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'The Effect of Correlation in Insulating Antiferromagnets*

R. LUZZI

Instituto de Física Gleb Watayhin, Universidade Estadual de Campinas, Campinas SP

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The effect of correlation in split-band antiferromagnets is considered. It is shown that the correlation enhances the stability of the insulating antiferromagnetic state.

O efeito de correlação na teoria de Slater de antiferromagnetismo em isolantes é considerado. Mostra-se que o efeito de correlação contribue para a estabilização da fase antiferromagnética isolante.

In previous papers[1,2], a discussion was given of Slater's split band model of antiferromagnetism and its comparison with Anderson's theory of superexchange. As previously stated[2], the effective intra-atomic electron-electron interaction U was consistently considered as independent of the state of the system. In this note we discuss the effect of correlation on U and therefore its influence on the stability conditions. To accomplish this purpose we introduce a method devised by Kanamori to study correlation in ferromagnetic metals[3].

Following Kanamori, we consider first the multiple scattering between two electrons, whose Hamiltonian is

$$H = H_0(\mathbf{r}_1) + H_0(\mathbf{r}_2) + U\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{1}$$

where H_0 is the one-electron Hamiltonian whose eigenvalues and eigenfunctions, $\omega_{\mathbf{k}}^{\pm}$ and $\Psi_{\mathbf{k}}^{\pm}$, are given in (2). Let us write $\Phi(\mathbf{k}-, \mathbf{k}'-)$ for the antisymmetric unperturbed wavefunction formed with functions $\Psi_{\mathbf{k}}^{-}$ and $\Psi_{\mathbf{k}'}^{-}$. We write

$$\Psi(\mathbf{k}, \mathrm{k}') = \Phi(\mathbf{k}-, \mathbf{k}'-) + \sum_{pap'a'} \mathscr{C}_{p\alpha, p'\alpha'}^{\mathbf{k}-, \mathbf{k}'-} \Phi(\mathbf{p}\alpha, \mathbf{p}'\alpha'), \tag{2}$$

with $\mathrm{a}, \alpha' = +$ or $-$ for the wavefunction, solution of the Schroedinger

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'Postal address: Caixa Postal 1170, 13100 - Campinas SP.

equation

$$\mathrm{HYQ}, \mathbf{k}') = E(\mathbf{k}, \mathbf{k}')\Psi(\mathbf{k}, \mathbf{k}'). \tag{3}$$

The equation in first order for the $\mathscr{C}$'s and the expression for the energy eigenvalue $E(\mathbf{k}, \mathbf{k}')$ are

$$\begin{aligned} &\langle \Phi(\mathbf{p}\alpha, \mathbf{p}'\,\mathbf{a}') | \mathrm{H} | \mathrm{k}-, \mathbf{k}'-) + \sum_{484'\beta'} \mathscr{C}^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{q}\beta,\mathbf{q}'\beta'} . \\ &\langle \mathbf{p}\alpha, \mathbf{p}'\alpha' | \mathbf{H} | \mathbf{q}\beta, \mathbf{q}'\beta' \rangle = \langle \mathbf{k}-, \mathbf{k}'- | H | \mathbf{k}-, \mathbf{k}'- \rangle \mathscr{C}^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{p}\alpha,\mathbf{p}'\alpha'} \end{aligned} \tag{4}$$

and

$$\begin{aligned} E(\mathbf{k}, \mathbf{k}') = {} & (\mathbf{k}-, \mathbf{k}'- | \mathbf{H} | \mathbf{k}-, \mathbf{k}'- \rangle + \\ & + \sum_{\mathbf{p}\alpha,\mathbf{p}'\alpha'} \mathscr{C}^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{p}\alpha,\mathbf{p}'\alpha'} (\mathbf{k}-, \mathbf{k}'- | \mathbf{H} | \mathbf{p}\alpha, \mathbf{p}'\alpha' \rangle. \end{aligned} \tag{5}$$

Evaluating the matrix elements in (4), one finds, after a straight-forward algebra the solution

$$\mathscr{C}^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{p}\alpha,\mathbf{p}'\alpha'} = - \frac{(U/N)}{\omega^{\alpha}_{\mathbf{p}} + \omega^{\alpha'}_{\mathbf{p}'} - \omega^{-}_{\mathbf{k}} - \omega^{-}_{\mathbf{k}'}} \left[1 + (U/N) F(^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{p}\alpha,\mathbf{p}'\alpha'})\right]^{-1} \tag{6}$$

where

$$F(^{\mathbf{k}-,\mathbf{k}'-}_{\mathbf{p}\alpha,\mathbf{p}'\alpha'}) = \sum_{\mathbf{q}\beta\mathbf{q}'\beta'} \frac{\sin^2(\theta_{\mathbf{q}} - \theta_{\mathbf{q}'}) \delta(\mathbf{p} + \mathbf{p}' - \mathbf{q} - \mathbf{q}')}{\omega^{\beta}_{\mathbf{q}} + \omega^{\beta'}_{\mathbf{q}'} - \omega^{-}_{\mathbf{k}} - \omega^{-}_{\mathbf{k}'}} \tag{7}$$

Replacing this result into Eq. (5), and taking into account that the only possible contributions are from those matrix elements between occupied States $(\mathbf{k}-, \mathbf{k}'-)$ and empty states $(\mathbf{p}+, \mathbf{p}'+)$, one gets

$$E(\mathbf{k}, \mathbf{k}') = \omega^{-}_{\mathbf{k}} + \omega^{-}_{\mathbf{k}'} + \frac{(U/N) \sin^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}'})}{1 + (U/N) F(\mathbf{k}, \mathbf{k}')}, \tag{8}$$

where

$$F(\mathbf{k}, \mathbf{k}') = \sum_{\mathbf{p},\mathbf{p}'} \frac{\sin^2(\theta_{\mathbf{p}} - \theta_{\mathbf{p}'}) \delta(\mathbf{p} + \mathbf{p}' - \mathbf{k} - \mathbf{k}')}{\omega^{+}_{\mathbf{p}} + \omega^{+}_{\mathbf{p}'} - \omega^{-}_{\mathbf{k}} - \omega^{-}_{\mathbf{k}'}} \tag{9}$$

The energies $\omega^{\pm}_{\mathbf{k}}$ must now be interpreted as the self-consistent one-electron energies already derived in the presence of the modified interaction. The last term in Eq. (8) is the matrix element $\langle \Psi(\mathbf{k}, \mathbf{k}') | \mathrm{H} | \Psi(\mathbf{k}, \mathbf{k}') \rangle$. The Hartree-Fock solution[2] for the matrix element of the electron-electron interaction is $(U/N) \sin^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}'})$. Therefore, the correlation effect produces a screening of the intra-atomic electron-electron interaction, which can be

redefined as

$$u_{eff}(\mathbf{k}, z') = U/[1 + F(\mathbf{k},\mathbf{k}')] \tag{10}$$

Thus, all the results of Slater theory remain unchanged except for the formal replacement of U by expression (10).

Recalling the form of o, A and θ (Refs. 1,2) one sees that in the limit of small b/U, the term $(U/N)F(\mathbf{k},\mathbf{k}')$ becomes negligible. Hence, the screening factor approaches one and then the correlation gives no meaningful modification to the intra-atomic interaction.

The ground state energy is now

$$E_0 = \sum \frac{1}{2}(\varepsilon_{k+Q} + \varepsilon_k) - \sum \frac{1}{2}(\varepsilon_{k+Q} - \varepsilon_k)\cos 2\tilde{\theta}_k + \\ + \frac{1}{2}\sum \langle \Psi(\mathbf{k},\mathbf{k}')|V|\Psi(\mathbf{k},\mathbf{k}')\rangle. \tag{11}$$

The tilde over θ means, of course, that it is now depending on $u_{eff}(\mathbf{k},\mathrm{k}')$. In the limit of small band width, $T/U \ll 1$, with the Bloch energies ε_k given in tight binding approximation and retaining only the transfer integral b to nearest neighbours, one obtains for the screening factor to secon order in b/U

$$1 + (b/U)^2 \sum_{\tau} \sin^2 \frac{\mathbf{Q}\cdot\tau}{2}[1 - \exp - i(\mathbf{k} + \mathrm{k})\,.\,\tau], \tag{12}$$

where τ is the vector connecting nearest neighbour sites.

Keeping terms to order b^4/U^3, the difference between correlated and uncorrelated energies of the AFM ground state results to be $(-2\eta^2 b^4/U^3)$, where $\eta = \sum_{\tau} \sin^2(\mathbf{Q}\cdot\tau/2)$. The effect of correlation is then to improve the stability of the AFM phase. This is strictly a kinetic contribution equivalent to Anderson's biquadratic exchange[4]. This result can also be obtained in second order perturbation theory. The second order energy correction is

$$\delta E_{\mathrm{AFM}} = -\sum_i |\langle 0|V|i\rangle|^2/(E_i - E_0) \\ = -(U/N)^2 \sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} \frac{\sin^2(\theta_k - \theta_{k'})\sin^2(\theta_p - \theta_{p'})}{\omega_p^+ + \omega_{p'}^+ - \omega_k^- - \omega_{k'}^-}$$

which for $b/U \ll 1$ reproduces the result $(-2\eta^2 b^4/U^3)$.

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