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# Some comments on Kondo lattices and the Mott transition

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**Abstract.** The so called exhaustion problem occurs when few electrons have to screen many spins in a metal with magnetic impurities. A singlet Fermi liquid ground state is possible only if all impurities are "isotropized" in such a way as to suppress their entropy. That takes a time $\tau_c$ and the corresponding energy $\epsilon_c = \hbar/\tau_c$ limits the Fermi liquid range. The present note explores that issue of time and energy scales, and it concludes that $\epsilon_c$ is much smaller than the single impurity Kondo temperature. Similarly the relevant energy scale is proportional to the number of electrons. Recent results on the Mott metal insulator transition in infinite dimension are reconsidered in the light of these results: controversies in that respect are shown to reduce to a simple physical question, with no firm answer as to now.

**PACS.** 75.20.Hr Local moment in compounds and alloys; Kondo effect, valence fluctuations, heavy fermions – 75.30.Mb Valence fluctuation, Kondo lattice, and heavy-fermion phenomena – 71.30.+h Metal insulator transitions and other electronic transitions

The physics of one single channel spin 1/2 impurity antiferromagnetically coupled to the conduction electrons in a metal is by now well understood [1]. The corresponding Kondo interaction Hamiltonian reads

$$H = \frac{J}{N_L} \sum_{k,k'} \sum_{\sigma,\sigma'} S_i s_{\sigma\sigma'} \; c^*_{k\sigma} c_{k'\sigma'} \; e^{i(k-k')R_i} \qquad (1)$$

where $N_L$ is the number of sites while $S_i$ and $R_i$ are the impurity spin and position. The dimensionless coupling is $z_o = \rho J/N_L \approx J/E_F$ where $E_F$ is the Fermi energy and $\rho$ the density of states at Fermi level. The physics is trivial in the strong coupling limit $z_o \gg 1$: the impurity traps an electron in order to build a singlet, the corresponding site is closed to other electrons and a Fermi liquid ensues, with one less electron and one less site (the only complication being a local interaction mediated by polarization of that singlet). Standard Kondo effect corresponds to the opposite weak coupling case: then logarithmic singularities act to increase the coupling $z(T)$ as the temperature decreases. The coupling approaches 1 when $T$ reaches a characteristic Kondo temperature $T_K \approx E_F \exp[-1/z_o]$. Thereafter $z$ evolves towards infinity and a Fermi liquid behaviour ensues again, with a temperature scale $T_K$ instead of $E_F$. The spin entropy Log2 is quenched on a temperature scale $T_K$.

The generalization to "Kondo alloys" with a finite concentration of magnetic impurities $N_{imp}$ is non trivial. First of all Kondo quenching competes with direct RKKY coupling $I$ between the impurity spins: that effect is already present for two impurities, and it has been extensively studied [2]. The ground state is always a singlet Fermi liquid, the only question for antiferromagnetic $J$ being whether it is driven by Kondo or RKKY. (The evolution is smooth except in restricted symmetric situations.) When the concentration of impurities is large, another issue arises, that of "exhaustion" [3]. It is best understood in the strong coupling limit in which Kondo quenching is a single site affair. Let us for a moment ignore direct exchange coupling between impurities: only electrons can quench the spins. If the number of electrons $N_{el}$ is larger than $N_{imp}$, singlet formation proceeds freely and the remaining carriers provide the low temperature Fermi liquid, admixed with magnetically neutral sites – the Kondo alloy resembles a single Kondo impurity. The physics is completely different in the opposite limit $N_{el} \ll N_{imp}$: then magnetic screening is necessarily collective. A Fermi liquid singlet ground state is still possible, but not on a one impurity basis. As an extreme situation, consider a lattice gas with one spin per site, $N_{imp} = N_L$: the ground state is a mixture of $N_{el}$ magnetically inert singlets and $(N_L - N_{el})$ "bachelor" spins, either up or down. The latter can hop around, exchanging with the singlets, thereby behaving as effective fermions (with a reduced bandwidth – see further). These new fermions have a hard core repulsion since they refer to the impurity spin. A singlet ground state means an isotropization of the spin structure of bachelors, with an energy scale that has nothing to do with the bare exchange $J$.

Real Kondo alloys usually correspond to weak coupling, $T_K \ll E_F$. The issue of exhaustion nevertheless remains, as the only electrons eligible to provide Kondo screening are those that lie within $T_K$ from the Fermi level: at relevant temperatures $\approx T_K$ the other ones are frozen

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by the exclusion principle and they cannot participate in real precession processes. Exhaustion is thus measured by the dimensionless ratio

$$p = \frac{N_{imp}}{N_{\mathit{eff}}} = \frac{N_{imp}}{\rho T_K} \tag{2}$$

$p$ is the number of spins that a single electron has to screen. In order to assess its importance we cannot ignore the RKKY interaction $I$, due to spin polarization of the conduction electrons *via* virtual excitation, which we may write as

$$I = \sum_{ij} \frac{J^2}{E_F} \frac{1}{\left(k_F R_{ij}\right)^3} \cos\left(2k_F R_{ij}\right) \, S_i S_j$$

($R_{ij}$ is the distance between impurities $i$ and $j$). The exchange is second order in $J$, it decays as $1/R^3$ and it displays the usual Friedel oscillation. Note that the reduction to a width $T_K$ around Fermi level does not apply to virtual excitation, as seen in the fact that the summation over intermediate states extends over the whole bandwidth ($I$ is not a scaling quantity). Since $1/\left(k_F R_{ij}\right)^3 \approx N_{imp}/\rho E_F$, three regimes ensue:

(i) $p \ll 1$: there is no exhaustion problem, impurities undergo an individual Kondo effect and the RKKY coupling is irrelevant.

(ii) $p \gg 1/z_o^2$, which implies $I \gg T_K$. Then RKKY coupling dominates, presumably leading to some frozen magnetic order that depends on geometry, whether antiferromagnetic, spin glass or other. That order kills the Kondo effect, as argued long ago [4].

(iii) $1 \ll p \ll 1/z_o^2$, which is the interesting case. The RKKY coupling should be minor – at least as long as the energy scale remains $T_K$. On the other hand exhaustion is a problem.

In the present paper we explore that last case in more detail. As a first approximation we ignore the RKKY interaction altogether, and we study qualitatively how an isotropic singlet state can be built up. We thereby ascertain the characteristic energy scales of the problem. We will see that the "coherence" temperature $T_c$ below which spin memory is quenched, allowing for Fermi liquid behaviour, is *at most* $T_K/p$, very much reduced as compared to $T_K$. A quick analysis of the energy and entropy of the system confirms that result. Such an idea that the characteristic temperature is reduced in alloys is not new: it was reached before in the framework of a periodic Anderson model, first using a crude mean field slave boson technique [5], then more recently using quantum Monte-Carlo simulation [6]. Such approximate methods, however, are not fully convincing: it is hard to assess the confidence one can have in slave bosons, and anyhow only a genuine Kondo model can ensure that charge fluctuations have no effect. We feel that a simple physical picture is useful.

We next look at the strong coupling limit. Then there is no real range of concentration where RKKY interactions are negligible. Since however that limit is rather unphysical, we take it as a theoretical model to ignore RKKY completely: we thereby pinpoint a "bare" Kondo effect in a very simple language (when $J$ is large the Kondo lattice is equivalent to a hard core Hubbard model). Details are slightly different as compared to the weak coupling case, but the final conclusion is essentially unchanged: the coherence temperature is very much reduced when few electrons act to screen many impurities. (As a bonus of that exact strong coupling solution, we show in the Appendix that the low temperature Fermi surface is the the so called "large" one, that encompasses a number of states $(N + N_{imp})$.) The standing question is then "what happens between $T_K$ and $T_c$": we offer a few suggestions.

The problem of Kondo alloys is interesting *per se*: it is supposed to control the physics of heavy fermions in rare earths alloys. But it also enters indirectly in the issue of Mott metal insulator transitions. In the canonical example of a half filled Hubbard model, with local repulsion $U$ on each site, a charge gap develops past a critical value $U_c$: two Mott-Hubbard sidebands correspond to localized carriers with up or down spins. Usually the residual superexchange interaction leads to antiferromagnetic order, but one may envisage a situation in which a large frustration would mean a paramagnetic configuration. The latter can be coherent, leading to an RVB like singlet ground state with no entropy. It may also be incoherent, retaining a magnetic entropy $N \operatorname{Log} 2$ at $T = 0$. We are concerned with the latter situation, whether it makes sense or not (we take it as a working hypothesis, which may be valid only at a small, but finite temperature[1]). The resulting state has been extensively studied in the limit of infinite dimensions [7]. In a recent review article [8] it is argued that the transition is first order, metallic and insulating solutions coexisting in a finite range of interaction strength $(U_{c1}, U_{c2})$. Free carriers near the transition lie in a resonant narrow band which disappears in the middle of a large preformed Mott-Hubbard gap when $U = U_{c2}$. When that resonant peak is present the metallic state may be viewed as a Kondo alloy process, the free carriers acting to screen the localized spins, thereby quenching their magnetic entropy [9]. That model is extremely appealing, as it explains naturally a number of striking features of numerical results – yet it has been questioned for a number of reasons [10,11]. It is therefore instructive to look at it from the vantage point of Kondo alloys. Near the transition, when the free carriers are few, the exhaustion problem is extreme: does it affect the energy balance that controls the appearance of free carriers inside the gap? We will show that the answer to that question indeed is crucial in choosing between conflicting models. The issue is by no means solved, but such an approach puts it in physical terms.

[1] Most of the existing theory is carried out for infinite dimension: it is not clear that the limits $T \to 0$ and $d \to \infty$ are interchangeable.

## 1 Collective Kondo screening in the weak coupling case

Assume that we perform real space renormalization until a single cell contains one impurity only. In the spirit of renormalization, each cell, $N_{imp}$ in number, contains a single state: we are left with an effective lattice gas with $N_{imp}$ sites. Each one of the $N_{eff}$ electrons hops from cell to cell, with a characteristic time scale $\tau_h$ which corresponds to a bandwidth $\epsilon_h \approx \hbar/\tau_h$. In order to estimate $\epsilon_h$ we require that the Fermi level density of states be preserved, *i.e.* $\rho \approx N_{imp}/\epsilon_h$. Using (2) it follows that

$$\epsilon_h \approx pT_K. \tag{3}$$

Only a fraction $1/p$ of the sites is visited at any given time, the duration of a visit being $\tau_h$. During a visit, the residual exchange with the host spin is $T_K$ [2]. It follows that the spin and its visitor precess around each other with a Larmor frequency $\omega_o \approx T_K/\hbar$. They rotate by an angle

$$\theta = \omega_o \tau_h \approx \frac{1}{p}\,. \tag{4}$$

It consequently takes at least $p$ visits in order to achieve a full turn.

A Fermi liquid ground state should be invariant upon spin rotation: it is a coherent superposition of all possible spin orientations. Let $\tau_c$ be the time needed in order to achieve such a full isotropization. The corresponding energy $T_c \approx \hbar/\tau_c$ defines a characteristic coherence temperature: Fermi liquid behaviour can only occur below $T_c$. At higher temperatures $T$, one can make wave packets that sweep in a time $\hbar/T$: they "see" a snapshot of the spins that is definitely anisotropic. The corresponding degeneracy is what builds the spin entropy $S(T)$. The central issue is thus an estimate of $\tau_c$, which in turn depends on whether successive visits to a given cell are coherent or not – put another way, does impurity precession resumes with the same rotation vector or not? In the former case it takes a time $p\tau_h$ to make a full turn – but since the rotation axis is fixed, it is not fully clear that the resulting state is really isotropic. In the latter case, impurity precession should instead be viewed as a Brownian motion on the sphere and it takes a time $p^2\tau_h$ to make a full turn. In either case one should remember that precession is stopped most of the time, being active only for a fraction of time $1/p$. Without a detailed theory one cannot really choose, but it is clear that the former choice yields a lower bound for $\tau_c$, *i.e.* an upper bound for $T_c$. That bound is

$$T_c = \frac{\epsilon_h}{p^2} = \frac{T_K}{p} = \frac{\rho T_K^2}{N_{imp}}\,. \tag{5}$$

[2] It would be exactly that if the number of cells would be $N_{eff}$ instead of $N_{imp}$: $T_K$ is by definition the band width for which the dimensionless coupling $z$ is $\approx 1$. For logarithmic scaling the difference is not much except if $p$ is exponentially large.

Well below $T_c$ we expect a Fermi liquid with no magnetic degrees of freedom, with an entropy $S = \gamma T$. Well above, the spins are essentially random, but possibly strongly correlated. The key issue is therefore the evolution of $S(T)$. It is definitely $N_{imp}\mathrm{Log}\,2$ above the single impurity Kondo temperature $T_K$: does it go to zero in one or two steps? In the former case $T_c$ is the only characteristic temperature of the problem and the Sommerfeld constant is

$$\gamma \approx \frac{N_{imp}}{T_c} \approx \rho\, p^2. \tag{6}$$

In the latter case part of the magnetic entropy could disappear due to spin correlations and $\gamma$ would be accordingly smaller.

Here again naive theories cannot decide. We nevertheless present a simple handwaving argument that pleads for a single energy scale. The entropy scale is $S_o = N_{imp}\mathrm{Log}\,2$. In order to identify the energy scale $E_o$ we note that the exchange energy is $T_K$ for each occupied site – hence $E_o \approx N_{eff}\, T_K$. Standard thermodynamic relations usually imply a temperature scale $T_o \approx E_o/S_o$: we recover the same scale $T_K/p$ found for the coherence energy $T_c$.

These arguments are by no means conclusive: they are meant to stimulate further thought. For instance it is quite possible that the actual coherence temperature $T_c$ (marking the onset of Fermi liquid behaviour) is even smaller, the precession by $2\pi$ around a *given* rotation axis being insufficient to achieve isotropy. The drop of entropy should then begin at the scale $T_K/p$ suggested by thermodynamics, what happens in the intermediate range remaining rather mysterious. It is also possible – and even likely – that RKKY interactions, while negligible above $T_K$, could become dominant around $T_c$: instead of being due to precession against rare visitors, the isotropization process would be due to direct interactions (to the extent that a real RVB state with no long range correlations does exist). To make life even more complicated, we may note that independent binary RKKY interactions do not make sense if many spins are coupled to few electrons: those interactions are strongly correlated. Altogether, the problem remains open, with many unclear facets.

## 2 The strong coupling limit

Since realistic Kondo alloys are complicated, it is instructive to look at a more artificial situation in which the theory is much better controlled: many of the ideas expounded above will reappear in another guise. Such a limit is that of an infinite $J$, much larger than the Fermi energy $E_F$. We assume an impurity on each of the $N_L$ lattice sites, and we put $N < N_L$ electrons that hop with a bandwidth $D$. The exhaustion parameter is $p = N_L/N$. Each available electron is trapped into a singlet with some impurity: the resulting energy – $(3NJ/4)$ is frozen and it disappears completely from the problem. Those singlet sites are magnetically inert, magnetism being concentrated onto the $(N_L - N)$ unscreened "bachelor" spins. We assume that there is no exchange whatsoever between these active spins: they can move only when they encounter a singlet site, with which they exchange (the screening electron

hops backwards from one site to the next). The overlap of two singlet states being 1/2, the bandwidth associated to these hops is $D/2$. Bachelor spins act as spin 1/2 fermions (indeed they are simply holes in a completely filled singlet lattice), but the new feature is that such fermions have a hard core: one cannot destroy two electrons on a singlet site that has only one! We thus have an exact isomorphism between two problems:

(i) A Kondo lattice with $N_L$ spins, $N$ electrons, bandwidth $D$, exchange $J = \infty$.
(ii) A Hubbard model with $N_L$ sites, $(N_L - N)$ electrons, (*i.e.* $N$ holes), bandwidth $D/2$, on site repulsion $U = \infty$.

Such an equivalence was noticed long ago [13]: we emphasize it here as it supports the previous discussion.

Let us first extend our precession argument. The hopping time is $\tau_h \approx \hbar/D$, the precession Larmor frequency is $\omega_o \approx J/\hbar$. During a visit the spin rotates by an angle $\theta \approx \omega_o \tau_h \approx J/D \gg 1$: a single visit on a given site is thus enough to achieve isotropy. But all sites must be visited: that takes a time $\tau_c \approx \tau_h N_L/N$. The corresponding coherence temperature is $T_c = \hbar/\tau_c \approx D/p$: we recover the same reduction by a factor $p$. Note that $T_c$ is proportional to the concentration of free electrons. We arrive at the same temperature scale comparing orders of magnitude for the energy $E_o$ and entropy $S_o$ in the ground state. If we exclude the frozen exchange energy, the remaining $E_o$ is due to singlet hopping, of order $ND$, while the entropy scale is of order $N_L$ Log2. The characteristic temperature over which $S_o$ is quenched should be $E_o/S_o$: we recover the same $T_c$.

Here we do have a reliable theory. The case of a nearly filled lattice, $(N_L - N) \ll N_L$, is essentially trivial: bachelor spins are few and their hard core makes little difference. In zeroth order they behave as ideal free fermions (the next order correction for a dilute Fermi gas is known, but it does not matter here). There is no exhaustion constraint, and the problem is dull. (We may notice however that the ground state Slater determinant allows an explicit calculation of all physical quantities, for instance the one particle distribution function $n_k$: this is done in the Appendix where we show that the resulting Fermi surface contains $(N_L + N)$ points, a modification of the usual Luttinger theorem that is here proven analytically.) The opposite limit $N \ll N_L$ implies extreme exhaustion. Then the motion is that of $N$ holes in a hard core Hubbard model. While there is no exact analytical solution to the problem due to spin disorder, everybody will agree that the energy scale is $ND$, the band width being somewhat reduced by the spin structure. That validates our precession argument.

## 3 Relevance to the Mott transition

We consider the standard one band Hubbard model on a lattice with $N_L$ sites

$$H = -t\, c^*_{i\sigma}\, c_{j\sigma} + U\, n_{i\uparrow} n_{i\downarrow}. \qquad (7)$$

The band is half filled, $N = N_L$. The physics is simple in two limits:

(i) *Strong coupling*, $U \gg t$: the ground state is an insulator with a large gap $\delta \approx U$. Localized spins are subject to an Anderson superexchange $J = 4t^2/U$, leading to an antiferromagnetic structure. The magnetic energy scale $J$ is much smaller than $\delta$: the insulating gap has nothing to do with magnetism, which is a minor correction.
(ii) *Weak coupling*, $U \ll t$: the ground state is a paramagnetic conducting Fermi liquid, except if the Fermi surface is nested (as it is for nearest neighbour hopping in a simple cubic lattice). In the latter case a spin density wave instability develops, formally very similar to the BCS instability (zone edge triplet particle hole pairs condense instead of zone center singlet particle pairs). The gap $\delta$ is due to Bragg scattering off the resulting antiferromagnetic order: the insulating behaviour is a direct consequence of the magnetic symmetry breaking, as shown by the fact that the Néel temperature is $\approx \delta$.

One goes smoothly from one limit to the other as $U$ is varied, but the physics is very different in the two limits. The same situation occurs in superconductors, where pairing is an "atomic" property for strong attractions $U$ (Bose-Einstein condensation is then a marginal detail), while $\delta$ is due to gauge symmetry breaking in the BCS weak coupling case[3].

Whether in strong or in weak coupling an insulator seems to imply antiferromagnetism: the real issue is whether a paramagnetic insulator can exist at zero temperature. More precisely one can imagine two situations:

(i) A coherent non degenerate ground state in which localized spins form a singlet state, invariant under spin rotation. That is easily achieved upon dimerization, but one then breaks translational invariance. The issue is whether one can achieve such a singlet state without breaking any symmetry, and without infinite range correlations: the answer is still a matter of debate[4].
(ii) An incoherent state, with residual entropy $N$ Log 2, in which localized spins are random.

We are here concerned with the second possibility, which has been supported recently by detailed calculations in the limit of infinite dimension [8] In that limit correlations are strictly local, and the surrounding world of a given site enters only through a single particle effective Lagrangian that is determined self consistently[5].

[3] In the electron-hole symmetric nested case the equivalence is actually an identity, since one can change the sign of $U$ performing an electron-hole transformation on one spin only.

[4] An equivalent question is whether a spin 1/2 lattice can have a singlet ground state – and since spins 1/2 are isomorphous to hard core bosons, whether a Bose liquid can have a *normal* ground state, which is neither superfluid (breakdown of gauge invariance), nor cristalline (breakdown of translation invariance). That question is open.

[5] That effective Lagrangian is supposed to ignore the state of the site considered: $\mathfrak{L}_\uparrow$ is the same whether a $\downarrow$ electron

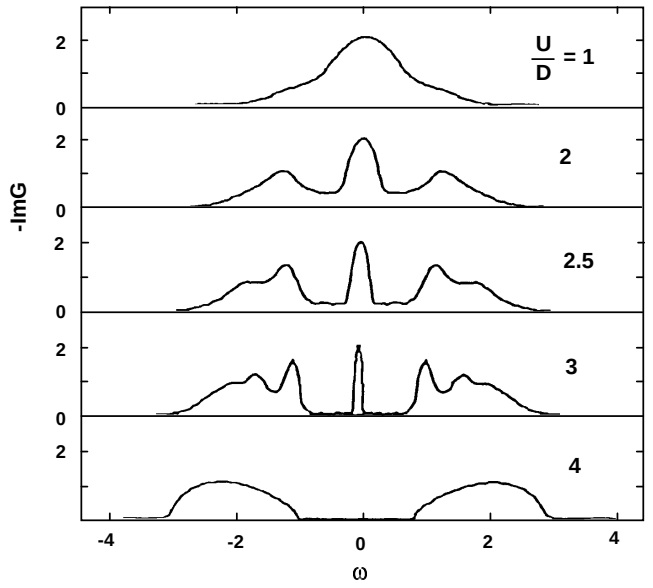


**Fig. 1.** The evolution of the one electron density of states $\rho(\omega)$ as a function of the Hubbard repulsion U for an electron-hole symmetric model at zero temperature, taken from reference [5]. Numbers refer to the value of U/D where D is the bandwidth.

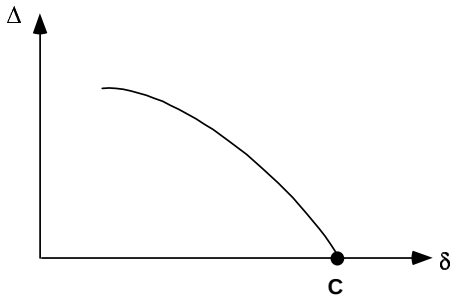


**Fig. 2.** The resonance width $\Delta$ as function of the gap $\delta$, parametrized by the interaction strength $U$. Note that both become fuzzy when $\Delta$ increases.

We take these results as granted and we explore their physical implications.

Let us first describe the salient results of Georges *et al.* They mostly consider an electron-hole symmetric case in which the density of states $\rho(\omega)$ is even with respect to the Fermi level. They first study the ground state $T = 0$: it is then easily shown that $\rho(0)$ is constant, unaffected by interactions. The evolution of $\rho(\omega)$ as the interaction $U$ is increased is shown in Figure 1. Starting from the usual single band at small $U$, two Mott sidebands develop

is there or not. While all right in a metallic state in which the memory time of a given site is finite, such an assumption is not obvious in the insulating state in which the spin structure is frozen. Then the relaxation time of the surrounding world, presumably $\approx 1/d$, must be compared to the free carrier energy scale $\Delta$: it is not clear that the limits $\Delta \to 0$ and $d \to \infty$ can be interchanged. That question deserves an answer, but it is not central to our argument.

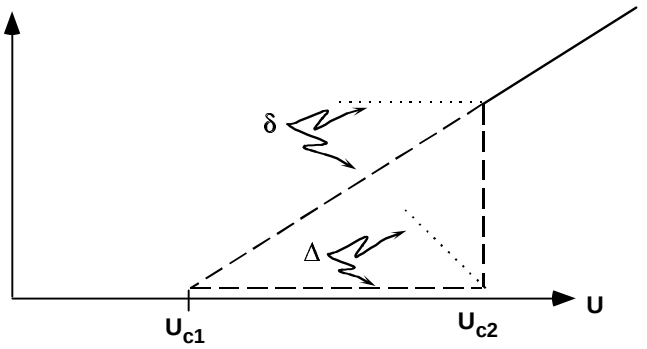


**Fig. 3.** Multistability at zero temperature: between $U_{c1}$ and $U_{c2}$ two solutions coexist for the gap $\delta$ and the resonance width $\Delta$, an insulating one (dashed curve) and a metallic one (dotted curve).

progressively, while a narrow resonance appears near Fermi level. Clearly the problem has two characteristic energies, the "gap" $\delta$ between the sidebands, and the width $\Delta$ of the resonance. As long as the central peak exists, these energies are not sharply defined: the central peak has tails and Auger processes fill in the gap! But they are better and better defined as $\Delta \to 0$. At some critical $U_{c2}$ the central peak disappears: beyond that a sharp gap $\delta$ exists, as in a semiconductor, and the ground state is insulating. Note that the weight (per crystal site) of the central peak is

$$z \approx \frac{\rho\Delta}{N} \approx \frac{\Delta}{D} \tag{8}$$

where $D$ is a typical bandwidth: the weight shrinks to zero at the transition. It does it in the middle of a large preformed gap: $\delta$ is of order $D$ at $U_{c2}$, as shown in Figure 2. That particular point is one of the standing controversies: we want to understand it better.

Because the insulating state has magnetic entropy, it is favoured at finite temperatures. It follows that the two states $\Delta \neq 0$ (metal) and $\Delta = 0$ (insulator) can coexist in a finite range $U_{c1} < U < U_{c2}$: the transition is first order. The evolution of $\delta$ and $\Delta$ as a function of $U$ is sketched in Figure 3, which clearly displays multistabilty. The corresponding phase diagram is shown in Figure 4, together with the Maxwell plateau. More interesting is the evolution of the central peak $\rho(\omega)$ as a function of $T$, sketched in Figure 5: the width does not vary much, but $\rho(0)$ decreases. When $T \approx \Delta$ the peak has a vanishing weight instead of broadening. That highly significant result must also be understood.

The Lagrangian $\mathfrak{L}$ describing retarded excursions into the surrounding world may be represented by an effective self energy $\sigma(\omega)$. The self consistency requirement implies that $\sigma(\omega) \approx D^2 G(\omega)$, where $G$ is the local full propagator and $D$ the bandwidth. $\sigma(\omega)$ may be mimicked assuming hybridization of the particular site 0 under study with a gas of fictitious drone fermions $\gamma_{\alpha\sigma}$, according to an

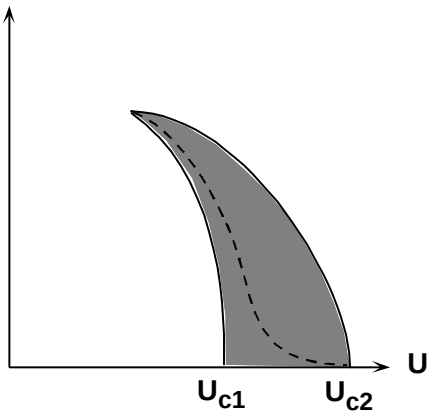


**Fig. 4.** Phase separation in the $T$, $U$ plane. The dashed curve is the Maxwell plateau.

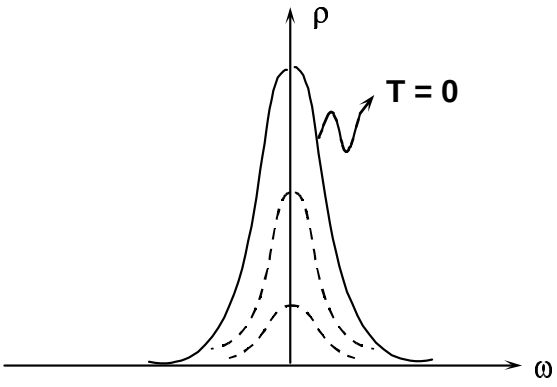


**Fig. 5.** Evolution of the central resonance peak in $\rho(\omega)$ as a function of temperature.

effective Anderson impurity model

$$H = U\left[c^*_{o\uparrow}c_{o\uparrow} - \frac{1}{2}\right]\left[c^*_{o\downarrow}c_{o\downarrow} - \frac{1}{2}\right] + \sum_{\alpha\sigma}\lambda_\alpha\left[c^*_{o\sigma}\gamma_{\alpha\sigma} + c.c.\right] + \sum_{\alpha\sigma}\epsilon_\alpha\gamma^*_{\alpha\sigma}\gamma_{\alpha\sigma}. \quad (9)$$

The resulting self energy is

$$\sigma(\omega) = \sum_\alpha \frac{\lambda_\alpha^2}{\epsilon_\alpha - \omega}\,. \quad (10)$$

The total weight of $\sigma$ is

$$\frac{1}{\pi}\int d\omega\,\mathrm{Im}\sigma = \sum_\alpha \lambda_\alpha^2. \quad (11)$$

Since $\mathrm{Im}\sigma \approx \pi D^2\rho$, it follows that the contribution of the central peak to (11) is of order $zD^2 \approx \Delta D$.

The level scheme of that problem is sketched on Figure 6: site 0 has the usual 4 states and the spectrum of $\sigma$ reflects that of $G$, with two sidebands and a narrow central peak. In the vicinity of $U_{c2}$ it is natural to focus on the central states, namely the spin doublet $n_o = 1$ (equivalent

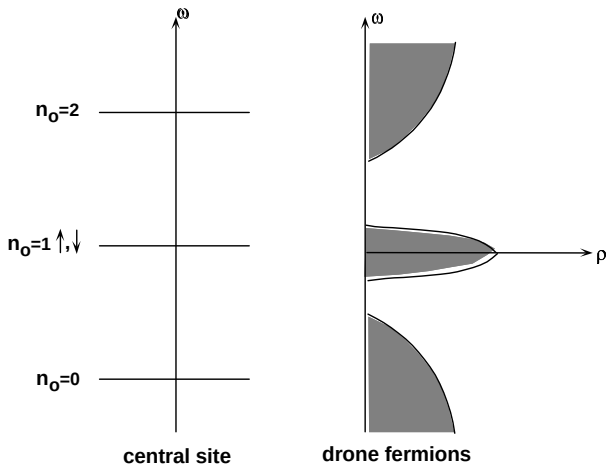


**Fig. 6.** The level scheme of the equivalent Anderson impurity model.

to a spin $S = 1/2$) and the resonance peak of $\sigma(\omega)$. This is achieved *via* a transformation "à la Schrieffer-Wolff", slightly more complicated as one must eliminate both the $n_o = 0, 2$ states *and* the Mott sidebands. The resulting Hamiltonian necessarily has a Kondo-like structure

$$H = \sum_{\alpha,\alpha'}\gamma^*_{\alpha\sigma}\gamma_{\alpha'\sigma'}\left[V_{\alpha\alpha'}\delta_{\sigma\sigma'} + J_{\alpha\alpha'}\,S s_{\sigma\sigma'}\right]. \quad (12)$$

Drone fermions scatter off the two level system. The scalar potential is identically zero if electron-hole symmetry holds (as known in usual Kondo physics). More generally it probably fixes the position of the resonance inside the gap. We ignore it altogether, focussing on the symmetric case. Since a typical energy denominator is of order $D$, the exchange coupling $J$ is of order

$$J_{\alpha\alpha'} \approx \frac{\lambda_\alpha\lambda_{\alpha'}}{D}\,. \quad (13)$$

Near $U_{c2}$ we expect it to be intermediate, corresponding to a Kondo temperature comparable to the band width $\Delta$ of the central peak. Indeed $\Delta$ is much smaller than all other energy scales: the shape of the central peak should be universal and the coupling can be neither weak nor strong. In order to substantiate this handwaving argument, we ignore the kinetic energy of the drone fermions and we calculate the spacing of the singlet and triplet states formed by $S$ with one trapped fermion: that should provide $T_K$. If we find $T_K \geq \Delta$ we justify *a posteriori* our starting approximation. We set

$$\sum_\alpha \lambda_\alpha\gamma_{\alpha\sigma} = A\eta_\sigma \quad (14)$$

where $A$ is a normalization factor such that $\eta$ has the usual anticommutation rules

$$A^2 = \sum_\alpha \lambda_\alpha^2. \quad (15)$$

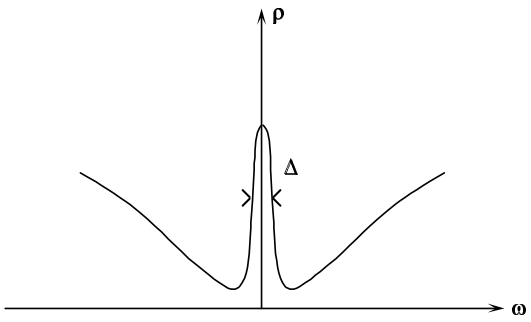


**Fig. 7.** The $T = 0$ density of states when $\delta$ and $\Delta$ are comparable (the value $\rho(0)$ is fixed).

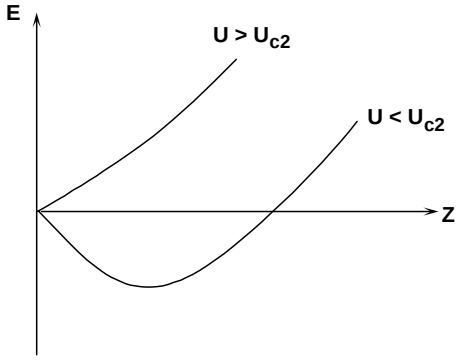


**Fig. 8.** The evolution of the ground state energy as a function of the resonance peak weight $z$ for various values of $U$.

Then the Kondo temperature is $A^2/D \approx \Delta$ , as expected. Note that this Kondo temperature is calculated in the presence of all other impurities, hidden in the self consistency condition for $\sigma(\omega)$, *i.e.* in the drone fermions.

Such a Kondo picture should capture all the low energy features of the Mott transition, as emphasized in [9]. We apply it to an energy balance argument. We start from an insulating state with a Mott-Hubbard gap $\delta$, and we bring $N_L$ $z$ states in the middle of the gap in order to build the resonant free fermion peak where the Fermi level sits. What is the cost in energy of such a process? If it is energetically favourable the insulator will turn spontaneously into a metal. If it is not, it may be that the insulating state is a local minimum, leading to a first order transition. The hope is to make a phenomenological description "à la Landau" of the Mott metal-insulator transition. Such an energy balance has two parts:

(i) An obvious cost in kinetic energy $N\,z\,\delta$, paid when occupied states are promoted from the lower Mott subband to the resonant peak.
(ii) A gain in exchange energy at $T = 0$ due to the formation of singlets. Each screened impurity gains a Kondo energy $T_K \approx \Delta$, but we are in an extreme exhaustion case: $N$ spins are screened by $N_{\mathit{eff}} = N\,z$ electrons, a much smaller number when $z \to 0$.

The key issue is whether one gains $\Delta$ once per spin or once per electron. The preceding sections plead for the latter – but here the fermions are constructs and the answer is not clear: we thus explore the two possibilities in succession.

*a) The Kondo energy is gained for all spins* – Since $z \approx \Delta/D$ the net energy cost is $N\,[\delta/\delta^* - 1]\,\Delta$, where $\delta^*$ is a threshold value of order $D$. The balance becomes favourable when $\delta = \delta^*$: the resonance peak appears in the middle of a large preformed gap, in accordance with [8].

*b) The Kondo energy is gained only once per electron* – The energy cost is then $N\,z\,[\delta - \Delta]$: the resonance peak disappears as soon as the gap opens. There is only one energy scale $\Delta$ in the problem and we recover the familiar band crossing picture for the metal–insulator transition [11]. Because $\rho(0)$ is fixed, there is still a peak at Fermi level, but in a closing gap as sketched in Figure 7. One expects no first order transition. Such a picture has advocates: it came out for instance from a slave boson treatment of the Hubbard model [12].

The two points of view are clearly contradictory, hence a controversy which is not easily settled opposing numerics to approximations. Here we provide the dilemma with a simple physical meaning. Let us for a moment assume that a) is the good choice. Such a Kondo picture has many appealing features:

(i) It has a built in *saturation mechanism* that describes the direct bifurcation at $U_{c2}$ the more states in the central peak, the more they repel the Mott sidebands, thereby increasing the gap $\delta$. The gap is thus an increasing function of $z$: the growth of the resonance peak stops when $\delta = \delta^*$. The evolution of the ground state energy as a function of $z$ is shown in Figure 8, which resembles the usual Gutzwiller approximation [14]. We recover the usual Landau picture of a phase transition.
(ii) It provides an obvious interpretation of the finite $T$ behaviour. While in the ground state each Kondo singlet gains an energy $\approx \Delta$, that gain disappears above the Kondo temperature. Then parallel and antiparallel spin configurations are equally probable and the net exchange energy vanishes. Only the cost in kinetic energy survives and the balance is unfavourable. The negative slope in Figure 8 changes sign, the *weight* $z$ going to zero.
(iii) The effect is enhanced by entropy. At a given temperature $T$ the spins decouple when $z \ll T/D$: the free energy goes down by $NT\mathrm{Log}2$. That drop is killed when $T \approx zD$, hence an initial slope of $F(z)$ near $T = 0$ of order $ND$ which adds to the kinetic energy contribution. It follows that $F(z)$ has a local minimum at $z = 0$, as sketched in Figure 9, the transition is first order.

All the results of [8] are thus natural consequences of a single assumption, namely that the Kondo energy $\Delta$ is gained at each spin site.

Where do we stand now? If the resonant peak free fermions were real particles, the discussion of the preceding section would claim that the Kondo energy is gained only once per carrier. In the author's opinion that remains

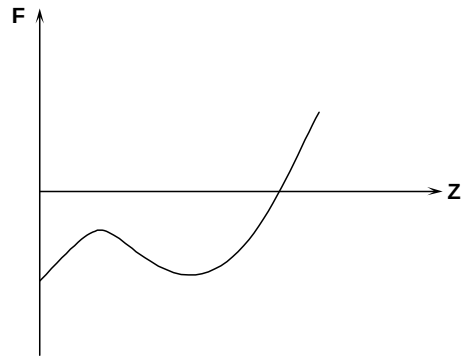


**Fig. 9.** The free energy at fixed $T \neq 0$ as a function of $z$.

a likely possibility. It should be admitted however that the $\gamma_{\alpha\sigma}$ are fictitious particles that mimick the excursion self energy $\sigma(\omega)$. Moreover their properties are calculated self consistently, so that they incorporate from the outset a certain amount of interactions. One may envisage a situation where the resonance width $\Delta$ would be already the *coherence energy* $T_c$ rather than the bare single impurity Kondo temperature $T_K$: then case (a) would hold. In such a situation the bare single site $T_K$ would be of order $D$ the band width – indeed a natural choice in an intermediate coupling situation where $D$, $U$ and $J$ are comparable. Exhaustion as described above would then reduce that large $T_K$ to $\Delta = zT_K$ as found in [8]. In the end the issue is whether the magnetic energy gain due to singlet formation is $\approx z$ or $\approx z^2$: the only purpose of the present discussion is to put the case in physical terms.

## 4 The strong magnetization limit

The Mott transition is usually discussed in non magnetized systems, $N_\uparrow = N_\downarrow$. Since the magnetization $M$ is a good quantum number, one can study the transition for a half filled band at any finite $M$, such that

$$N_\downarrow = N_L - N_\uparrow \neq N_\uparrow.$$

That has been done recently [15]. Although not achievable experimentally the limit of large magnetizations, $N_\downarrow \ll N_\uparrow$, is particularly interesting as the nature of the Mott transition becomes very clear. Assume first that there is a single $\downarrow$ spin: it may dissociate into an empty site (0) and a doubly occupied site (2), with a cost in energy $U$. That is equivalent to a local *attraction* $-U$ between (0) and (2). In 1 or 2 dimensions such an attraction always produces a bound state: charge dissociation does not occur at $T = 0$ and the system is an insulator. If $d \geq 3$ the bound state appears instead at a finite $U_c$: charges are free below $U_c$ and the system is a metal. The bound state has a characteristic radius $\xi$ which is easily calculated: the interaction between bound pairs should have a small effect if their distance is large, $N_\downarrow \xi^d \ll 1$ (we set the volume equal to 1): the Mott transition then occurs at $U_c$.

When the density increases, the pairs begin overlapping: their binding diminishes according to the old picture of Mott (screening is one mechanism, but "saturation" of the fermion distribution due to the exclusion principle is another one [16]). That should make the metallic state more favourable and as a result the threshold $U_c(M)$ for the Mott transition should *grow* as $M$ is reduced from 1 to 0. In the limit $M = 0$ we recover the previous "collective" picture of the transition. The evolution as a function of $M$ is continuous, the crossover corresponding to $N_\downarrow \xi^d \approx 1$.

When pairs are dilute (*i.e.* a magnetization close to saturation, $N_\downarrow \ll N_L$ ), the metal–insulator transition corresponds to closing of the gap (when binding is destroyed): in that limit, free carriers do not disappear in the middle of a large preformed gap as they seem to do in the paramagnetic case $M = 0$. It would then be most interesting to extend the $d = \infty$ calculation to the magnetized case, in order to see explicitly how the spectral density evolves as a function of $M$. If it is found that the preformed gap at $U_{c2}$ disappears as $M$ grows, then the results of [8] will gain additional support[6].

The above discussion does not pay attention to magnetism: it does indeed occur for a simple cubic lattice and it is interesting to consider its evolution. When down spins are few, they form effective dilute bosons. The latter will undergo Bose-Einstein condensation at $T = 0$, in the state with minimum center of mass energy. Since the two body problem is trivially solved, it easily verified that the lowest state corresponds to a center of mass momentum at zone corner rather than $P = 0$. Creating a bound boson means flipping a spin: the Bose-Einstein order parameter is thus the transverse magnetization. For $M$ close to saturation, the ground state is consequently a small canting of the spins opposite on the two sublattices, as shown in Figure 10: that is just the remnant of antiferromagnetism as $N_\downarrow \to 0$. Note that for such a cubic lattice the ground state is always antiferromagnetic, with a continuous evolution between two limits:

(i) The dilute case where binding is an atomic property that has nothing to do with magnetism. The gap is the binding energy $\gg T_N$.
(ii) The dense case $N_\uparrow = N_\downarrow = N_L/2$, in which the gap is due to Bragg scattering (there is only one energy scale).

The situation is similar to that found in superconductors, in which the ground state goes continuously from

[6] Such an extension has another more technical interest. One of the methods used in [8] is based on "iterated perturbation theory", where local interactions are treated within second order perturbation theory (IPT), and then calculated self consistently within the iteration scheme. The justification for that second order crude theory is that it interpolates between weak and strong coupling. Such an interpolation, however, is due to electron-hole symmetry and it disappears if $N_\uparrow \neq N_\downarrow$: a calculation as a function of $M$ should allow an assessment of IPT.

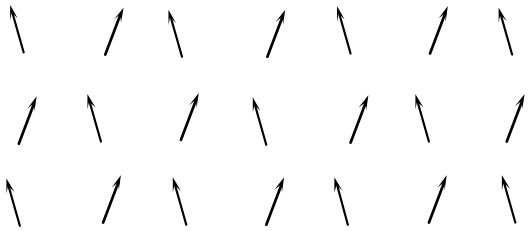

**Fig. 10.** The canted antiferromagnetic spin configuration for large net magnetization $M$, equivalent to Bose-Einstein condensation of triplet pairs.

a Bose-Einstein condensation of preformed pairs to the BCS state[7].

## 5 Conclusion

In this brief note we tried to throw a fresh look at two problems, both of which have been intensively studied in the past:

(i) How can a few electrons screen many magnetic impurities, the so called "exhaustion problem" in Kondo lattices? We claim that the characteristic temperature scale $T_c$ is much smaller than the single impurity Kondo temperature. The standing issue is whether there are one or two characteristic temperatures in the evolution of the entropy $S(T)$: we suspect there is only one, but that is only a guess.

(ii) Can the physics of Kondo lattices shed light on the Mott metal-insulator transition in half filled Hubbard lattices? Usually such a transition is accompanied by antiferromagnetic order, and the two effects are intermingled: where is the hen and where is the egg? Recent work in infinite dimension [8] has focussed on possible *paramagnetic* insulators, in which localized spins are incoherent and retain magnetic entropy at zero temperature. The prediction is that the transition is first order, free carriers appearing as a narrow resonance in the middle of a large preformed gap. We view that prediction as resulting from a Kondo quenching of the localized spins: the claim of [8] would then be either that exhaustion does not matter, or that the bare $T_K$. is actually the band width.

If true, such a statement deserves a detailed justification – the more so as different experts have different views. At that stage qualitative arguments are of no avail: only playing with explicit calculations in different contexts can yield a convincing answer. Two such calculations are particularly desirable:

(i) The exhaustion issue is neat and clean in the real Kondo lattice, in which carriers are true ones instead of constructs. Can one study the $d = \infty$ limit of a Kondo lattice with one spin per site and a variable number of electrons, *using the same approach as for the Hubbard model* (in a first approximation one can choose $J = \infty$)? Can one compare the lattice problem with a single impurity? That should straighten out the exhaustion issue without any havoc on the definition of fermions.

(ii) Returning to the Hubbard model, can one apply the $d = \infty$ calculation to the evolution of the Mott transition as a function of the magnetization $M$? The results can be checked against the known limit of saturation; moreover the presence of an additional parameter allows for a good check of the computational procedures.

Only experts can carry that program: this conclusion is a standing order!

The author has greatly enjoyed many stimulating discussions with A. Georges, F. Gebhard, G. Kotliar and D. Logan.

## Appendix

A standing issue has been the Fermi surface of a Kondo lattice, with a spin 1/2 on each of the $N_L$ sites and with $N$ electrons (the spins must be regularly spaced in order to preserve translational invariance and to have a well defined Fermi surface). Is the Fermi surface the "small" one encompassing $N$ states, or the "large" one encompassing $(N_L + N)$ states? If the spins 1/2 are made up from an underlying Anderson lattice with local $f$-orbitals, continuity with the perturbative limit strongly suggests the latter choice of a "large" Fermi surface. Indeed that result has been established variationnally [17]. But a direct proof within the $s$-$d$ language would be nice. The $J = \infty$ limit does provide such a proof in the limit of a nearly filled band, $(N_L - N) \ll N_L$. That limit is complementary to the small $J$ characteristic of Anderson hybridization. We sketch the argument which, although not general, is enlightening.

The $p = (N_L - N)$ bachelor spins act as free fermions with a bandwidth half that of the original ones. The corresponding ground state is characterized by the positions $i_m, j_n$ of the $\uparrow$ and $\downarrow$ holes, respectively $p_\uparrow$ and $p_\downarrow$ in number. It may be written as [13]

$$\mid \Psi_o \rangle = \phi\,(\alpha_m, \beta_n)\ \ c_{\alpha_m \uparrow}\, c_{\beta_n \downarrow} \mid \mathrm{sing}\rangle \qquad \text{(A.1)}$$

where $|\mathrm{sing}\rangle$ denotes the state with $N_L$ electrons and a singlet at each site. If $p$ is small the hard core repulsion between holes is irrelevant and $\phi$ is just a Slater determinant. One may then calculate the one particle density matrix explicitly,

$$n_{ij,\sigma} = \langle\, \Psi_o \mid c^*_{i\sigma}\, c_{j\sigma} \mid \Psi_o \,\rangle. \qquad \text{(A.2)}$$

The Fourier transform of $n_{ij,\sigma}$ yields the distribution $n_{k\sigma}$. If there is no hole, we find at once $n_{ij,\sigma} = 1/2\delta_{ij}$, as befits a singlet state where $\uparrow$ and $\downarrow$ are equally populated.

[7] Indeed the two problems can be mapped on each other performing an electron hole transformation on the $\uparrow$ spin only. The interaction $U$ goes to $-U$ and the magnetized repulsive system with $N_\downarrow = N_L - N_\uparrow$ goes into an attractive gas $N_\uparrow = N_\downarrow$.

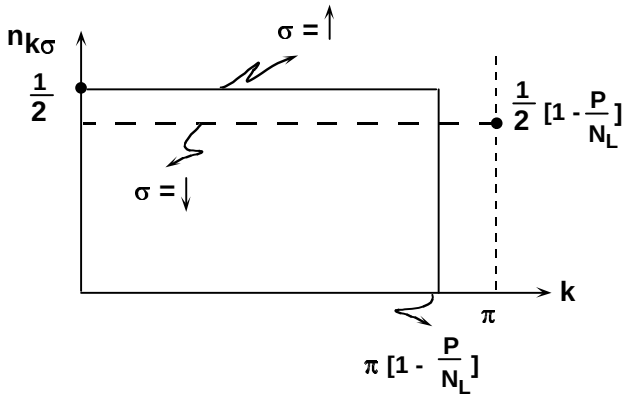


**Fig. 11.** The distribution $n_{k\sigma}$ of real fermions for $p$ bachelor spins all aligned $\sigma = \uparrow$.

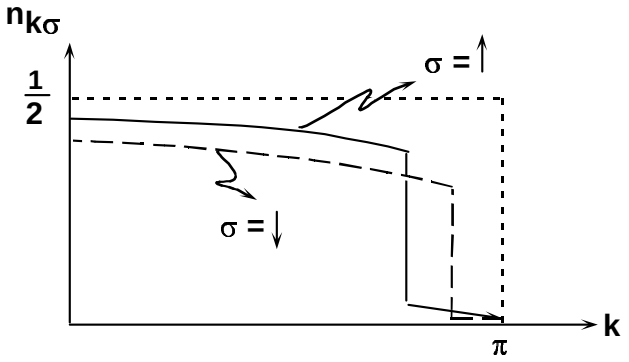


**Fig. 12.** A sketch of the distribution $n_{k\sigma}$ of real fermions when bachelor spins have different spins, with densities $p\uparrow$ and $p\downarrow$.

Assume next that all the holes are $\uparrow$: the Slater determinant is the exact ground state. Equation (A.2) becomes

$$n_{ij,\sigma} = \phi^*(\alpha_m)\ \phi(\alpha'_m)\ \langle \text{sing} \mid c^*_{\alpha_m\uparrow} c^*_{i\sigma}\ c_{j\sigma} c_{\alpha'_m\uparrow} \mid \text{sing}\rangle. \tag{A.3}$$

Consider first the "spectator" spins $\sigma = \downarrow$: in order to return to the singlet state the $(\alpha)$ and $(\alpha')$ sets must be identical, $i$ must be equal to $j$ and it should not belong to the set $(\alpha)$ (a singlet has only one electron). It follows that

$$n_{ij,\downarrow} = \frac{1}{2}\delta_{ij}\left[1 - \frac{p}{N_L}\right]. \tag{A.4}$$

When $\sigma = \uparrow$ two contributions emerge:

(i) Either $i$ does not belong to $(\alpha)$ while $j$ does not belong to $(\alpha')$: then $(\alpha) = (\alpha')$ and $i = j$. That part is just the contribution we had for $\sigma = \downarrow$.

(ii) Or $(\alpha) = (\gamma, j)$ and $(\alpha') = (\gamma, i)$ where $(\gamma)$ does contain neither $i$ nor $j$ and $i \neq j$. The corresponding contribution is

$$-\frac{1}{2}\sum_{\gamma \neq i,j} \phi^*(\gamma, j)\ \phi(\gamma, i)\ [1 - \delta_{ij}] \tag{A.5}$$

(the minus sign comes from anticommuting operators). The $\delta_{ij}$ term cancels the $p$ in the bracket of (A.4) and the final result for $n_{k\uparrow}$ is just the usual Fermi step function. These results are summarized in Figure 11 for a 1d system for which $k_{F\uparrow} = \pi[1 - p/N_L]$. Note that the total number of real $\uparrow$ and $\downarrow$ fermions are the same

$$N_\uparrow = N_\downarrow = N_L \frac{1}{2}\left[1 - \frac{p}{N_L}\right]$$

as it should (real fermions sit on the singlets).

The situation is more complicated when $p_\uparrow$ and $p_\downarrow$ are both $\neq 0$. Then the hard core repulsion between $\uparrow$ and $\downarrow$ holes cannot be ignored (if it were, $n_{k\sigma}$ would become negative). But we know that dilute holes are well represented by a product of Slater determinants, appropriately normalized by the hard core (the normalization constant is $\approx \left[1 - p_\uparrow p_\downarrow / N_L^2\right]$). The Fermi levels (for 1d) are

$$k_{F\sigma} = \pi\left[1 - \frac{p_\sigma}{N_L}\right] \tag{A.6}$$

while the plateaux are to first order

$$n_{k\sigma} = \frac{1}{2}\left[1 - \frac{p_{-\sigma}}{N_L}\right]. \tag{A.7}$$

We expect the distribution shown in Figure 12, which roughly goes from 1/2 to 0. The number of true fermions for $\uparrow$ and $\downarrow$ spins is equal to $1/2\,[1 - p/N_L]$, as expected for singlets (to first order: normalization makes for the second order term). The number of $k$ values inside the Fermi surface is

$$N_L\ [2 - p_\uparrow - p_\downarrow] = N_L + N. \tag{A.8}$$

As expected we find the large Fermi surface.

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