A Comment on the Local Magnetic Moment in Ferromagnetic Dilute Alloys

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Recently, the magnetic properties in ferromagnetic dilute alloys have been studied in the Wolff-Clogston model for dilute alloys by taking into account exchange interactions among electrons in the host atoms.[1,2] (Hereafter, references 1 and 2 are referred to as W and YS, respectively.) The existence of a local magnetic moment and an off-diagonal spin correlation in the impurity ground state have been shown to be closely related to the occurence of localized spin excitations in W. In this short note, the local magnetic moment is calculated, by making use of the Green's function obtained in YS, and is compared with the result of W.

The one-particle Green's function up to the first-order terms with respect to Vo (the impurity potential) and δU (the difference between intra-atomic Coulomb integrals at the impurity and host atoms) in the Hartree-Fock approximation is given by

$$G_\sigma(k, k'; z)=\delta_{k,k'} G_{o\sigma}(k; z)+\frac{1}{N}G_{o\sigma}(k; z)v_\sigma(k-k')G_{o\sigma}(k'; z), \tag{1}$$

where $G_{o\sigma}(k; z)$ is the pure medium propagator given by (3. 8) in YS and $v_\sigma(k)$ is the screened impurity potential given by (3.13) in YS. In (1), the off-diagonal spin correlation is neglected. By making use of the Fourier transformed Green's function defined by

$$G_\sigma(R_l, R_j; z)=\frac{1}{N}\sum_{k,k'} G_\sigma(k, k'; z)\exp\left\{i(k\cdot R_l-k'\cdot R_j)\right\}, \tag{2}$$

and the expectation value of the number of electrons with spin σ on the Wannier site i given by

$$\langle n_{l\sigma}\rangle=-\frac{1}{\pi N}\int d\varepsilon f(\varepsilon)\mathrm{Im}G_\sigma(R_l, R_l; \varepsilon+i0^+), \tag{3}$$

we get

$$\langle n_{l\sigma}\rangle=\frac{1}{N}\sum_k f\left\{\varepsilon_\sigma(k)\right\}+\frac{1}{N^3}\sum_{k,k'}\frac{f\left\{\varepsilon_\sigma(k)\right\}-f\left\{\varepsilon_\sigma(k')\right\}}{\varepsilon_\sigma(k)-\varepsilon_\sigma(k')}$$

$$\times\sum_j v_\sigma(R_j)\cos\left\{k\cdot(R_l-R_j)\right\}\cos\left\{k'\cdot(R_l-R_j)\right\}, \tag{4}$$

where $f(\varepsilon)$ is the Fermi distribution function and

$$v_\sigma(R_j)=\frac{1}{N}\sum_k v_\sigma(k)\exp\left\{i(k\cdot R_j)\right\},$$

The second term in (4) gives $\Delta n_{i\sigma}(=\langle n_{i\sigma}\rangle - n_\sigma)$, where n_σ is the uniform value of $\langle n_{i\sigma}\rangle$ for the unperturbed ferromagnet. For the sake of simplicity, we assume that the unperturbed state is a saturated ferromagnetic one, so that the impurity potential of electrons with up spin cannot be screened. When the effective mass approximation is taken for $\varepsilon_\sigma(k)$, we get $\Delta n_{i\sigma}$ at OK as the similar expression as that obtained by Friedel[3] for a thin spherical well potential. In more general case, i. e., unsaturated ferromagnetic state including the higher-order terms with respect to V_0 and δU than the first-order terms, $\Delta n_{i\sigma}$ is non-zero. This result is inconsistent with the Wolfram's assumption of the existence of critical values of V_0 and δU for nonvanishing value of $\Delta n_{i\sigma}$.

Next, we discuss the one-particle Green's function $\hat{G}^b{}_{\sigma\sigma}(\omega)$ in W. In the region IIb in W where $\Delta n_{i\sigma}=0$, the one-particle Green's function $\hat{G}^b{}_{\sigma\sigma}(\omega)$ is obtained from the following equation of motion;

$$\hat{G}^b{}_{\sigma\sigma}(\omega)=\frac{1}{2\pi}\hat{I}+(\hat{E}+\hat{P}^b{}_\sigma)\hat{G}^b{}_{\sigma\sigma}(\omega), \tag{5}$$

where off-diagonal spin correlation is neglected and $\hat{I}$, $\hat{E}$ and $\hat{P}^b{}_\sigma$ are given by (7) and (19) in W. The diagonal matrix element of the Green's function $\left[\hat{G}^b{}_{\sigma\sigma}(\omega)\right]_{i,i}$ can be obtained from (5) and we get it as the same expression as (88) in W replacing ν_σ by

$$\nu_\sigma=2\pi(V_0+\delta U n_{-\sigma}). \tag{6}$$

From this Green's function and (3), we can obtain $\langle n_{i\sigma}\rangle$. For instance, when ν_σ in (6) is small, we can obtain the same one-particle Green's function as (1) replaced $v_\sigma(k)$ by ν_σ and $\langle n_{i\sigma}\rangle$ is obtained as (4). Then the Green's function $\hat{G}^b{}_{\sigma\sigma}(\omega)$ obtained in the region IIb of W (where $\Delta n_{i\sigma}=0$) gives the nonvanishing value of $\Delta n_{i\sigma}$.

It is concluded that $\Delta n_{i\sigma}$ is nonvanishing unless both values of V_0 and δU are zero and there is no critical value of V_0 and δU for the existence of the local magnetic moments. However, the induced moments obtained in (4) cannot be called as the "localized moments", because induced moments are proportional to the first-order terms with respect to V_0 and δU which are assumed to be small. For large values of V_0 and δU, the localized electronic state exists as discussed in W, so that there may exist localized magnetic moments.[4] In this case, the large moments in the host metal are induced near the impurity atom and decrease with increasing R_i.

References

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3) J. Friedel: Nuovo Ciment, Suppl. **2** (1958) 287.
4) T. Moriya: Proceedings of the International School of Physics "E. Fermi", Course 37, 1966 (Academic Press Inc., New York 1967) p. 206.