Fermi distribution function. Since the local approximation makes the self-energy independent of wavevector $\boldsymbol{k}$ we may rewrite (2) as

$$D(E) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\infty}\frac{D_0(\eta)}{E^{+} - \Sigma(E) - \eta}\,\mathrm{d}\eta \tag{5}$$

where $D_0(\eta)$ is the uncorrelated LDOS corresponding to the band structure $\varepsilon(\boldsymbol{k})$.

To find $D(E)$ and E_{F} in a self-consistent way we start with the LDOS per site $D_0(E)$ and calculate the self-energy from (4). Then quasiparticle LDOS and Fermi level E_{F} are found from (5) and (3) and used as input data for an iteration process carried out using (4), (5) and (3).

We have solved (3)–(5) numerically for the paramagnetic state using d-band BCC canonical and d-band nickel realistic shapes of the uncorrelated LDOS with band fillings $N_{\mathrm{e}} = 7.3$ electrons/site (iron case) and 9.4 electrons/site (nickel case), respectively (Treglia *et al* 1982). The results are displayed in figures 1–4. The origin of the energy scale is set at the Fermi level in each case and one half of the one-electron band width is used as an energy unit.

In figures 1 and 2 we present the nickel and iron one-particle spectra calculated for various values of the parameter U/W. One can observe that for weak correlation strength, $U/W \leqslant 0.125$, there is practically no difference between the spectra obtained in SC and NSC ways. For stronger correlation strength, $U/W \geqslant 0.250$ in the iron case and $U/W \geqslant 0.5$ in the nickel one, a satellite stucture in the NSC one-particle spectra becomes clearly apparent. However, this structure is completely removed by the SC process and the SC one-particle spectra become almost structureless in comparison with the initial band density of states. From our previous results (Taranko *et al* 1987, 1988a, b) we expect that the satellite-like structure will appear in the NSC approach regardless of the shape of the uncorrelated LDOS and will always be smoothed out by the SC process.

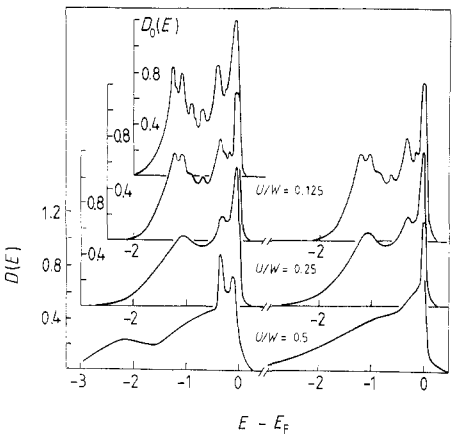

Figure 1. The nickel one-particle spectrum for different values of the correlation strength U/W. The NSC results are depicted on the left-hand side, and the SC results on the right-hand side.

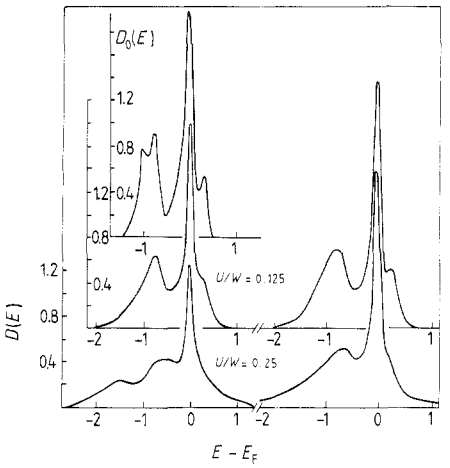

Figure 2. As figure 1, except that this is for the d-band BCC canonical LDOS (iron case).

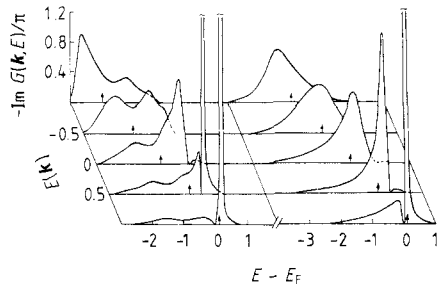

Figure 3. The nickel one-particle spectral density for $U/W = 0.5$ calculated in the NSC way (left-hand side) and the SC way (right-hand side).

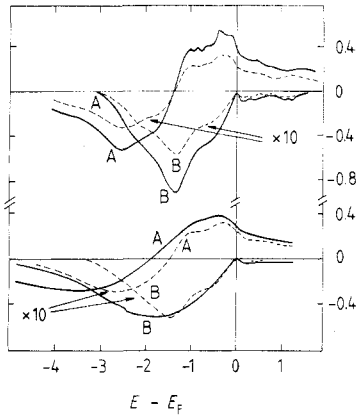

Figure 4. The imaginary (B) and real (A) components of the nickel self-energy calculated in the NSC way (upper part) and the SC way (lower part) for $U/V = 0.125$ (broken curve) and $U/W = 0.5$ (full curve).

In figure 3 we present the nickel spectral density of states calculated for $U/W = 0.5$ and plotted for several values of band energies between the bottom and top of the energy band. As is well known, the spectral density of one-electron band states leads to a set of δ-functions centred at energies denoted in figure 3 by arrows. The correlation effects make these functions shift and broaden. In the NSC approach, it follows from figure 3 that the quasiparticles are not well defined. However, the spectral density obtained in the SC way exhibits well defined peaks (although they are rather broad for energies near the bottom of the band) and one can obtain the correlated band structure from peak positions in a relatively simple way. As should be expected, for weak correlation strength

(typically $U/W \leqslant 0.125$), the differences between the shapes of spectral densities obtained in the NSC and SC ways are negligible and in both approaches we find well defined peaked structures centred at the corresponding band energies.

Finally, in figure 4, we give the nickel self-energy $\Sigma(E)$ curves (without the first-order term—see (4)) calculated for $U/W = 0.125$ and 0.5. Once again, one can observe that in the case of weak correlation strength the NSC approach gives quite satisfactory results. For stronger Coulomb correlations the self-energy calculated in the SC way differs significantly from the NSC one—in particular, we note its strongly delocalised character for states far below the Fermi energy.

In conclusion, there is no additional structure due to Coulomb correlations in the one-particle spectrum arising from the d-band BCC canonical and d-band nickel realistic uncorrelated LDOS when the correlation problem for the degenerate Hubbard Hamiltonian is studied using the SC SOPT. The details of the band LDOS survive in the SC one-particle spectrum for correlation strength $U/W \leqslant 0.125$. For a larger correlation strength the resulting SC one-electron spectrum is rather structureless.

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