Phase Transitions in the Symmetric Kondo Lattice Model  
in Two and Three Dimensions  
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Abstract  
We present an application of high-order series expansion in the coupling  
constants for the ground state properties of correlated lattice fermion systems.  
Expansions have been generated up to order $(t/J)^{14}$ for $d = 1$ and $(t/J)^8$  
for $d = 2, 3$ for certain properties of the symmetric Kondo lattice model.  
Analyzing the susceptibility series, we find evidence for a continuous phase  
transition from the “spin liquid” phase characteristic of a “Kondo Insulator”  
to an antiferromagnetically ordered phase in dimensions $d \geq 2$ as the antiferromagnetic Kondo coupling is decreased. The critical point is estimated to  
be at $(t/J)_c \approx 0.7$ for square lattice and $(t/J)_c \approx 0.5$ for simple-cubic lattice.

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The interplay between magnetic Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction and the Kondo effect is a central unresolved problem in the physics of valence fluctuation and heavy fermion compounds [1]. The development of magnetic long-range order in heavy fermion metals has been a subject of intensive experimental investigation. On the theoretical side, aside from an early conjecture made by Doniach [2] and Varma [3] that a state with antiferromagnetic (AF) long-range order is energetically more favorable than the non-magnetic Kondo state for small enough AF Kondo couplings, such basic issues as the location of the critical point, the order of the transition, and the transport properties in the critical regime remain to be understood [1]. The recent revival of interest in the class of stoichiometric insulating compounds known as “Kondo insulators” [4] has uncovered both non-magnetic semiconducting and AF-ordered materials at low temperatures. Examples of the former are CeNiSn, Ce₃Bi₄Pt₃, and CeRhSb [4], whereas those of the latter are UNiSn [5], CePdSn and CePtSn [6]. Furthermore, susceptibility and transport measurements on ternary compounds CeNi₁₋ₓ(Pd,Pt)ₓSn suggest a continuous AF transition as a function of isoelectronic substitutions x [6]. In this context, the periodic Anderson model and the symmetric Kondo lattice model (KLM) may be considered as prototypical models that plausibly captures some of the essential physics of electronic correlations in stoichiometric Kondo insulators [7]. The possibility of a continuous transition between an insulating, spin-liquid phase and an AF phase in these models has been investigated recently by mean-field approximations [8], variational wavefunction calculations [9,10] and large-scale quantum Monte Carlo simulations [11].

In this Communication we apply high-order Rayleigh-Schrödinger perturbation theory [18], about the strong-coupling limit, to the zero-temperature properties of the symmetric KLM. In particular, we address the possibility of a continuous transition in dimensions \( d \geq 2 \). The Hamiltonian of the symmetric KLM is given by

\[
H = -t \sum_{\langle ij \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} + J \sum_i S_i \cdot s_i,
\]

which describes a half-filled band of conduction electrons (with creation operator \( c_{i \sigma}^\dagger \) and nearest neighbor hopping amplitude \( t \)) interacting with a lattice of spin-half local moments.
$S_i$ through an intra-site Kondo coupling $J$ (taken to be AF, i.e. $J > 0$); $s_i = \frac{1}{2}c_i^{\dagger} \tau_{\sigma \sigma'} c_{i \sigma'}$ (where $\tau$ are the Pauli matrices) denotes the conduction electron spin at site $i$. We will consider only the simplest lattice structures in this paper, so that $d = 2, 3$ is shorthand for the square and simple-cubic lattices, respectively.

In one dimension, the symmetric KLM possesses an insulating spin-liquid ground state characteristic of a “Kondo insulator” for all values of the Kondo coupling $J > 0$. The spin and charge excitations exhibit interesting properties found through quantum Monte Carlo (QMC) simulations [12,13], exact diagonalization [14], variational wavefunction [15], and density matrix renormalization group (DMRG) [16] studies. For an $N$-site symmetric KLM, the number of states with $\sum_i (S^z_i + s^z_i) = 0$ (that is, the dimension of the space within which finite-lattice calculations are generally done in the absence of any spatial symmetries) is given by $\sum_m (\frac{N}{m})^3$, a number which reaches roughly 740,000 for $N = 8$. Exact diagonalization is therefore limited to systems with $N \leq 10$ [14], which suggests that approach is only suited to the study of the one-dimensional KLM. The DMRG, which has been applied to the symmetric KLM with $N$ up to 24 [16], is also effectively restricted to one-dimensional (or quasi-one-dimensional) systems so far [17]. The large Hilbert space makes the generalization of these methods to $d > 1$ impractical at the present time.

The series expansions, unlike other $T = 0$ numerical approaches, is not restricted to $d = 1$, and it is a method well-suited to locating critical points (which there is reason to believe exist in $d \geq 2$). Its primary requirement is that the unperturbed Hamiltonian have a nondegenerate (or finitely degenerate) ground state, which is fulfilled by the symmetric KLM in the strong-coupling ($t/J = 0$) limit. To demonstrate the validity of our series expansions, the $d = 1$ symmetric KLM will be first considered and our results compared with others’ in the literature. For $d \geq 2$, our calculations suggest that AF spin susceptibilities for both local moments and conduction electrons diverge at a critical value of $t/J$, indicative of a continuous AF-ordering phase transition. Our estimates of the critical points are $(t/J)_c \approx 0.7$ for $d = 2$ and $(t/J)_c \approx 0.5$ for $d = 3$. 
In the strong coupling limit, the ground state is non-degenerate and describes a state in which the conduction electron spin and the local moment are locked into local singlets at every site. The series calculations involve perturbative diagonalization of finite-cluster Hamiltonians, with the hopping term \( t \) as the perturbation, followed by evaluation of relevant matrix elements. In contrast with exact diagonalization, perturbative diagonalization is a noniterative process: with \( m \) matrix multiplications one obtains the ground state eigenvector to order \( (t/J)^m \) and the ground state energy to order \( (t/J)^{m+1} \).

Properties of the KLM for which series have been constructed include: the ground state energy per site \( E \); the zero-frequency local moment and conduction electron antiferromagnetic spin susceptibilities \( \chi_l(Q) \) and \( \chi_c(Q) \) (where \( Q \) is the zone-corner wavevector, and it is assumed that \( g = 2 \) for both conduction and localized electrons); equal-time two-point density correlations \( \mathcal{N}(\mathbf{r}) = \langle (n(\mathbf{r}) - 1)(n(\mathbf{0}) - 1) \rangle \) (with \( n = \sum_\sigma c_\sigma^\dagger c_\sigma \)); equal-time single-particle Green’s functions \( \mathcal{G}(\mathbf{r}) = \langle \sum_\sigma (c_\sigma^\dagger(\mathbf{r})c_\sigma(\mathbf{0}) + c_\sigma^\dagger(\mathbf{0})c_\sigma(\mathbf{r})) \rangle \) and thence the momentum distribution function \( n(\mathbf{k}) = \sum_\mathbf{r} \mathcal{G}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \); and local moment correlations \( S_l(\mathbf{r}) = \langle S^z(\mathbf{r}) \rangle \). Above, \( \langle \cdot \rangle \) denotes the ground-state expectation value.

The cluster method (connected graph expansion) is used to carry out the series expansion. For a description of the cluster method in the context of quantum spin systems see Ref. [18] (but note that substantial technical improvements have been made in the weight-calculation algorithms since that writing). The essence of the cluster method is that one can express quantities such as those listed above in terms of sums over clusters \( \sum_g L(g)W(g, t/J) \), where \( L \) is the “lattice constant” which describes the number of embeddings of the cluster into the lattice and \( W \), a power series in \( t/J \), is the “weight” of the cluster \( g \). For all of the above properties, the clusters one must consider are just the naively connected ones, in which lattice sites correspond to nodes of a graph and the terms in the kinetic energy correspond to edges. For the one-dimensional case, the clusters are simply open chains. One knows on quite general grounds that the leading nonzero term in \( W \) for a cluster with \( n \) edges is of order \( (t/J)^n \). Thus, by considering all distinct clusters with up to \( n \) sites one can determine the coefficients in the expansion for some property to order \( (t/J)^n \). In the
following presentation, the results for physical quantities are expressed as $J^\alpha \sum_n c_n (t/J)^n$, where $c_n$ are the series coefficients while $\alpha = -1$ for the susceptibilities, $\alpha = 1$ for the energy $E$, and $\alpha = 0$ for other expectation values.

We note in passing that the series presented here have some special properties which follow from particle-hole symmetry of the symmetric KLM on a bipartite lattice. Most of the series contain only even powers of $t/J$; most graphs (for most properties) have leading nonzero terms in their weights of higher order than $(t/J)^n$. In consequence, although we are presently limited to calculations for 8-site clusters, we know the exact expansions to order $(t/J)^{14}$ in $d = 1$; and exact expansions to order $(t/J)^8$ in $d = 2$ (3) are obtained by consideration of only 17 (18) topologically distinct clusters of which only 1 (2) has 8 sites.

Next we present the results, beginning with $d = 1$. The first test of the series comes from an examination of the ground-state energy; the coefficients are listed in Table I. To obtain estimates of $E$ at finite $t$, ordinary Padé approximants are employed; a comparison of the best-behaved ($[4/3]$) approximant with the result from the DMRG calculation for a 24-site chain is displayed in Fig. 1. The agreement is excellent up to $t/J \sim 0.75$. One can also compare $S_l$ with the DMRG results; at $t/J = 0.5$, series estimates of the nearest and second-neighbor correlations differ from DMRG estimates by only 0.2%. We have calculated the conduction electron momentum distribution $n(k)$ for different values of $t/J$. The results shown in Fig. 2 are typical for an insulator. The results for $t/J = 0.625$ compare well with those obtained using quantum Monte Carlo for systems with up to eight sites Ref. [12]. To illustrate what one gains by going to the effort of calculating a high-order series, comparisons are provided in Table II to the results of lowest-order perturbation theory and other numerical calculations.

With the results for one dimensional systems validating the accuracy of the series calculations, we now turn to $d \geq 2$. The relevant physical distinction between $d = 1$ and $d \geq 2$ is that an $S = 1/2$ antiferromagnet orders at $T = 0$ only for $d \geq 2$. The question at hand, as discussed in the introduction, is whether there is evidence for a transition to an AF-ordered phase as $t/J$ increases from zero, and, if so, what is the value of $t/J$ at the
transition. Let us first consider \( d = 2 \). Series for \( E \), the local-spin structure factor \( \hat{S}_l(Q) \) (the Fourier transform of \( S_l \)), \( \chi_l(Q) \) and \( \chi_c(Q) \) are listed in Table III.

The AF susceptibility series have positive, monotonically increasing terms and are thus strongly suggestive of a critical point at some \( (t/J)_c < 1 \) at which the AF correlations become long-ranged. The ratios of consecutive terms \( c_n/c_{n-2} \) do not vary smoothly with \( n \), so from these rather short series it is difficult to obtain a precise estimate of \( (t/J)_c \). Analysis of the \( \chi_l \) series by means of differential approximants \[20\] yields no reasonable approximants. For the \( \chi_c \) series, there are three plausible approximants with singularities at \( (t/J)^2 = 0.60, 0.84, \) and 0.48; and there is a correlation between the locations of the singularities and the values of the associated exponents. If the charge excitations remain gapful at this magnetic transition (as naively expected, and also supported by the variational calculation \[10\]), the transition should lie in the \( d = 3 \) classical Heisenberg model universality class with known exponent \( \gamma \approx 1.4 \). Interpolating to this value of \( \gamma \) yields an estimate for \( (t/J)_c^2 \) of 0.53, with an uncertainty of 0.02 associated with the interpolation alone.

Because the series are short, it is worthwhile to also examine the direct Padé approximants to the series. Doing so is tantamount to biasing \( \gamma \) to the value 1; since the correct value is not too much different the locations of the poles might not be too far off, for our purposes. (In fact, one can apply this method to first five or six terms of the classical, simple cubic lattice Ising model susceptibility high-temperature expansion, and find that consistent estimates of the critical coupling are obtained which are only 10% too small.) The \([2/2]\) approximants for the series yield poles at \( (t/J)^2 = 0.44 \) and 0.69 for the conduction and local electron susceptibilities, respectively.

The bottom line is that our best estimate for the AF ordering critical point in \( d = 2 \) comes from consideration of \( \chi_c(Q) \): \( (t/J)_c \approx 0.7 \), with an uncertainty of roughly 0.1. This is in excellent agreement with the variational calculation of Wang et al. \[10,13\], but differs from the estimate (a value near 2.1) of Fazekas and Müller-Hartmann \[9\]. The underlying reason for that agreement with Wang et al. is not obvious; let us just note that that class
of variational wavefunctions becomes exact in the strong-coupling limit, which is also the starting point of the series expansion.

An analogous analysis has been carried out for the \( d = 3 \) susceptibility series listed in Table IV. In this case it is appropriate to bias the critical exponent to “1 plus logarithmic corrections” which we take to mean somewhere in the range 1 to 1.1. The differential approximants are more consistent than in \( d = 2 \): the plausible approximants for \( \chi_c(Q) \) have poles at 0.235, 0.256 and 0.281 with corresponding exponents 1.02, 1.36, and 1.51. The same is true for the ordinary Padé: the [2/2] approximants for \( \chi_c(Q) \) and \( \chi_l(Q) \) have poles at \((t/J)^2 = 0.23\) and \(0.22\), respectively. Our preferred estimate is \((t/J)_c = 0.49\) with a conservative uncertainty of 0.04.

In summary, a cluster expansion technique for generating high-order \( T = 0 \) perturbation expansions for quantum many-body systems has been successfully applied to the symmetric KLM in \( d = 1, 2, \) and 3. For \( d = 1 \), physical quantities estimated by appropriately extrapolated perturbation expansions are reliable up to intermediate values of \( t/J \). In \( d \geq 2 \), we have obtained estimates of the critical coupling separating the Kondo-insulating, spin-liquid phase at small \( t/J \) from an antiferromagnetically ordered phase; the transition results from competition between the Kondo effect and RKKY interactions. This property of the symmetric KLM may be relevant to the observed AF compounds and the transition from nonmagnetic insulator to antiferromagnet in the class of heavy fermion insulators \[1,6\]. The properties of the charge excitations across this transition is an interesting issue that remains to be addressed.

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by Keith Briggs, to calculate the differential approximants.

**Figure Captions**

FIG. 1. Ground state energy $E$ for the one-dimensional symmetric KLM, comparing the best
Padé approximant (solid line) to the series with the nearly exact results from the DMRG (filled
circles with a dashed line as guide to the eye) [16].

FIG. 2. Momentum distribution $n(k)$ for the one-dimensional symmetric KLM for several values
of $t/J$, as determined from the series expansions for $G(r)$. 
Tables

TABLE I. Series coefficients $c_n$ for the energy and first and second neighbor local spin correlations of the one-dimensional KLM. Note that the coefficients of odd powers vanish for these properties.

| $n$ | $E$         | $S(1)$       | $S(2)$       |
|-----|-------------|--------------|--------------|
| 0   | $-0.75$     | 0.0          | 0.0          |
| 2   | $-0.6666666667$ | $-0.2777777778$ | 0.0          |
| 4   | $-0.3111111111$ | 0.0111111111 | 0.2911111111 |
| 6   | 0.7114685479  | 1.0581324823 | $-0.3128030682$ |
| 8   | 0.1925692156  | $-1.2088861341$ | $-1.2886446333$ |
| 10  | $-2.8528410569$ | $-5.5271656257$ | 3.7729247608  |
| 12  | 2.2809484235  | 16.5201887345 | 4.1162298390  |
| 14  | 12.8828505218 | 19.6847763427 | $-35.1869342747$ |
TABLE II. Comparison of lowest nontrivial order in perturbation theory (PT) (second order, except for $S_l(2)$ for which it is fourth); extrapolated high-order perturbation theory (with uncertainties of 1 in the last digit, as estimated by the consistency of various Padé approximants); and other calculations of selected properties of the one-dimensional KLM.

| $t/J$ | Property | Lowest-order PT | Extrapolated PT | Other calculations |
|-------|----------|-----------------|-----------------|-------------------|
| 0.5   | $E$      | −0.9167         | −0.9261         | −0.9261<sup>a</sup> |
| 0.5   | $S_l(1)$ | −0.0695         | −0.0587         | −0.05875<sup>b</sup> |
| 0.625 | $S_l(1)$ | −0.1085         | −0.0788         | −0.088(10)<sup>c</sup> |
| 0.5   | $S_l(2)$ | 0.01819         | 0.01157         | 0.01155<sup>b</sup> |
| 0.625 | $S_l(2)$ | 0.04442         | 0.0212          | 0.021(5)<sup>c</sup> |

<sup>a</sup>Obtained by extrapolating, versus $1/N$, the DMRG<sup>16</sup> results for open chains consisting of $N = 16$ and 24 sites. Note that for an open 24-site ring $E = −0.919159$, so extrapolation is necessary to obtain an accurate estimate of $E$ from open-chain calculations.

<sup>b</sup>DMRG for 24-site open chain.<sup>16</sup>

<sup>c</sup>Quantum Monte Carlo for closed 8-site rings, with boundary-condition averaging.<sup>19</sup>

TABLE III. Series coefficients $c_n$ for the antiferromagnetic local-spin structure factor, and the zero-frequency antiferromagnetic spin susceptibilities for the localized and conduction electrons, in the square-lattice KLM. The coefficients for odd $n$ all vanish.

| $n$ | $\tilde{S}_l(Q)$ | $\chi_l(Q)$ | $\chi_c(Q)$ |
|-----|------------------|--------------|--------------|
| 0   | −0.25            | 2.0          | 2.0          |
| 2   | 1.555555556      | 26.07407407  | 7.11111111   |
| 4   | 1.43506173       | 154.03667490 | 18.53155556  |
| 6   | −16.90670160     | 162.70126205 | 24.94787492  |
| 8   | 105.05854716     | 267.49655192 | 173.60536516 |
TABLE IV. Same as in Table III, but for simple-cubic-lattice KLM

| $n$ | $\chi_t(Q)$       | $\chi_c(Q)$       |
|-----|-------------------|-------------------|
| 0   | 2.0               | 2.0               |
| 2   | 39.111111111      | 10.666666667      |
| 4   | 326.9517696       | 49.2918518        |
| 6   | 746.1135610       | 171.9991437       |
| 8   | 6739.6417011      | 1493.2844373      |