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THEORY OF PRESSURE-INDUCED MAGNETIC AND
METAL-INSULATOR TRANSITIONS*

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ABSTRACT

A theory of pressure-induced simultaneous metal-insulator and magnetic phase transitions is presented. It is based on a model consisting of a periodic lattice with (1) an itinerant-electron band; (2) a narrow dispersionless band (localized states); (3) a hybridization term; (4) a very strong short-ranged repulsion between electrons of opposite spin in the localized states; and (5) a moderately strong short-ranged repulsion between electrons in the itinerant and localized bands. The problem is treated in the Hartree-Fock approximation, allowing spontaneous ferromagnetic broken symmetry. Pressure, which mainly changes the energy separation between the two bands, induces transitions from insulating, (ferro)-magnetic states, to metallic states with no localized moments. The transition may be continuous or discontinuous, depending on the values of the interaction parameters. A richly structured phase diagram is obtained. For some values of the parameters the model reproduces in a reasonable fashion the complex transition recently found in NiI_2 at pressures of about 19 GPa.

1. INTRODUCTION

The metal-insulator transition is a phenomenon of great interest in solid-state physics¹⁻³. It appears in a large variety of substances, including some elements, doped semiconductors, and transition-metal, rare-earth and actinide compounds, and as a function of a variety of external parameters: pressure, temperature and chemical composition. The conductivity transition can be discontinuous (first order) or continuous, and is many times associated with crystal structure modifications and/or drastic changes in the magnetic properties of the substance.

The Diamond Anvil Cell⁴, with its great capabilities, has allowed to explore new systems under pressure. In particular, a combination of techniques (Diamond Anvil Cell, Mössbauer spectroscopy, conductivity and X-ray structural measurements) has produced the discovery of a simultaneous metal-insulator and magnetic phase transition⁵ in NiI_2 , a layered transition-metal insulating compound at ordinary pressures. This compound consists of alternating hexagonal single- Ni and double- I atomic layers stacked along the c -axis; it can be thought of, in the first approximation, as being made of face-centered-cubic I^- ions, intercalated every other layer by hexagonal monolayers of Ni^{++} . The magnetic structure arises principally from the Ni^{++} ions: each layer is ferromagnetically ordered, with successive layers being antiferromagnetically ordered with respect to each other. At ordinary pressures the Néel temperature is approximately 80 K.

Under pressure the antiferromagnetism becomes stronger, with the Néel temperature increasing by approximately a factor of four at pressures of about 19 GPa. At 19 GPa there is a phase transition with several well defined characteristics: (1) the substance is no longer antiferromagnetic, (2) it becomes metallic, and (3) there is no observable change either in the crystal structure, the atomic volume or the lattice parameters.

Electronic band-structure calculations^{6,7} of NiI_2 and the isostructural $NiBr_2$ and $NiCl_2$ yield metals for all three substances, with the Fermi level falling in the middle of the Ni 3d-bands. The fact that all three are insulators indicates the failure of band theory, and the fact that correlation effects in the Ni 3d-bands do produce a Mott insulator.^{1,2} The application of pressure, similarly to the substitution of a light halogen for a heavier one, reduces the energy difference between the halogen np and the Ni 3d-

states. The crystal Hamiltonian produces a hybridization between the various atomic-like orbitals, and favors the existence of itinerant states, *i.e.*, metals. The effect of hybridization is paramount in states with the same or very close orbital energies. Therefore the application of pressure, by decreasing the energy difference between the *Ni* and the halogen orbital energies, might produce an insulator-to-metal transition, as it does in the specific case of *NiI₂*.

It is the purpose of this contribution to present a calculation in which these effects are explicitly modeled. The calculation is based on the Hartree-Fock approximation of a two-band Hamiltonian which includes hybridization and short range interactions: a strong one for electrons in the "localized" band, and a weaker one between electrons in the localized and the extended bands. The model has been called in the past the Falicov-Kimball model^{3,8}, and can be considered a straightforward extension of the periodic Anderson model^{9,10}, with an additional short-range interaction between electrons in the two different states.

Section 2 describes briefly the model. Section 3 contains the approximations and the method of solution. Section 4 presents the results, the discussion and conclusions.

2. THE MODEL

A model that describes the concurrent magnetic and metal-insulator phase transition in *NiI₂* must contain the following basic ingredients:

- (1) An electronic structure which contains extended, only weakly correlated band states. In case of *NiI₂*, the *I* 5*p*-bands are of this kind. For simplicity, the present model takes only a single band, with dispersion ϵ_k , into consideration. The operators $c_{k\sigma}$ ($c_{k\sigma}^\dagger$) annihilate (create) particles in the extended band states with wavevector k , spin σ , and energy ϵ_k .
- (2) The most energetic electrons of the *Ni⁺⁺* ions form a highly correlated, localized (3*d*)⁸-configuration, *i.e.*, each *Ni⁺⁺* ion sustains two holes in the 3*d* shell, as opposed to a collective *Ni* 3*d* conduction band. For two holes the lowest energy term corresponds to total spin $S = 1$. The strong Coulomb repulsion between localized holes on the same site eliminates fluctuations between different configurations, and produces the Mott insulator, *i.e.*, a non-conducting, localized picture for *Ni* 3*d* states. In the model considered here, only one spin-degenerate localized orbital per unit cell is taken

into account. This is a crude approximation, because it is only capable of describing spin magnetic moments, with no contribution arising from the orbital part and the degeneracy of the d -band. The operators $d_{k\sigma}$ ($d_{k\sigma}^\dagger$) annihilate (create) particles in the localized states with wavevector k , spin σ , and energy E . This orbital has no dispersion.

(3) Excess occupancy of the localized orbital is energetically not favorable because of the strong intrasite Coulomb interaction. The model includes this property by a short-range repulsion term, of magnitude U , that describes the strong screened Coulomb interaction for two holes in the same site.

(4) The periodic potential of the lattice is responsible for a hybridization term, of strength V , between the extended c , and the localized d orbitals of the crystal.

(5) The experimental situation⁵ clearly indicates that the magnetization changes discontinuously at the transition pressure. A first-order non-continuous transition can only be obtained, if a repulsion between particles in localized and extended states (of strength G) is included into the model.

In summary the Hamilton operator is:

$$\begin{aligned}
 H = & \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} E d_{k\sigma}^\dagger d_{k\sigma} \\
 & + V \sum_{k,\sigma} (d_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_{k\sigma}) \\
 & + \frac{U}{N} \sum_{k,k',q} d_{k+q\uparrow}^\dagger d_{k'-q\downarrow}^\dagger d_{k'\downarrow} d_{k\uparrow} \\
 & + \frac{G}{N} \sum_{\sigma,\sigma'} \sum_{k,k',q} d_{k+q\sigma}^\dagger c_{k'-q\sigma'}^\dagger c_{k'\sigma'} d_{k\sigma} ,
 \end{aligned} \tag{1}$$

where N denotes the number of unit cells in the crystal.

The function ϵ_k and the four parameters E , V , U , and G , depend directly on the volume of the unit cell, and, through an equation of state, on the applied pressure. A direct study of the pressure dependence is not possible in the framework of this approach. It is therefore assumed that the main effect of an external pressure is a shift of the parameter E , *i.e.*, a decrease in the difference between the average energy value of the extended and localized states, which leads to a significant band overlap and a growing importance of the hybridization. This assumption is supported by existing band-structure calculations.^{6,7}, and by the experimentally found increase of Néel

temperature with pressure⁵.

The model introduced above and its numerous relatives have been studied for the last thirty years in the context of the intermediate-valence systems,¹⁰ the Kondo problem,¹¹ and heavy-fermion systems.¹²

3. THE HARTREE-FOCK APPROXIMATION

A Hartree-Fock approximation H_{HF} to the many-body Hamiltonian (1) is given by

$$H_{HF} = \sum_{k,\sigma} \tilde{\epsilon}_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} \tilde{U}_\sigma d_{k\sigma}^\dagger d_{k\sigma} + \sum_{k\sigma} \tilde{V}_\sigma (d_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_{k\sigma}) - N U \Delta_\uparrow \Delta_\downarrow - N G \Lambda (\Delta_\uparrow + \Delta_\downarrow) + N G (|\Gamma_\uparrow|^2 + |\Gamma_\downarrow|^2) , \quad (2)$$

where the new mean-field, one-particle parameters $\tilde{\epsilon}_k$, $\tilde{U}_\sigma$, and $\tilde{V}_\sigma$ are defined by

$$\tilde{\epsilon}_k := \epsilon_k + G (\Delta_\uparrow + \Delta_\downarrow) , \quad (3a)$$

$$\tilde{U}_\sigma := E + U \Delta_{-\sigma} + G \Lambda , \quad (3b)$$

$$\tilde{V}_\sigma := V - G \Gamma_\sigma . \quad (3c)$$

They depend on the expectation values

$$\Lambda := \Lambda_\uparrow + \Lambda_\downarrow , \quad (4a)$$

$$\Lambda_\sigma := \frac{1}{N} \sum_k \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle , \quad (4b)$$

$$\Delta := \Delta_\uparrow + \Delta_\downarrow , \quad (4c)$$

$$\Delta_\sigma := \frac{1}{N} \sum_k \langle d_{k\sigma}^\dagger d_{k\sigma} \rangle , \quad (4d)$$

and

$$\Gamma_\sigma := \frac{1}{N} \sum_k \langle d_{k\sigma}^\dagger c_{k\sigma} \rangle . \quad (4e)$$

All Hartree-Fock states are assumed to conserve translational symmetry, an approximation that is valid for paramagnetic and ferromagnetic states, but not for antiferromagnets, ferrimagnets, and charge- and spin-density waves. Although NiI_2 is an antiferromagnet, each Ni plane is *ferromagnetic*, with alternating planes arranged

antiferromagnetically with respect to each other. In the present contribution the detailed antiferromagnetic correlation between *Ni*-planes is neglected (it is a smaller effect, arising from Anderson superexchange¹³), and the magnetization *m* discussed below refers exclusively to the single-*Ni*-plane magnetization. It should be noted that if the system were allowed to break the translational symmetry, then there would be an infinite number of possible Λ , Δ_σ , and Γ_σ functions that depend on a given wavevector *q*; these functions are obtained by replacing the angular brackets in (4b), (4d) and (4e) above by $\langle c^\dagger_{k+q\sigma} c_{k\sigma} \rangle$, $\langle d^\dagger_{k+q\sigma} d_{k\sigma} \rangle$, and $\langle d^\dagger_{k+q\sigma} c_{k\sigma} \rangle$ respectively. The self-consistent diagonalization of H_{HF} would then require the solution of an integral equation.

The physical interpretation of the expectation values (4a-e) is obvious: The quantity Δ in (4c) measures the total density of electrons in localized orbitals. Because of the repulsion between band and localized states [*G*-term in (1)], the shift (3a) in band energy from ϵ_k to $\tilde{\epsilon}_k$ is proportional to this density multiplied by the coupling constant *G*. Similarly, Λ measures the total density of band electrons. The effective field resulting from the *G*-term shifts the energy of the localized orbitals, as given in (3b) by a term $G\Lambda$. These energies are also shifted by the repulsion between electrons in the same localized orbital with different spin by the $U\Delta$ -term in (3b). The exchange in the *G*-term leads to an extra spin-dependent contribution to the hybridization *V*, as seen in (3c).

Diagonalization of H_{HF} is straightforward. The linear combinations of the $c^\dagger_{k\sigma}$ and $d^\dagger_{k\sigma}$ operators

$$\Psi^\dagger_{+,k\sigma} = \cos\gamma_{k\sigma} c^\dagger_{k\sigma} + \sin\gamma_{k\sigma} d^\dagger_{k\sigma} , \quad (5a)$$

$$\Psi^\dagger_{-,k\sigma} = -\sin\gamma_{k\sigma} c^\dagger_{k\sigma} + \cos\gamma_{k\sigma} d^\dagger_{k\sigma} , \quad (5b)$$

that diagonalize H_{HF} may be obtained by the standard equation-of-motion technique

$$\left[H_{HF}, \Psi^\dagger_{\pm,k\sigma} \right] = E_{\pm,k\sigma} \Psi^\dagger_{\pm,k\sigma} . \quad (6)$$

The square bracket denotes the usual commutator and the creation (destruction) operators $\Psi^\dagger_{\pm,k\sigma}$ ($\Psi_{\pm,k\sigma}$) create (annihilate) a particle with energy $E_{\pm,k\sigma}$:

$$E_{\pm,k\sigma} = \frac{1}{2} (\tilde{\epsilon}_k + \tilde{U}_\sigma) \pm \left[\frac{1}{4} (\tilde{\epsilon}_k - \tilde{U}_\sigma)^2 + \tilde{V}_\sigma^2 \right]^{\frac{1}{2}} \quad (7)$$

and spin σ . It is easy to see that the excitation spectrum $E_{\pm, k \sigma}$ develops the familiar hybridization gap for non-vanishing $\tilde{V}_{\sigma}$.

The quantities of physical interest here are the total magnetization m

$$m = | [\Lambda_{\uparrow} + \Delta_{\uparrow}] - [\Lambda_{\downarrow} + \Delta_{\downarrow}] | , \quad (8)$$

and the concentration (4a) of particles in the extended states Λ as a function of the various parameters, E in particular. The calculation (a non-linear problem) requires self-consistency. It is equivalent to finding roots of five transcendental equations¹⁴ that depend on the five variables E_F (Fermi energy), Δ , $\eta := \Delta_{\uparrow} - \Delta_{\downarrow}$, $\Gamma_{\uparrow}$, and $\Gamma_{\downarrow}$. The solution for the first two variables, E_F and Δ , as a function of the latter three is always unique, whereas η , $\Gamma_{\uparrow}$, and $\Gamma_{\downarrow}$ may have multiple solutions. Results are presented in the following section.

In order to understand the structure and physical content of the resulting Hartree-Fock ground-state, the quasi-particle density of states:

$$\rho_{\sigma}(\omega) := \frac{1}{N} \sum_k \left[\delta(E_{+, k \sigma} - \omega) + \delta(E_{-, k \sigma} - \omega) \right] \quad (9)$$

is very useful. Some examples are also given in the following section.

4. RESULTS AND DISCUSSION

Results for particular values of the parameters are shown in Figures 1-3. In these figures the total number of electrons in the system is one per formula unit; the density of itinerant states (per spin, per formula unit) was assumed to take the form

$$\rho_0(\epsilon) := \frac{8}{\pi W^2} \left[\epsilon (W - \epsilon) \right]^{\frac{1}{2}} , \quad (10)$$

where W , the bandwidth [directly related to the band energies ϵ_k of (1)], is taken to be the energy unit of the problem. The value of W should be interpreted, rather than the actual bandwidth of the problem, as the value of the energy interval which contains one electron per spin per formula unit in the density of states¹⁵.

The other parameters were taken to be $U = 5 W$ and $V = 0.1 W$. Figure 1 shows the values of m and Λ for the cases of $G = 0.1 W$, and $G = 0.5 W$, as functions of the increasing values of E , i.e., increasing overlap between itinerant and localized states (increasing pressure). The $G = 0.1 W$ case exhibits a smooth increase in Λ

and a continuous decrease in m . In particular m is equal to 1 for values of E smaller than $E = 0.09379 W$, and equal to 0 for values of E greater than $E = 0.46814 W$. These two values of E can be considered those corresponding to pressures at which there are second-order phase transitions¹⁶. The $G = 0.5 W$ case exhibits a discontinuous (first-order) transition from $m = 1$ to $m = 0$ for $E = 0.31549 W$; there is also a corresponding discontinuity in Λ . Figures 2 and 3 show the densities of quasi-particle states for two particular situations close to the transition: $G = 0.5 W$ and $E = 0.31 W$, and $G = 0.5 W$ and $E = 0.32 W$. It can be seen that the former corresponds to a fully magnetized insulator, whereas the latter is an unmagnetized metal. Hybridization plays an important role in all cases.

Figure 4 shows two other cases, intermediate between those depicted in Figure 1. They correspond to $G = 0.3 W$, and $G = 0.4 W$. Whereas the former still exhibits the two second-order transitions characteristic of small G values, the latter presents a new situation. There are in this case, as E (or equivalently the pressure) increases, *three* phase transitions: a second-order one, where m departs from the $m = 1$ value; a discontinuous one, where m jumps between two intermediate values; and another second-order transition when m finally attains the $m = 0$ value.

It is instructive to plot the contours of constant m in the G - E plane. This plot divides the G - E plane into three regions: $m = 1$, the first high-symmetry region; $m = 0$, the second high-symmetry region, and intermediate values of m , the low-symmetry region. There are in this plane three lines of singularities, and three singular points. A second-order line separates regions of $m = 0$ and non-zero m values, in which m varies continuously. Another second-order line divides regions of $m = 1$ and $m < 1$ values, in which m also varies continuously. There is a third line along which m has jump discontinuities; these can be between $m = 1$ and $m = 0$, between intermediate values of m and $m = 0$, or between two intermediate values of m . The separation of these three regimes are given by singular points where the second-order lines meet the line of discontinuities. Finally the line of discontinuities, where it separates two regions of low and identical symmetry, terminates at a *classical* critical point.

Even though only a few cases have been explored in detail, it is evident that the model described by (1) exhibits a great richness of structure and possibilities. The

examples studied here, in any case, encompass that which motivated this study: The simultaneous magnetic and insulator-metal transition in NiI_2 . The graph of Figure 4, case (2) seems to reproduce fairly well the behavior of the hyperfine field, *i.e.*, the Ni -plane magnetization, as determined by Mössbauer spectroscopy, and reported in Reference 5. The densities of quasi-particle states shown in Figures 2 and 3, when account is taken for the difference in band structure between the present model and the Ni halogenides, describe qualitatively the electronic changes expected in these transitions.

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- ¹⁴ In the self-consistency problem only Λ , as given by (4a), rather than the individual spin components Λ_{σ} , given by (4b), appear. In addition the self-consistent equation for Λ is automatically satisfied with the determination of the Fermi level

E_F , and Δ , because $(\Lambda + \Delta)$ equals the total number of particles per site.

- 15 It should be emphasized that even though the present formulation treats itinerant and localized *electrons*, the actual case of NiI_2 corresponds to itinerant *holes* derived from the $5p$ -electrons of I , and localized *holes* in the $(3d)^8$ configuration of Ni^{++} . The transformation from electrons to holes is elementary; the multiplicity of states on the localized $(3d)^8$ configuration, caused by the orbital angular momentum, is not included in the present model. For the particular case of NiI_2 , where the conduction band derives from the $5p$ -electrons of I and there are two I per formula unit, the value of W should be approximately one sixth of the total $5p$ -bandwidth, or probably smaller, given the accumulation of states at the top of the $5p$ -band.
- 16 Second-order phase transitions, as used here, are in the sense defined by Landau [see for instance L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley, Reading MA, 1958), Chapter XIV]. The order parameter in this case is the magnetization, with the values of $m = 0$ and $m = 1$ constituting two distinct high-symmetry phases, and intermediate values of m being the low-symmetry phase.

FIGURE CAPTIONS

Figure 1.

The magnetization m (upper graph) and the extended-band occupation number Λ (lower graph) for $U = 5 W$ and $V = 0.1 W$, as functions of E ; (1) $G = 0.1 W$; (2) $G = 0.5 W$. Case (1) exhibits two second-order transitions. Case (2) shows only a discontinuous transition.

Figure 2.

Schematic representation of the density of quasi-particle states for the case $U = 5 W$, $V = 0.1 W$, $G = 0.5 W$, and $E = 0.31 W$. The horizontal thin full line indicates the energy of the last occupied state. The dashed lines represent the densities of spin states in the absence of interactions and hybridization (the dashed straight lines are the localized states). Note that the system is fully magnetized (no down-spin states occupied) and is an insulator, with an energy gap between last occupied (up-spin) states and first empty (down-spin) states. There are additional localized down-spin states at higher energies, not included in the graph.

Figure 3.

Schematic representation of the density of quasi-particle states for the case $U = 5 W$, $V = 0.1 W$, $G = 0.5 W$, and $E = 0.32 W$. The horizontal thin full line indicates the energy of the last occupied state. The dashed lines represent the densities of spin states in the absence of interactions and hybridization (the dashed straight lines are the localized states). Note that the system is not magnetic, with identical bands and identical occupation of both spins. It is also metallic, since the Fermi level falls in the middle of the lower band. There is considerable hybridization, and no clear distinction can be made between localized and extended states.

Figure 4.

The magnetization m (upper graph) and the extended-band occupation number Λ (lower graph) for $U = 5 W$ and $V = 0.1 W$, as functions of E ; (1) $G = 0.3 W$; (2) $G = 0.4 W$. Case (1) exhibits two second-order transitions. Case (2) shows three

singularities: two second-order transitions and, at an intermediate value of E , a discontinuous change.

Figure 5.

The regions in the G - E plane where, for $U = 5 W$ and $V = 0.1 W$, m takes specific values: $m = 1$, the first high-symmetry region; $m = 0$, the second high-symmetry region, and intermediate values of m , the low-symmetry region. Thin lines indicate second order transitions, where m departs from one of the high-symmetry values and varies continuously. The thick line indicates discontinuous changes in the values of m . The open circles show the intersection of the line of discontinuities with the second-order-transition lines, and separate regions where m jumps from 1 to 0, from an intermediate value to zero, and between two intermediate values. The black dot indicates the "classical" critical point, where the line of discontinuities stops, *i.e.*, the discontinuities vanish.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

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