Ground-state Phase Diagram of the One-dimensional Kondo Lattice Model

Nichols A. Romero†

University of Illinois at Urbana-Champaign
Department of Physics
1110 West Green Street
Urbana, Illinois 61801–3080

The Kondo lattice model (KLM) is the canonical model of strongly correlated electron systems. It is of particular interest because it is the simplest model that describes the physics of heavy fermion materials which show a rich variety of phases. In this review, we summarize the salient features and underlying physics of the one-dimensional KLM. The zero-temperature phase diagram exhibits three phases: a ferromagnetic metallic, insulating spin liquid, and a paramagnetic metallic state. Results are presented for the transitions between these phases as obtained through a variety of analytic and numerical techniques.

CONTENTS

I. INTRODUCTION

This review article is written in a pedagogical manner so that any graduate-level physics student with no background in strongly-correlated electron systems can understand the salient features of the Kondo lattice model (KLM). In Section I.A, I motivate the study of heavy-fermion materials by presenting the properties of the diverse ground state. There is a interesting history behind the KLM which is being the scope of this paper. To begin understanding the KLM requires knowledge of the single-impurity problem which is discussed in Section I.B. I conclude Section I by bridging the gap between the Kondo problem and heavy fermions. The focus of Section II is to present the models for heavy fermions and the interactions which lead to the diversity in their physical properties. The ground-state phase diagram of the one-dimensional KLM is presented in Section III. Further avenues of exploration are discussed in section (IV) of this review article.

A. Motivation

Since the discovery of heavy-fermion compounds, condensed matter physicists have pursued the problem of understanding the strong correlation effects which determine the physical properties of these interesting materials. In general, these materials are intermetallic compounds containing rare-earth or actinide elements. It is the diversity of the heavy fermion ground state which has generated excitement in recent years. It has now been experimentally observed that there are four known ground states: (i) normal heavy-fermion states, (ii) antiferromagnetically ordered states, (iii) unconventional superconducting states and (iv) Kondo insulators

The low temperature behavior of these materials is at odds with that expected for Fermi liquids (FL). Table I gives a comparison of the leading low temperature behavior of specific heat coefficient $\gamma = C/T$, the magnetic susceptibility χ, and the temperature dependent resistivity $\Delta\rho$ for $CeCu_{6-x}Au_x$. Table II gives characteristics numbers which explain why these heavy-fermion materials have produced so much excitement. The behavior of these thermodynamic and transport properties are described next.

TABLE I Comparison of physical properties for a heavy fermion material $CeCu_{6-x}Au_x$ and those of a Fermi liquid Lavagna and Pépin (1999).

property	heavy-fermion state	Fermi liquid
γ	$-\ln T/T_0$	const
χ	$1-\alpha\sqrt{T}$	const
$\Delta\rho$	T	T^2

TABLE II Comparison of data between heavy-fermion materials and those of conventional metals. Lee *et al.* (1986)

Kind	Specific-Heat Coefficient $\gamma(0)$ [mJ/mole-K^2]	Magnetic Susceptibility $\chi(0)$ [memu/mole]	Room-Temperature Resistivity $\rho(298K)$ [$\mu\Omega$-cm]	T^2-Coefficient of Resistivity A [$\mu\Omega$-cm/K^2]
superconductor (UPt_3)	450	7	150	3
magnet (U_2Zn_{17})	400	12	110	
normal ($CeAl_3$)	1600	40	170	35
conventional (Pd)	9.4	0.8	20	10^{-5}

There are two ways the heat coefficient enhancement can be interpreted. (i) Interpreting the specific heat in terms of the fraction of electrons in the band that are thermally excited $C \sim nk_B(T/T_0)$, where $T_0 \sim 10K$ is the characteristic bandwidth temperature. (ii) Comparing with a free-electron-type formula for $\gamma(0) = m^* k_F/\pi^2\hbar^2)(k_B^2/3)$, one determines a large effective mass $m^*/m_e \sim 10^3$. It is generally accepted that the strong-correlations and not band-structure effects are predominately responsible for the interesting low temperature properties of these materials. It is the coherent propagation of these very-heavy-fermionic quasiparticles that leads to the formation of the heavy-fermion state.

In contrast to conventional metals, the magnetic susceptibility for heave-fermion metals exhibits considerable temperature dependence. At high temperatures χ is well fit by a Curie-Weiss Law $\chi = C/(T+\theta)$. While at low temperatures, χ flattens out into a relatively constant susceptibility which is quite enhanced over that of conventional metals as the values in Table II indicate.

We know turn away from considering thermodynamic properties and investigating the resistivity ρ, a transport properties which especially characterizes metals. Figure 1 exemplifies the most striking physical property of the heavy-fermion materials. The resistivity increases with decreasing temperature, while that for conventional metals decreases. At high temperatures ($T > 30$ K), all the curves show Kondo-$\ln T$ behavior. At low temperature there is a transition from saturation of the resistivity at ~ 60 $\mu\Omega$-cm for dilute samples ($x > 0.2$) to coherent behavior for dense samples $x < 0.15$.

Particularly stimulating and controversial is the ongoing discussion on the origin of superconductivity in these heavy-fermion materials, e.g. UPt_3, $CeCu_2Si_2$ and UBe_{13}. The central question is whether electron-electron mechanism could be operative in heavy-fermion superconductivity. The possibility of non-phononic mechanism and exotic pairing states has fascinated experimentalists and theorists alike.

B. Spin Hamiltonians

The starting point for studying any strongly-correlated electronic systems is to write down a simple Hamiltonian $\mathcal{H}$ which captures the physics interest. In Section I.B.1, I introduce the simplest model for studying magnetic properties. The homogeneous spins systems are in fact to simple to describe any strongly-correlated electron systems. This will leads us into the single-impurity models (Section I.B.2) which is the starting point for studying heavy-fermions in the dilute impurity limit. I follow a presentation similar to Mahan (1990) and Hewson (1993).

1. Homogeneous Spin Systems

The Heisenberg model is the most generic zero field ($H = 0$) Hamiltonian for treating spins which are identical on each site.

$$\mathcal{H}_{\text{Heisenberg}} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \tag{1}$$

where the sum is evaluated over the nearest-neighbors $\langle ij \rangle$. If the system of interest posses anisotropies, equation 1 can be generalized,

$$\mathcal{H}_{\text{Heisenberg}} = -J_{\parallel} \sum_{\langle ij \rangle} S_i^z S_j^z - J_{\perp} \sum_{\langle ij \rangle} \left(S_j^x S_j^x + S_i^y S_j^y \right) . \tag{2}$$

When $J_{\perp} = 0$ the Heisenberg model reduces to the well-known Ising model,

$$\mathcal{H}_{\text{Ising}} = -J_{\parallel} \sum_{\langle ij \rangle} S_i^z S_j^z , \tag{3}$$

and when $J_{\parallel} = 0$, we have the XY model

$$\mathcal{H}_{\text{XY}} = -J_{\perp} \sum_{\langle ij \rangle} \left(S_j^x S_j^x + S_i^y S_j^y \right) . \tag{4}$$

These homogeneous spin Hamiltonian are capable of qualitatively describing where strong electron correlations are non-existent.

2. Single-Impurity Models

In these models the spin is an isolated impurity in an otherwise homogeneous electron gas. They allow one to

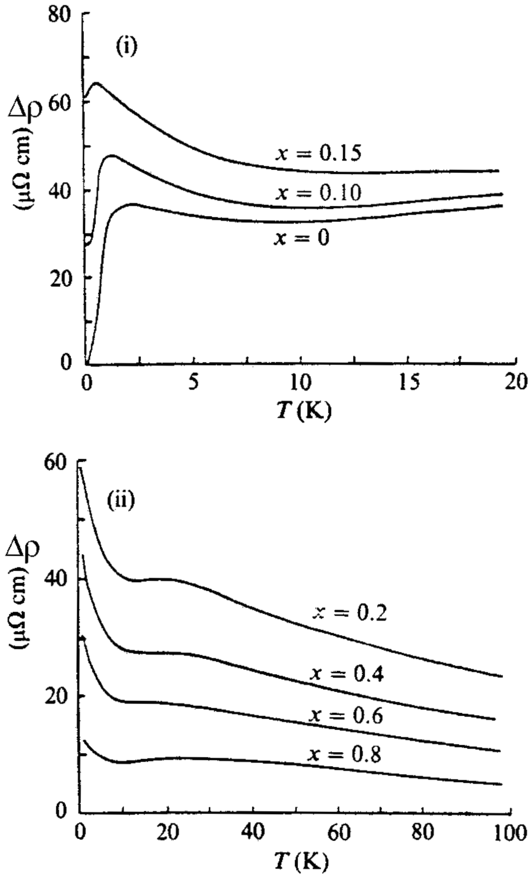

FIG. 1 The resistivity difference $\Delta\rho(T)$ of $Ce_{1-x}La_xPb_3$ minus that of $LaPb_3$ for the concentrations x indicated, (i) shows the on-set of coherence for small La concentrations and, (ii) the loss of the maximum and impurity-like behavior for small concentrations of Ce from Lin *et al.* (1987).Note that $x = 0$ corresponds to the lattice case.

study the formation of local moment on the impurity as well as scattering of the conduction electrons from the localized spin. As in Section I.B.1, I continue to present these Hamiltonians with site-independent coupling constants.

The $\mathcal{H}_{\rm sd}$ interaction is a model of localized f electrons interacting with s-like continuum wave functions.

$$\mathcal{H}_{\rm sf} = J\sum_{\vec{k}}\left[S^z\left(n_\uparrow^{\vec{k}} - n_\downarrow^{\vec{k}}\right) + S^+ c^\dagger_{\vec{k}\uparrow}c_{\vec{k}\downarrow} + S^- c^\dagger_{\vec{k}\uparrow}c_{\vec{k}\downarrow}\right] \quad (5)$$

where the spin$-\frac{1}{2}$ operators can be defined through the creation and annihilation operators of localized electrons in f orbitals:

$$S^z = \frac{1}{2}\left(n_\uparrow^f - n_\downarrow^f\right) \quad (6)$$

$$S^+ = f_\uparrow^\dagger f_\downarrow \quad (7)$$

$$S^- = f_\downarrow^\dagger f_\uparrow. \quad (8)$$

The first term is an interaction between the z-component of the spin of both the impurity and continuum wave function. The last two terms flip the spin of the continuum electrons while flipping the localized spin of the impurity in the opposite direction.

This leads us to the simplest Hamiltonian that can be constructed for a correlated-electronic system. It includes the energetics of both the conduction electrons and the localized spins plus the mixing term Eq.5. It was Zener (1951) and not Kondo himself, who proposed the Hamiltonian,

$$\mathcal{H}_{\rm Kondo} = \sum_{\vec{k},\alpha}\varepsilon_{\vec{k}}n_\alpha^{\vec{k}} + \varepsilon_f\sum_\alpha n_\alpha^f + \mathcal{H}_{\rm sf} \quad (9)$$

where $\alpha = \uparrow,\downarrow$. The Kondo Hamiltonian applies to a localized spin with 2 degrees of freedom, the generalization to N degrees of freedom is given by the Coqblin-Schrieffer model,

$$\mathcal{H}_{\rm CSM} = \sum_{m=1}^{N}\sum_{\vec{k}}\varepsilon_{\vec{k}}n_\alpha^{\vec{k}} + \frac{J}{N}\sum_{m,m'=1}^{N}\sum_i f^\dagger_{im}c_{im}c^\dagger_{im'}f_{im'}. \quad (10)$$

No discussion of impurity models would be complete without mention of Anderson's model,

$$\mathcal{H}_{\rm Anderson} = \sum_{\vec{k},\alpha}\varepsilon_{\vec{k}}n_\alpha^{\vec{k}} + \varepsilon_f\sum_\alpha n_\alpha^f + Un_\uparrow^f n_\downarrow^f + V\sum_{\vec{k},\alpha}\left(c^\dagger_{\vec{k}\alpha}f_{\vec{k}\alpha} + \text{H.c.}\right) \quad (11)$$

where H.c. denotes Hermitian conjugate.

The Anderson and Kondo models describe the interactions of conduction electrons with those of localized spins. These two apparently distinct models are not totally different. There exist canonical transformation which prove that the Kondo Hamiltonian is a subset of the Anderson Hamiltonian. This transformation produces an infinite number of terms which exemplify some of the rich phenomena that are Anderson model describes includes (i) potential scattering of conduction electrons, (ii) non-spin-flip interaction between a conduction electron and an impurity electron, (iii) interactions between impurity electrons and (iv) a process by which two localized electrons hop off the impurity site to become two conduction electrons.

C. The Kondo Problem to Heavy Fermions

This is a brief historical digression which explains the state of the so-called Kondo problem. I've avoided the frequent use of the adjective "Kondo" because the word tends to be used loosely in the literature. In Section I.B.2 I described the models for a single magnetic impurity in a host metal. These theories were developed over a period of thirty years and most of the models for explaining these systems are well understood. Concepts such a scaling trajectories, fixed points, spin compensation, quasi-particles, FLT and Kondo resonances were successful in providing exact solutions to their thermodynamic behavior.[1] Figure 2 exemplifies the excellent agreement between theory (solid-line) and experiment (dots) using the Coqblin-Schrieffer model.

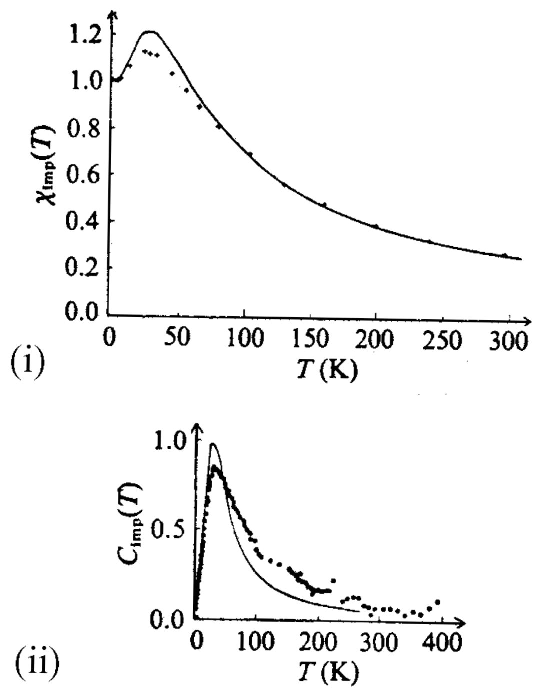

FIG. 2 Comparison of experimental results for the compound YbCuAl with exact results for the $N = 7$ Coqblin-Schrieffer model with $T_K = 66$ from Rajan (1983).

Using the Hamiltonian given by Eq.9, Kondo formulated an elegant explanation for the long-standing mystery known as the resistance minimum observed in metals like Cu and Al doped with small concentration of Fe or Ni. A spin-flip scattering mechanism between the conduction electrons (near the Fermi level) and the localized spins which resulted in the *Kondo effect*, the screening of the impurity spin by the conduction electrons. Kondo showed using third order perturbation theory in the coupling constant J, that this interaction led to the $\ln T$ contribution to the resistivity. It also gave rise to the temperature-dependent susceptibility as described in Section I.A.

There were difficulties with the theory near low temperatures because of the $\ln T$ divergence. The search for a comprehensive theory to explain the resistance minimum became known as the *Kondo problem.* It was K. G. Wilson application of the numerical renormalization group that gave definitive results for the low temperature enhancement of ξ and γ. This was shortly followed by Noziéres (1999) exact calculation for the T^2 for the resistivity using only FLT. The Kondo single-impurity problem was solved.

The solution to any good problem always leads to questions and further problems. The difficult with the single-impurity model is that it fails to develop coherence effects. The most striking example is depicted in Fig.1. Here the resistivity due to single impurity saturates at low temperatures while that of the heavy-fermions decreases as T^2. It was pointed out by Noziéres (1999) that the compensation of a localized moment in an impurity-like way would be impossible for concentrated systems as there would not be enough occupied electron states in the region of the Fermi level for this to be possible. There is agreement with the impurity models on certain aspects of the behavior of dense systems, however the transport properties at low temperatures are not predicted correctly. The study of the single-impurity model has led to further investigation into *Kondo lattices*, periodic arrays of magnetic impurities interacting with conduction electrons.

II. HEAVY-FERMION MODELS

The discussion of heavy-fermion models closely follows the treatment by Tsunetsugu *et al.* (1997).

A. PAM and KLM

The minimum requirement for a theoretical model of heavy-fermion systems is to consider two types of orbitals for the electrons. The conduction electrons which can be in s,p or d orbitals and the localized electrons in f orbitals. The generic Hamiltonian which be written down is the orbitally nondegenerate periodic Anderson Model (PAM),

$$\mathcal{H}_{\rm PAM} = -t \sum_{\langle ij\rangle,\alpha} \left(c^\dagger_{i\alpha} c_{j\alpha} + {\rm H.c.}\right) + \sum_{i,\alpha} \varepsilon_f n^f_{i,\alpha} + V \sum_{i,\alpha} \left(c^\dagger_{i\alpha} f^\dagger_{i\alpha} + {\rm H.c.}\right) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow}. \quad (12)$$

The first term represents the hopping processes of the conduction electrons, ε_f is the energy of the f level, the third term describes the local mixing between the two

[1] This is a resonance in the quasi-particle density of states at T_0.

orbitals, and finally U is the on-site Coulomb interaction for the f orbitals. Note that when we consider the f orbital on a single site, Eq.12 reduces to the single-impurity Anderson model Eq.11. If the charge fluctuations of the f electrons are omitted and the lowest f-ion multiplet is taken into account as a localized spin, the PAM can be effectively treated as the Kondo Lattice Model (KLM),

$$\mathcal{H}_{\rm KLM} = -t \sum_{\langle ij\rangle,\alpha} \left(c^\dagger_{i\alpha} c_{j\alpha} + \text{H.c.} \right) + J \sum_i S^f_i S^c_i \quad \text{(13a)}$$

$$\begin{aligned}\mathcal{H}_{\rm KLM} = &-t \sum_{\langle ij\rangle,\alpha} \left(c^\dagger_{i\alpha} c_{j\alpha} + \text{H.c.} \right) \\ &+\frac{J}{2} \sum_i \left(c^\dagger_{i\uparrow} c_{i\downarrow} f^\dagger_{i\downarrow} f_{i\uparrow} + \text{H.c.} \right) \\ &+\frac{J}{4} \sum_i \left(n^c_{i\uparrow} - n^c_{i\downarrow} \right) \left(n^f_{i\uparrow} - n^f_{i\downarrow} \right) \end{aligned} \quad \text{(13b)}$$

where $\vec{S}^c_i = \frac{1}{2}\sum_{\alpha,\alpha'} \sigma_{\alpha,\alpha'} c^\dagger_{i\alpha} c_{i\alpha'}$ are the spin density operators for the conduction electrons and $\vec{S}^f_i = \frac{1}{2}\sum_{\alpha,\alpha'} \sigma_{\alpha,\alpha'} f^\dagger_{i\alpha} f_{i\alpha'}$.[2] The KLM model which was originally proposed by Doniach (1977) can obtained from the PAM using second-order perturbation theory with respect to V. The exchange interaction derived in this way gives $J = 8V^2/U$. Therefore the small-J limit of the KLM corresponds to the limit of the strong Coulomb interaction.

B. Kondo effect vs. RKKY interaction

In the KLM, the exchange coupling is the source of interesting many-body effects. Again much like the PAM, when only a single f-spin is considered, Eq.13 reduces to the single-impurity case Eq.9. It was shown by Yosida (1966) that the ground state of the Eq.13 is a many-body singlet composed of the localized spin and the local spin polarization of conduction electrons. Wilson (1975) showed that the anomalous temperature dependences of physical quantities was a result of the crossover from the weak-coupling regime at high temperatures to the strong-coupling nature at low temperatures.

As discussed in Section I.C, the Kondo effect is essentially understood. The study of the lattice problem has a longer history than that of the Kondo effect. It began with the study of nuclear-spin ordering in a metal. In this context the localized spins S_i are the nuclear spins, and the exchange coupling in 13 is to be understood as a hyperfine coupling. Ruderman and Kittel (1954) derived the indirect nuclear spin-spin interaction by second-order perturbation theory,

$$\begin{aligned}\mathcal{H}_{\rm RKKY} = &-\frac{9\pi}{8} n_c^2 \frac{J^2}{\varepsilon_F} \sum_{\langle ij\rangle} \frac{\vec{S}_i \cdot \vec{S}_j}{r^3_{ij}} \Big[2k_F \cos\left(2k_F r_{ij}\right) \\ &- \frac{\sin\left(2k_F r_{ij}\right)}{r_{ij}} \Big], \end{aligned} \quad (14)$$

where n_c is the conduction electron density and k_F is the Fermi wave number. The Ruderman-Kittel-Kasuya-Yosida (RKKY) Hamiltonian is a long ranged spin-spin interaction which changes its spin depending on the distance between spin pairs.

The RKKY interaction was introduced to complete our broad picture of the KLM. The main physical idea behind the KLM: (i) the competition between the Kondo effect and the RKKY interactions and (ii) the nature of the screening of the localized spins in the lattice. The former point tells us that with decreasing temperature, the Kondo effect on each site tends to suppress magnetic moments,i.e. favor the paramagnetic state, while the RKKY interactions tends to magnetically order the localized spins. It was Noziéres (1999) who pointed up the possibility of an exhaustion of the conduction electrons in the screening of the localized spins. As discussed in Section I.C, in the single-impurity Kondo case the localized spins are screened by the conduction electrons leading to the formation of a singlet state. The number of conduction electrons in the Kondo effect is equal to 1. In the Kondo lattice case, the number of conduction of electrons within $k_B T$ of the Fermi surface maybe insufficient to screen all the localized spins. This "incomplete" Kondo effect and the residual unscreened localized spin that leads to some of the interesting low temperature behavior.

III. PHASE DIAGRAM

Obtaining the phase diagram of the one-dimensional KLM proved to be a non-trivial task. Earlier investigation by Doniach (1977) using mean field theory (MFT) and those of Jullien *et al.* (1979) using real-space renormalization-group analysis led to controversial results. It was the disagreement with the quantum Monte Carlo (QMC) study of the 1D KLM below half-filling ($n_c < 1$) by Troyer and Würtz (1993) that led to the re-examination of the phase-diagram.

A. Ferromagnetic-Paramagnetic Phase

Because the physics of the KLM is a competition between the Kondo effect and the RKKY interaction, there are two limits of primary interest. In the large-J regime, the localized spins are essentially screened by the conduction favoring a paramagnetic (PM) state while in the small-J regime, the magnetic ordering of the localized

[2] This J is different from the one defined in the $\mathcal{H}_{\rm sd}$. They are related as follows $J_{\rm KLM} = 2J_{\rm sd}$.

spsins favor a ferromagnetic (FM) state. Further investigation concluded that a ferromagnetic phase (FM) existed at strong- and intermediate coupling J/t regions for all conduction electron densities n_c and that a spin-liquid insulator phase existed at half-filling $n_c = 1$ for all values of J. For some time, the FM-PM phase boundary was unknown. Tsunetsugu *et al.* (1993) determined the first reliable phase diagram using numerical diagonalization. Even with these results several issues remained:

1. Does a FM phase exists in an infinite-size system?
2. What does the FM-PM phase boundary look like near half-filling?
3. Is the FM-PM phase transitions first or second-order?
4. Is there any phase separation?

These questions were not answered until quite recently. McCulloch *et al.* (1999) used an infinite-size density matrix renormalization group (DMRG) to study the 1D KLM. Figure 3 confirms the FM-PM phase boundary up to $n_c = 0.95$. Their findings also agree with the proposal of Tsunetsugu *et al.* (1993) that PM-FM transition is of second-order. They determined that for $J < 0$, the ferromagnetic phase only asymptotically approaches half-filling due to phase separation between ferromagnetism and spin-liquid insulating phase at *exactly* half-filling.

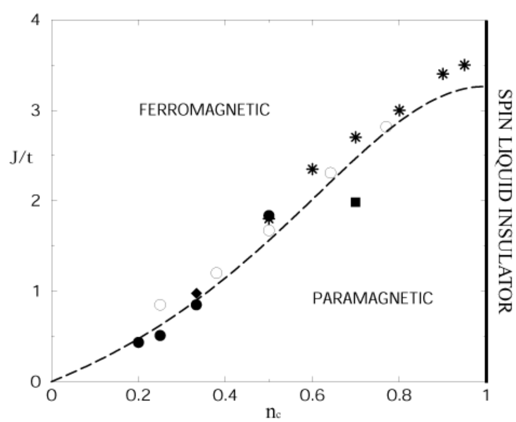

FIG. 3 Phase diagram of the 1D KLM. The stars are the recent results of McCulloch *et al.* (1999) using the DMRG. The data is superimposed on the results of Tsunetsugu *et al.* (1993) calculated by numeric diagonalization. The open circles are the boundary of $S_{\text{total}} = \frac{1}{2}(L - n_c)$ and the solids circles are the intermediate S_{total}.

B. Spin-liquid Insulator

In bipartite lattices, the physics at carrier density $n_c > 1$ is identical to that that at $1 - n_c < 1$, due to particle-hole symmetry. The properties of the KLM at half-filling $n_c = 1$ are very different from those at $n_c \neq 1$. There is a quantum-disordered phase in which spin and charge correlation decay exponentially in space and time. This spin-liquid insulator is characterized by finite energy gap in both charge and spin excitations.

The half-filled KLM is a simple model for a group of recently discovered compounds called "Kondo insulators." At high temperatures they exhibit Curie-Weiss behavior in the magnetic susceptibility, and evolve into a semi-conducting phase with small gaps at low temperatures. Some of these compounds are listed in Table III).

TABLE III Example of Kondo Insulators Aeppli and Fisk (1992).

Compound	Gap[K]
$Ce_3Bi_4Pt_3$	42
SmB_6	27
CeNiSn	3
YbB_{12}	62

IV. CONCLUSIONS

An important issue that has not been addressed in this review is heavy-fermion superconductivity. It is known that there is no long-range order of superconductivity in one dimension. Nonetheless, a good starting point for investigation is a comparison of the correlation functions for KLM with the non-interacting case $J = 0$.

Obviously, the ultimate goal is to understand real three-dimensional heavy-fermion systems. Since there are no $ab-initio$ approaches for studying strongly correlated electron systems in site, these heavy-fermion models will be continue to be used in further investigation. Based on the progress made in one-dimensional systems, some of these techniques have been successfully applied to higher dimensions. Vekiíc *et al.* (1995) applied QMC to study the transition between the spin-liquid phase and the antiferromagnetically order phase in a two-dimensional KLM.

Whatever the dimensionality of the study, it is essential to go beyond the mean-field level to study the low energy properties of heavy fermions.

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†Electronic address: `nromero@uiuc.edu`; URL: `http://www.uiuc.edu/~nromero/`

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