Progress of Theoretical Physics, Vol. 68, No. 4, October 1982

Disordered Electronic Models and Impurity Spin Dynamics. I

—— *Ferromagnetic Ensemble and Mott Transition in an Exactly Solved Limit* ——

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(Received May 4, 1982)

Local gauge invariant n orbital models for elastic scattering of electrons in random potentials are extended to include local exchange interactions between electrons and magnetic impurities. The cooperation between local exchange interaction and electron hopping leads to ferromagnetic order in a low temperature phase for both the electronic and ionic subsystems. The critical temperature is proportional to the ensemble averaged exchange coupling. Ferromagnetic order implies spin split impurity bands in the electronic density of states. This as well as *dc* conductivity, internal energy, and magnetization is calculated exactly in the large n limit. The quasielectron states at E_F, wherever E_F comes to lie within the bands, can be classified as extended, i.e., conducting, in this limit. In the ferromagnetic phase, the proper variation of interaction parameters generates a Mott transition. The temperature- and magnetic field-dependence of the electronic magnetization is shown to be mean field like by using a high temperature expansion. It is also shown that an antiferromagnetic ensemble is always unstable and a spin glass phase is suppressed in the present models. The exact large n limit solutions render possible a future joint study in $O(1/n)$ of both the Kondo effect in the nonmagnetic phase of a disordered system and of the Anderson metal insulator transition.

§ 1. Introduction, results and expectations

Hope for problem formulation and solution in physics is often linked to the recognition of basic symmetries. For disordered electronic tight binding models Wegner discovered local gauge invariance as such a symmetry.[1] $1/n$ expansions for such n orbital models describing elastic electron scattering in random potentials revealed two (orthogonal or unitary) types of Anderson localization[2)~6)] and a related yet different universality class with symplectic symmetry.[7] There is extensive literature on related problems in the different and independent approach using weakly damped metallic electrons in lowest order approximation, e.g., Refs. 8), 9). The purpose of this paper is not to review or compare these different methods but to report on progress made in the many body theory for tight binding models with both elastic spinindependent scattering and local interactions of electron and impurity spins.

In the case of long range (Coulomb) electron electron interactions the author has previously given evidence for the Anderson metal insulator transition to become rather like an ordinary phase transition.[10] This is because firstly in-

elastic processes couple the diffusively singular particle hole channel of the density correlation into one particle observables. Thus the density of states $\rho(E_F)$ as the order parameter acquires critical behaviour. And secondly the long range of the interaction enhances the diffusion but the depletion of states at E_F cancels this effect.' These are effects in first order in $1/n$, while the large n limit only contains trivial Coulomb interaction effects like a shift of the chemical potential.

In this paper generalizations of the Kondo interaction between electronic spins and magnetic impurities are introduced in addition to local gauge invariant electronic submodels (mainly the real matrix ensemble[1),2),4)]) and rich behaviour already emerges in the large n limit. It is hoped that in a future study one can proceed beyond this leading order of the $1/n$-expansion in order to examine the Kondo effect in disordered systems (without the perturbative breakdown experienced when one or a very low concentration of magnetic impurities is implanted in pure systems[11)]) as well as the Anderson metal-insulator transition.

The models under consideration in this paper are based on the following grand canonical hamiltonian (where, as justified above, we omit the long range Coulomb interaction):

$$K=-\mu N_{\mathrm{el}}+H_0+H_{\mathrm{dis}}+H_{\sigma S} \tag{1·1}$$

with

$$H_0=-\omega_0\{\sum_{r\alpha}\hat{\sigma}^z_{r\alpha}+\sum_{r\bar{\alpha}}\hat{S}^z_{r\bar{\alpha}}\}, \tag{1·2a}$$

$$H_{\mathrm{dis}}=n^{-1/2}\sum_{r\alpha r'\beta\lambda}f_{r\alpha\lambda r'\beta\lambda}a^\dagger_{r\alpha\lambda}a_{r'\beta\lambda} \tag{1·2b}$$

and

$$H_{\sigma S}=-n^{-1}\sum_{r\alpha\bar{\alpha}}J^{\alpha\bar{\alpha}}_r\hat{\sigma}_{r\alpha}\cdot\hat{S}_{r\bar{\alpha}}\,. \tag{1·2c}$$

The electron spin operators $\hat{\sigma}_{r\alpha}$, where $\alpha=1\cdots n$ labels the n orbitals per site r, are given in terms of the electronic fermi operators $a_{r\alpha\lambda}$ by

$$\hat{\sigma}_{r\alpha}=\sum_{\lambda\lambda'}a^\dagger_{r\alpha\lambda}\sigma_{\lambda\lambda'}a_{r\alpha\lambda'} \tag{1·3}$$

with Pauli matrices σ and λ being the spin projection.

In (1·1) μ denotes the chemical potential and N_{el} is the conserved total number of electrons. The free hamiltonian H_0 determines the trivial spin dynamics in a small magnetic field h^z with the Larmor frequency $\omega_0=g\mu_B h^z$. The elastic scattering of electrons in spin-independent random potentials is represented by H_{dis}, where the $f_{r\alpha r'\beta}$ are independent, short-ranged, and gaussian

distributed random matrix elements with zero mean value. $H_{\rm dis}$ and the f-distribution form a disordered electronic submodel by itself, which is supposed to obey local gauge invariance as given in Ref. 1). In the large n limit, the real matrix (orthogonal) ensemble and the phase invariant (unitary) ensemble yield the same results, since they agree in the only contributing moment

$$\langle f_{ra r'\beta} f_{r'\beta ra}\rangle_{\rm Ens} = M_{r-r'} . \tag{1·4}$$

For the spin interaction $H_{\sigma s}$ we assume $\tilde{n}=n/k$ ionic spins labelled by $\tilde{\alpha}$ per occupied site. Instead of (1·3), the drone fermion representation[12),13)] is used for these spin operators, which is discussed in § 2.

We may distinguish two models:

i) $J_r^{a\tilde{a}}=J$ nonrandom, $\tilde{n}$ ionic spins per site: Model A, (1·5a)

ii) $J_r^{a\tilde{a}}$ random in Model B, (1·5b)

where in Model B the $J_r^{a\tilde{a}}$ are independent, gaussian distributed random variables with mean value J. Only in the large n limit the results for both models are identical, since for the present choice of normalization in (1·2c) the variance of J appears in $O(1/n)$ for the first time.

The ensemble averaged one electron propagator is local due to the local gauge invariance (see, e.g., Ref. 1)) and is defined by

$$\mathcal{G}_\lambda(\tau) = -\langle\langle T_\tau\{a_{ra\lambda}(\tau) a^\dagger_{ra\lambda}(0)\}\rangle_K\rangle_{\rm Ens} \tag{1·6}$$

in the Heisenberg picture of the finite temperature technique. The exact large n limit result for arbitrary temperature becomes

$$\mathcal{G}_\lambda^\infty(z_m) = \frac{2}{E_0^{\,2}}\{iz_m+\mu_\lambda-\sqrt{(iz_m+\mu_\lambda)^2-E_0^{\,2}}\}, \quad z_m=(2m+1)\pi k_B T , \tag{1·7}$$

where the temperature dependence is completely absorbed in the chemical potential given by

$$\mu_\lambda-\mu-\frac{1}{2}\lambda\omega_0 = \lambda\frac{J}{k}\langle\!\langle \tilde{S}^z\rangle\!\rangle^\infty_{\rm Ens} = \lambda\frac{J}{2k}\tanh(\beta\omega_0/2+\beta J m_{\rm el}/2), \tag{1·8}$$

while the integrated second moment (1·4) or $M(q)=E_0^{\,2}/4-Aq^2$ in Fourier space fixes E_0. The electronic magnetization $\frac{1}{2}m_{\rm el}$ per orbital is obtained from

$$m_{\rm el} = \frac{1}{V}\langle\!\langle \tilde{\sigma}^z\rangle\!\rangle^\infty_{\rm Ens} \tag{1·9a}$$

$$= \sum_\lambda \lambda T\sum_{z_m}\mathcal{G}_\lambda^\infty(z_m) e^{-iz_{m0-}} . \tag{1·9b}$$

Equations (1·7)~(1·9) form a self-consistency problem which as such becomes

trivial at $T=0$ and one finds, e.g., for $h^z=0$ and $E_F>E_0-J/(2k)$, $-E_0+J/(2k)<E_F<E_0+J/(2k)$,

$$m_{el}=\frac{1}{2}-\frac{E_F-\frac{J}{2k}}{E_0^2}\sqrt{E_0^2-\left(E_F-\frac{J}{2k}\right)^2}-\frac{1}{\pi}\arcsin\left(\left(E_F-\frac{J}{2k}\right)\Big/E_0\right). \quad (1\cdot10)$$

This is indeed the stable solution as shown in § 4. A high temperature expansion for

$$m_{el}=2/(\pi E_0^2)\int_{-E_0}^{E_0}d\varepsilon\{f(\varepsilon-\mu_\uparrow)-f(\varepsilon-\mu_\downarrow)\}\sqrt{E_0^2-\varepsilon^2} \quad (1\cdot11)$$

shows that the ferromagnetic phase transition occurs at

$$T_c=\frac{1}{2}\sqrt{\frac{1}{2k}}J\,, \quad (1\cdot12)$$

and that the magnetization behaves mean field like

$$(m_{el})^2=3t/k+O(t^2) \quad \text{for } t=(T_c-T)/T_c>0 \text{ and } h^z=0 \quad (1\cdot13a)$$

and

$$m_{el}\propto(h^z)^{1/3} \quad \text{for } T=T_c\,. \quad (1\cdot13b)$$

Below T_c the impurity band becomes spin split even in zero magnetic field. The density of states as derived from

$$\rho_\lambda(E)=-\pi^{-1}\,\mathrm{Im}\;G_\lambda^R(E+io) \quad (1\cdot14)$$

shows semi circular behaviour with

$$\rho_\lambda^\infty(\varepsilon)=2/(\pi E_0^2)\sqrt{E_0^2-(\varepsilon+\mu_\lambda)^2}\,, \quad |\varepsilon+\mu_\lambda|<E_0\,, \quad \varepsilon=E-\mu\,. \quad (1\cdot15)$$

The bands can be shifted relative to one another by variation of the exchange coupling J. Thus, e.g., for half filled bands at $J=0$, i.e., $E_F=0$, and for $T=h^z=0$, a Mott transition occurs at

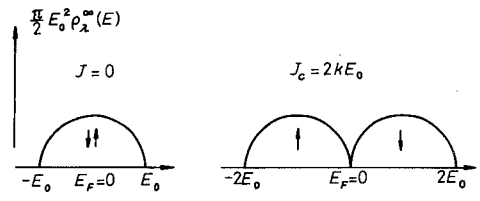

Fig. 1. Half-filled spin-up and -down bands for $J=0$ (a) and spin-splitting for the critical value $J_c=2kE_0$ of the Mott transition.

$$J_{c_M}=2kE_0 \tag{1·16}$$

as illustrated in Fig. 1.

§ 2. Models

a. *Probability distributions*

The number of random variables in the models (1·1)~(1·5) is different according to the different intentions. In any case, however, the disordered electronic submodel (1·2b) is contained. Its random matrix elements $f_{ra r'\beta}$ are distributed by

$$P_1(\{f\})=(2\pi M_{r-r'})^{-1/2}\exp\{-|f_{ra r'\beta}|^2/(2M_{r-r'})\}, \tag{2·1}$$

where the f's are assumed to be short ranged in $r-r'$ (and so is $M_{r-r'}$), but infinitely long ranged in the orbital labels. Spin orbit coupling and hence spin-dependent f's are not considered in this paper. In the case of time reversal invariance the f's are real, and the electronic submodel (1·2b)/(2·1) is just the real matrix (orthogonal) ensemble.[3] In the presence of a small magnetic field however, the f's change into[14]

$$f^H_{ra r'\beta}=\exp\Big(-\frac{ie}{2\hbar c}H\cdot(r'\times r)\Big)f^{H=0}_{ra r'\beta}\,. \tag{2·2}$$

In contrast to the Zeeman term this phase factor, which represents the orbital effect, cancels out, e.g., in the large n limit and survives only in particle-particle type scattering in the form of accumulating phase factors.[15]

The introduction of a nonrandom exchange interaction $H_{\sigma s}$ in the definition of Model A forms the simplest way to include many body effects from short ranged spin interactions. In the more realistic model B the exchange couplings $J_r^{\alpha\beta}$ are assumed to be independent and gaussian distributed by

$$P_2(\{J_r^{\alpha\beta}\})=(2\pi\Delta)^{-1/2}\exp(-(J_r^{\alpha\beta}-J)^2/(2\Delta)). \tag{2·3}$$

We also assume that each complex has $\tilde{n}=O(n)$ spins, i.e., $k=O(1)$. Thus in an extrapolation of the $1/n$ expansion one may think of one impurity spin at one R_i and an arbitrary finite number of electronic orbitals at the same site. The total probability distribution for the ensemble is given by the product

$$P_1(\{f\})P_2(\{J_r^{\alpha\beta}\}). \tag{2·4}$$

Finally it is worth noting the difference between the distribution $P_2(\{J_r^{\alpha\beta}\})$ and the one used in the Sherrington-Kirkpatrick model.[16] The present choice of the normalization factor $1/n$ in $H_{\sigma s}$ (n corresponds to the number N of spins in the

SK model) and the intrinsic character of J and Δ (in contrast to the N-scaled quantities in the SK-model) suppresses a spin glass phase for all J at least in the large n limit.

b. *Fermion representation of* $H_{\sigma s}$

Several years ago Spencer discussed the use of the drone-fermion representation of spin operators of arbitrary quantum number. The Wick theorem and the linked cluster theorem are still valid in the new representation. The spin commutation rules, which are fermi-like at equal sites and bose-like at different sites, are reproduced by two independent fermion fields. Even for $S=1/2$, where (with $\tilde{\alpha}=1, 2, \cdots, n/k$)

$$\hat{S}^z_{r\tilde{\alpha}}=c^\dagger_{r\tilde{\alpha}}c_{r\tilde{\alpha}}-\frac{1}{2}, \quad \hat{S}^+_{r\tilde{\alpha}}=\hat{S}^x_{r\tilde{\alpha}}+i\hat{S}^y_{r\tilde{\alpha}}=c^\dagger_{r\tilde{\alpha}}\phi_{r\tilde{\alpha}}=c^\dagger_{r\tilde{\alpha}}(d_{r\tilde{\alpha}}+d^\dagger_{r\tilde{\alpha}}), \tag{2·5}$$

if $c_{r\tilde{\alpha}}$, $d_{r\tilde{\alpha}}$ (drones) are the two independent fermi (destruction) operators in occupation number space, this representation is useful, since it separates spin-flipping and nonflipping terms. By insertion of (2·5) the explicit fermion representation of the grand canonical hamiltonian (with $S=1/2$ magnetic impurities) becomes

$$\begin{aligned}K=&-\mu N_{\mathrm{el}}-\frac{1}{2}\omega_0\sum_\lambda \lambda N_\lambda-\omega_0\sum_{r\tilde{\alpha}}(c^\dagger_{r\tilde{\alpha}}c_{r\tilde{\alpha}}-1/2)\\&+n^{-1/2}\sum f_{r\alpha r'\beta}a^\dagger_{r\alpha\lambda}a_{r'\beta\lambda}\\&-n^{-1}\sum J^{\tilde{\alpha}\beta}_r\{c^\dagger_{r\tilde{\alpha}}(d_{r\tilde{\alpha}}+d^\dagger{}_{r\tilde{\alpha}})a^\dagger_{r\beta\downarrow}a_{r\beta\uparrow}+(d_{r\tilde{\alpha}}+d^\dagger{}_{r\tilde{\alpha}})c_{r\tilde{\alpha}}a^\dagger_{r\beta\uparrow}a_{r\beta\downarrow}\}\\&-n^{-1}\sum J^{\tilde{\alpha}\beta}_r\lambda(c^\dagger_{r\tilde{\alpha}}c_{r\tilde{\alpha}}-1/2)\hat{n}_{r\beta\lambda},\end{aligned} \tag{2·6}$$

where $\hat{n}$ is the electron density operator, while N_{el} is a c-number, since the total number of electrons is conserved. There is also a particle hole symmetry in the model. Moreover, a spin-independent local gauge invariance, as primarily required for the second line only is naturally maintained in the whole hamiltonian.

§ 3. Propagators in the large n limit

The propagators are calculated in the interaction picture with a free grand canonical hamiltonian K_0 and the U-matrix

$$U(\beta)=T_\tau\exp\left(-\int_0^\beta d\tau'(K(\tau')-K_0(\tau'))\right) \tag{3·1}$$

of standard finite temperature technique.[17] The one particle Greens functions for the three fermion fields are local leaving propagation in space exclusively to

the impurity-induced 'electron interaction' $M_{r-r'}$. From

i) $$\mathcal{G}_\lambda(\tau)=-\langle\langle T_\tau\{a_{r\alpha\lambda}(\tau)a^\dagger_{r\alpha\lambda}(0)U(\beta)\}\rangle_0/\langle U(\beta)\rangle_0\rangle_{\mathrm{Ens}} \tag{3·2a}$$

with $$a^\dagger_{r\alpha\lambda}(\tau)=\exp(K_0\tau)a^\dagger_{r\alpha\lambda}\exp(-K_0\tau)=\exp((\lambda\omega_0/2+\mu)\tau)a^\dagger_{r\alpha\lambda}\,, \tag{3·2b}$$

ii) $$C(\tau)=-\langle\langle T_\tau\{c_{r\alpha}(\tau)c^\dagger_{r\alpha}(0)U(\beta)\}\rangle_0/\langle U(\beta)\rangle_0\rangle_{\mathrm{Ens}} \tag{3·3a}$$

with $$c^\dagger_{r\alpha}(\tau)=\exp(-\omega_0\tau)c^\dagger_{r\alpha}\,,\quad \langle c^\dagger_{r\alpha}c_{r\alpha}\rangle_0=(\exp(-\beta\omega_0)+1)^{-1}\,, \tag{3·3b}$$

iii) $$F(\tau)=-\langle\langle T_\tau\{\phi_{r\alpha}(\tau)\phi_{r\alpha}(0)U(\beta)\}\rangle_0/\langle U(\beta)\rangle_0\rangle_{\mathrm{Ens}} \tag{3·4a}$$

with $$\phi_{r\alpha}(\tau)=\phi_{r\alpha}\quad\text{and}\quad\langle d^\dagger_{r\alpha}d_{r\alpha}\rangle_0=1/2\,, \tag{3·4b}$$

one obtains the interaction-free (not yet large n limit) solutions

i) $$\mathcal{G}_\lambda{}^0(z_m)=(iz_m+\mu+\lambda\omega_0/2)^{-1} \tag{3·5}$$

ii) $$C^0(z_m)=(iz_m+\omega_0)^{-1} \tag{3·6}$$

and

iii) $$F^0(z_m)=2/(iz_m). \tag{3·7}$$

For the results of § 1 we need neither $F^0(z_m)=F^\infty(z_m)$ nor the spin flip propagator, which becomes $C^0(\tau)F^0(\tau)$ for $K=K_0$. To obtain the large n limit for i) and ii) we have to sum all combinations of tree insertions from disorder scattering and of Hartree-like terms from the spin interaction. This is shown in Figs. 2(a) and (b) for Model A and Model B respectively. In the latter model the

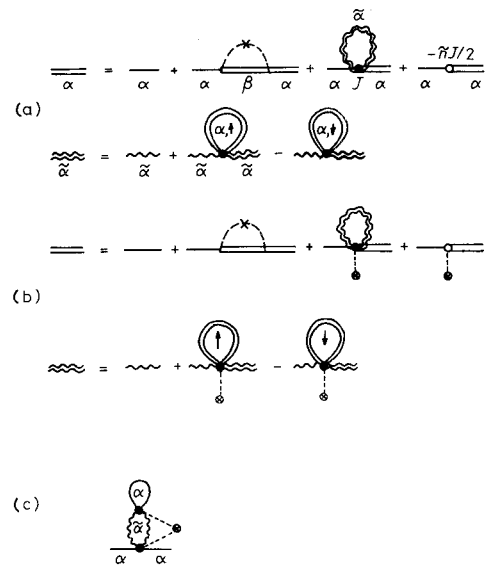

Fig. 2. Large n limit Dyson equations for the one particle Greens functions $\mathcal{G}$ (straight lines) and C (wavy lines) are shown for Model A and Model B in (a) and (b) respectively. In (b) the exchange coupling is a random field and is represented by a dotted line with crossed circle end for the ensemble average. A simple cross means an f-average and α stands for (r,α). (c) shows an $O(1/n)$ graph of Model B.

exchange constant is a random field itself, but writing out diagrams like in Fig. 2(c) one finds that nontrivial averages of these fields are eliminated in the large n limit. Note that this does no longer hold, if we change the normalization factor $1/n$ of $H_{\sigma s}$ into $1/\sqrt{n}$ which is possible for the special case of a zero mean value of the exchange coupling. Diagram summations are then highly nontrivial, which is probably related to the spin glass problem as in the Sherrington-Kirkpatrick model.[14),15)]

For the present model B, however, Fig. 2(b) yields the following exactly solvable coupled integral equations (according to the usual diagrammatic rules)

$$\mathcal{G}_\lambda^\infty(z_m)=\mathcal{G}_\lambda^0(z_m)+(\sum_r M_{r-r'})\mathcal{G}_\lambda^0(z_m)(\mathcal{G}_\lambda^\infty(z_m))^2$$
$$+J/k\,\mathcal{G}_\lambda^0(z_m)\mathcal{G}_\lambda^\infty(z_m)T\sum_n(C^\infty(z_n)-1/2), \tag{3·8}$$

$$C^\infty(z_m)=C^0(z_m)+\sum_\lambda \lambda JT\sum_n \mathcal{G}_\lambda^\infty(z_n)C^0(z_m)C^\infty(z_m). \tag{3·9}$$

The large n solution for C, which is essentially the S^z-propagator, becomes

$$C^\infty(z_m)=(iz_m+\omega_0+Jm_{\mathrm{el}})^{-1}, \tag{3·10}$$

while the result for $\mathcal{G}_\lambda^\infty$ is given by (1·7).

§ 4. Ferromagnetic order and a Mott transition

The present models contain electron hopping and local interactions $H_{\sigma s}$ between electronic spins and impurity spins. As a combined effect this implies nonlocal spin spin interactions of the form $\hat{\sigma}_{r\alpha}\hat{\sigma}_{r'\beta}$ and $\hat{S}_{r\alpha}\hat{S}_{r'\beta}$ respectively, whence the question of long range magnetic order arises. Recalling the still unsolved problems of the transition between atomic limit and band limit of the Hubbard model[11)] our disordered models offer an exactly solvable limit (and the possibility of systematic expansions) for this and other problems in a modified physical context.

In order not to rule out antiferromagnetic order artificially, one has to allow for an r-dependence of one particle Green's functions, thus assuming the restricted antiferro-translational invariance for the ensemble. In the Appendix it is shown however that the antiferromagnetic solution is not stable. Since a spin glass phase can also be ruled out, the full translational invariance as contained in Eqs. (3·2) is a correct choice.

The selfconsistent solution for the electronic magnetization derived from (1·7)~(1·9) becomes

$$m_{\mathrm{el}}=\sum_\lambda \lambda\left(\frac{1}{\pi E_0{}^2}\mu_\lambda\sqrt{E_0{}^2-\mu_\lambda{}^2}+\frac{1}{\pi}\arcsin\left\{\frac{\min(\mu_\lambda, E_0)}{E_0}\right\}\right)\theta(E_0{}^2-\mu_\lambda{}^2) \tag{4·1}$$

with μ_λ given by (1·8). This is valid at finite temperatures too and obviously contains a nonmagnetized solution as well. The selfconsistent structure simplifies in the zero temperature limit and one finds for $h^z=0$ Eq. (4·1) with

$$\mu_\lambda=E_F+\lambda\frac{J}{2k}\{\theta(Jm)-\theta(-Jm)\},\qquad \theta(0)=1/2\,. \tag{4·2}$$

The sign of J only determines the relative direction of electronic and ionic magnetization and for $J\neq 0$ there is always a solution with finite $m_{\rm el}$, whereof Eq. (1·10) gives one example. That these ferromagnetic solutions are indeed the stable ones is shown by a calculation of the energy (in the large n limit)

$$\begin{aligned}U^\infty=\langle\!\langle H\rangle\!\rangle^\infty_{\rm Ens}&=n^{-1/2}\sum\langle f_{ra r'\beta}\langle a^\dagger_{ra\lambda}a_{r'\beta\lambda}\rangle_K\rangle_{\rm Ens}\\&-n^{-1}\sum\langle J_r^{\alpha\beta}\langle(c^\dagger_{ra}c_{r\alpha}-1/2)\lambda a^\dagger_{r\beta\lambda}a_{r\beta\lambda}\rangle_K\rangle_{\rm Ens}\,.\end{aligned} \tag{4·3}$$

For finite spontaneous magnetization we obtain at $T=0$ and $h=0$

$$\begin{aligned}U^\infty=&-nV\frac{2}{3\pi E_0{}^2}\sum_\lambda\left(E_0{}^2-\left(E_F+\lambda\frac{J}{2k}\right)^2\right)^{3/2}\theta\left(E_0{}^2-\left(E_F+\lambda\frac{J}{2k}\right)^2\right)\\&-nVJk^{-1}\langle\!\langle\hat{S}^z\rangle\!\rangle^\infty m_{\rm el}\,,\end{aligned} \tag{4·4}$$

while $U^\infty(m_{\rm el}=0)$ can be formally obtained by putting $J=0$ in (4·4). Comparing these contributions shows that ferromagnetic ordering lowers the energy for all finite J.

Ferromagnetic order means that the density of states for up and down spin of electrons are no longer equal. The shift of the centers of the impurity bands relative to each other depends on J. Thus by varying the interaction strength one can induce a *Mott transition,* which occurs when the impurity bands have zero overlap and the Fermi energy happens to coincide with one of the band edges. The symmetric case was discussed in the introduction. Note that the same Mott transition could also be generated by variation of, e.g., E_0, ω_0, or k keeping J fixed.

The *dc* conductivity can be obtained from a 'many body theoretic analog' (which is derived elsewhere[18]) of the Kubo-Greenwood formula

$$\mathrm{Re}\,\sigma(\omega+io)=-V^{-1}e^2\omega\sum_{\mu\nu}\frac{\partial^2}{\partial q^2}\,\mathrm{Im}\,D_R^{\mu\nu}(q,\omega)\Big|_{q=0}\,, \tag{4·5}$$

where $D_R^{\mu\nu}$ is the proper density response function obtained from the Matsubara density fluctuation propagator

$$\mathcal{D}^{\mu\nu}(r,\tau)=-\langle\langle T_\tau\{\tilde{n}_{r\mu}(\tau)\tilde{n}_{0\nu}(0)\}\rangle_K\rangle_{\rm Ens}\,,\quad \tilde{n}=\hat{n}-\langle\hat{n}\rangle\,. \tag{4·6}$$

In the large n limit we obtain

$$\sigma_{dc}=2\pi ne^2 A V^{-1}\sum_{\lambda}\{\rho_{\lambda}^{\infty}(E_F)\}^2 . \tag{4·7}$$

Let us finally analyze the destruction of ferromagnetic order near the critical point T_c. We may apply a high temperature expansion to (1·11) for a qualitative study.

Then we find

$$m_{\mathrm{el}}=\frac{\beta}{4}(1-\beta^2 E_0{}^2/16)(\mu_{\uparrow}-\mu_{\downarrow})-\frac{\beta^3}{48}(\mu_{\uparrow}{}^3-\mu_{\downarrow}{}^3)+O(\beta^5)$$

with

$$\mu_{\lambda}=\mu+\lambda\frac{\beta}{4k}J^2 m_{\mathrm{el}}-\lambda\frac{\beta^3}{48k}J^4 m_{\mathrm{el}}^3+O(\beta^5). \tag{4·8}$$

Thus, for $\beta E_0\ll 1$, the magnetization vanishes mean field like as given by (1·12) and (1·13).

Acknowledgements

The author wishes to thank H. Horner, F. Wegner and K. Ziegler for discussion. He is especially grateful to A. Khurana for careful reading and to H. Horner for pointing out the relationship with the Sherrington-Kirkpatrick model.

This work has been supported in part by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereigh 123 (Heidelberg).

Appendix

The ensembles considered here do not exclude antiferromagnetic order a priori but it will be shown that this state is thermodynamically unstable. But let us anticipate a plausible argument which favours a ferromagnetic ensemble in comparison with the antiferromagnetic solution: Since an electron cannot flip its spin while hopping from site to site by elastic disorder scattering (with $M_{r-r'}$ as given by (1·4)) and since in an antiferromagnetic state the nearest neighbour site offers a higher density of states for the flipped spin, the antiferro-order hinders this hopping for a majority of electrons. And since all energies within the impurity bands are conducting in the large n limit, hopping is expected to lower the energy and hence the ferromagnetic order should lower the energy in comparison with the antiferro-ensemble.

The calculation of the energy starts again from Eq. (4·3). Under the assumption of antiferro-order one has translational invariance of the ensemble with twice the lattice constant. Let $r+\delta$ denote the nearest neighbour sites of r, then

$$\mathcal{G}_{r+\delta,\lambda}=\mathcal{G}_{r,-\lambda} \tag{A·1}$$

because, according to $m_r=\mathcal{G}_{r\uparrow}(\tau=0_-)-\mathcal{G}_{r\downarrow}(0_-)$, the magnetization m_r reverses its sign under $\lambda\to-\lambda$. Let us moreover assume $M_{r-r'}$ to be of very short range and expand about its maximum M_0

$$M_{r-r'}=M_0+\nabla M_0\delta+\frac{1}{2}\Delta M_0\delta^2+O(\delta^3),\qquad \delta=r-r', \tag{A·2}$$

in order to study the contribution from nearest neighbour hopping explicitly. The decisive part of U^∞ is the first line in (4·3) which now becomes proportional to

$$\sum_{rr'}M_{r-r'}T\sum_{\lambda,\varepsilon_n}\mathcal{G}_{r,\lambda}(\varepsilon_n)\mathcal{G}_{r'\lambda}(\varepsilon_n)$$
$$=zVM_0\Pi_1(0)+zV(M_0+\Delta M_0a^2/2)\Pi_2(0) \tag{A·3}$$

with the polarization parts (a: lattice constant)

$$\Pi_1(0)=T\sum_{\varepsilon_n,\lambda}\mathcal{G}^2_{r\lambda}(\varepsilon_n),\quad \Pi_2(0)=T\sum_{\varepsilon_n,\lambda}\mathcal{G}_{r\lambda}(\varepsilon_n)\mathcal{G}_{r,-\lambda}(\varepsilon_n). \tag{A·4}$$

In the ferromagnetic case only Π_1 appears in (A·3) and we thus have to calculate the change due to Π_2. Gathering contributions from the cuts of the integrand in the complex plane we obtain

$$\Pi_2{}^R(0)=\frac{4}{\pi F_0{}^4}\sum_\lambda\int_{-E_0-\mu_\lambda}^{E_0-\mu_\lambda}d\varepsilon f(\varepsilon)(\varepsilon+\mu_{-\lambda})\sqrt{E_0{}^2-(\varepsilon+\mu_\lambda)^2}$$
$$+\frac{4}{\pi E_0{}^4}\sum_\lambda\int_{\lambda E_0-\mu_\lambda}^{\lambda E_0-\mu_\lambda}d\varepsilon f(\varepsilon)\sqrt{(\varepsilon+\mu_\lambda)^2-E_0{}^2}\,\sqrt{E_0{}^2-(\varepsilon+\mu_{-\lambda})^2}\,. \tag{A·5}$$

At $T=h^z=0$ and for $-E_0<\mu_\downarrow<\mu_\uparrow<E_0$ we obtain for the first line of (A·5)

$$-\frac{8}{3\pi E_0{}^4}\sum_\lambda(E_0{}^2-\mu_\lambda{}^2)^{3/2}+8\frac{J}{k}\langle\!\langle\hat{S}^z\rangle\!\rangle_m\,, \tag{A·6}$$

where the first term equals $\Pi_1{}^R(0)$ and the second term is always positive as is the second line of (A·5). Note that $\langle\!\langle\hat{S}^z\rangle\!\rangle_r m_r$ is r-independent. The final conclusion is that the ferromagnetic ground state has a lower energy than the hypothetical antiferromagnetic state.

References

1) F. Wegner, Phys. Rev. **19** (1979), 783.
2) R. Oppermann and F. Wegner, Z. Phys. **B34** (1979), 327.
3) F. Wegner, Z. Phys. **B35** (1979), 207.
4) L. Schäfer and F. Wegner, Z. Phys. **B38** (1980), 113.
5) K. Jüngling and R. Oppermann, Z. Phys. **B38** (1980), 93.
6) R. Oppermann and K. Jüngling, J. of Phys. **C14** (1981), 3745, 3757.

7) Ref. 5) and S. Hikami, A. I. Larkin and Y. Nagaoka, Prog. Theor. Phys. **63** (1980), 707.
8) E. Abrahams, P. W. Anderson, D. C. Licciardello and T. V. Ramakrishnan, Phys. Rev. Letters **42** (1979), 673.
9) S. Hikami, Prog. Theor. Phys. **64** (1980), 1466.
10) R. Oppermann, *Proc. Int. Conf. 'Disordered systems and localization' Rome, Lecture Notes in Physics* (1981), 257.
11) S. Doniach and E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin, London, 1974).
12) H. J. Spencer, Phys. Rev. **171** (1968), 515.
13) D. C. Mattis, *Theory of Magnetism* (Harper and Row, New York, 1965).
14) T. Matsubara and T. Kaneyoshi, Prog. Theor. Phys. **40** (1968), 1257.
15) B. L. Altshuler, D. Khmelnitskii, A. I. Larkin and P. A. Lee, Phys. Rev. **B22** (1980), 5142.
16) D. Sherrington and S. Kirkpatrick, Phys. Rev. Letters **35** (1975), 1972.
17) A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, 1971).
18) R. Oppermann, "Habilitationsschrift" (in German), (Heidelberg, 1981), unpublished.