Zero Temperature Series Expansions for the Kondo Lattice Model

Weihong Zheng and J. Oitmaa
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia.
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We present new results for the Kondo lattice model of strongly correlated electrons, in 1-, 2-, and 3-dimensions, obtained from high-order linked-cluster series expansions. Results are given for various ground state properties at half-filling, and for spin and charge excitations. The existence and nature of the predicted quantum phase transition are explored.

I. INTRODUCTION

The Kondo lattice model, described by the usual Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_i^\sigma c_j^\sigma + h.c.) + J \sum_i S_i \cdot s_i$$

(1)

represents a band of conduction electrons, interacting via a spin-exchange term with a set of immobile (f electrons).

The model has been extensively studied in connection with a class of materials known as “Kondo insulators” (J > 0), and in connection with the manganites (J < 0). Despite the apparent simplicity of the model, in which neither the conduction electrons nor localized spins interact directly among themselves, the spin exchange leads to a strongly-correlated many-body system. No exact results are known for either ground state or thermodynamic properties for general J/t, in any dimension.

The model incorporates two competing physical processes. In the strong-coupling (large |J|) limit, the conduction electrons are “frozen out” via the formation of local singlets (J > 0) or triplets (J < 0). In either case there will be a gap to spin excitations and spin correlations will be short ranged. On the other hand, at weak coupling, the conduction electrons can induce the usual RKKY interaction between localized spins, giving rise to possible magnetically ordered phases with no spin gap and long-range correlations. In one dimension there will be a smooth crossover from large |J| to small |J| behaviour, but in higher dimension a quantum phase transition is expected.

A great deal of work has been carried out on the one dimensional model, using a variety of analytic and numerical methods, and we refer the reader to a recent review. In higher dimension there have been mean-field approaches, quantum Monte Carlo calculations, and a series expansion study. These studies, which are all for the half-filled case, conclude that a quantum phase transition, at which the spin gap vanishes continuously, occurs at (J/t)\text{c} \approx 1.45 \pm 0.05 in the 2D J > 0 case, while Refs. give (J/t)\text{c} \approx 1.833, 2.0 respectively for the 3D J > 0 case. There have not been, to our knowledge, any similar studies for the case of ferromagnetic coupling.

Our aim in this paper is to study the Kondo lattice model in 1, 2, and 3-dimensions via series expansion methods. We have considerably extended the calculations of Ref. by obtaining longer series, by using also expansions about the Ising limit, and by studying also the energies of elementary excitations.

Linked-cluster series expansions have been used successfully for many years to study strongly interacting lattice models. A recent review describes the basic approach and some of the results which have been obtained. The method is applicable in any dimension, is particularly suited to locating critical points and is free from finite size corrections or minus sign problems which hamper other numerical approaches. On the other hand good convergence may be limited to particular regions of the phase diagram.

The Hamiltonian is written in the generic form $H = H_0 + \lambda \Sigma$ where $H_0$ has a simple known ground state. The remaining term(s) $\Sigma$ in $H$ are treated perturbatively, to high order. In this way the ground state energy, correlations, susceptibilities, etc, are expressed as power series in $\lambda$. These are then analysed by standard methods. An extension of the basic linked-cluster method allows the computation of the full dispersion relation for elementary excitations, which can yield energy gaps.

For the present model the simplest choice is to take $H_0 = J \sum_i S_i \cdot s_i$, a sum of single-site exchange terms. The unperturbed ground state is then a simple product state of dimer states. This is the approach used in Ref. and also our first method here. We refer to these as “dimer expansions”. An alternative is to write the exchange term as

$$J \sum_i [S_i^z \tilde{s}_i^z + \frac{1}{2}(S_i^+ \tilde{s}_i^- + S_i^- \tilde{s}_i^+)]$$

(2)

and to take only the first term as $H_0$. In such an “Ising expansion” both the spin-fluctuation and hopping terms are
treated perturbatively. To remove the degeneracy in $H_0$, we add following two terms for conduction spins into $H_0$

$$J' \sum_{ij} (s^z_i s^z_j + 1/4) + h \sum_i [(-1)^i s^z_i + 1/2]$$

and subtract them from the perturbation term, so the overall Hamiltonian is

$$H = H_0 + \lambda V$$

$$H_0 = J \sum_i (S^z_i s^z_i) + J' \sum_{ij} (s^z_i s^z_j + 1/4) + h \sum_i [(-1)^i s^z_i + 1/2]$$

$$V = J \sum_i (S^x_i s^x_i + S^y_i s^y_i) - J' \sum_{ij} (s^z_i s^z_j + 1/4) - h/2 \sum_i [(-1)^i s^z_i + 1/2] - t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)$$

Series in power of $\lambda$ are computed for given values of $J, t, J'$ and $h$, and extrapolated to $\lambda = 1$ where the original Hamiltonian is recovered. Such expansions are appropriate for magnetically ordered phases, although they can also yield accurate results in other cases.

In the remainder of this paper we will present and discuss our results for the 1D case (Section II), for the 2D square lattice and for the 3D simple cubic lattice (Section III). An overall summary is given at the end.

II. THE 1D KONDO LATTICE MODEL

Using the dimer expansion approach we have computed series for the ground state energy in the form

$$E_0/NJ = \sum_{s=0}^{\infty} e_s (t/J)^s$$

and the coefficients, to order 20, are given in Appendix A. Our coefficients agree exactly with Ref. 8, and add three new terms (odd coefficients vanish for this series). Integrated differential approximants are used to evaluated the series for particular $t/J$, and the resulting energy is shown in Figure 1. The different approximants agree well up to $t/J \approx 1.2$, but then splay outwards. We also show, for comparison, the energy obtained from an early DMRG calculation.

Next we turn to the spin excitations. In the strong-coupling limit a spin excitation corresponds to a spin-triplet at one site, which is able to propagate coherently via the conduction electron hoping term. The dispersion relation can be expressed in the form

$$\Delta_s(k) = \sum_n t_n(\lambda) \cos nk$$

FIG. 1: The ground state energy for the 1D Kondo lattice model. The solid points are the DMRG results.
where the quantities $t_n(\lambda)$ are expressed as power series in $\lambda = t/J$. For the 1D case we have computed these up to $n = 9$ (order 18 in $\lambda$), and for the interested reader we provide this data in Appendix A. Figure 2(a) shows the triplet spin-excitation energy vs $k$, for value of $t/J = 0.25, 0.4, 0.5$. For $t/J = 0$ the excitation will, of course, have energy $J$ and will be dispersionless. Increasing the hopping amplitude gives increasing bandwidth, with the energy at $k = 0$ raised slightly and a minimum at $k = \pi$. We are unaware of any previous reported calculations of this dispersion relation, apart from the second order result given in Ref. 3.

From eq. 8 at $k = \pi$ we obtain a series in $\lambda$ for the spin gap, which is again evaluated using integrated differential approximants. Results are shown in Figure 3. The series is well converged up to $t/J \simeq 1.1$. For comparison we show spin-gaps calculated by DMRG [13] and a mean-field approach [14]. Agreement with DMRG is excellent over the range shown, while the mean-field method appear to seriously underestimate the size of the gap. All of the results, including ours, are consistent with a spin-gap which decreases rapidly but does not vanish until $J = 0$.

Next we consider the so-called “quasiparticle” excitation, which we prefer to call a one-hole excitation. This corresponds to the removal of an electron from the half-filled band and thus, in the strong-coupling limit, to a single localized spin on one site with singlets on the others. For $t = 0$ the energy gap is thus $3J/4$. For the 1D case we have computed this series up to order 12 in $\lambda$. Figure 2(b) shows the one-hole excitation spectrum for values $t/J = 0.25$, $0.4$, and $0.5$. For $t/J = 0$ the excitation will, of course, have energy $J$ and will be dispersionless. Increasing the hopping amplitude gives increasing bandwidth, with the energy at $k = 0$ raised slightly. For $t/J = 0.25$ the excitation will, of course, have energy $J$ and will be dispersionless.
0.4 and 0.5. The minimum occurs at $k = 0$ and the bandwidth seems roughly proportional to $t/J$. We are, again, not aware of any previous calculations of this dispersion curve. The series at $k = 0$ allow us to compute the one-hole gap, and our results are plotted in Figure 2. A notable feature is that $\Delta_{qp}$ becomes approximately constant for $t/J > 0.5$. We know of no previous calculations for the one-hole gap apart, again, from the second order strong-coupling result in Ref. 8. There is yet another gap, the “charge gap”, which corresponds to an excitation in which the system remains half-filled, but with a doubly occupied site and an empty site. We are not able to compute this via series, at this stage. However, in the strong coupling limit $\Delta_c = 2\Delta_{qp}$ (this is valid to at least second-order in $t/J$). The charge gap has been computed by DMRG and we show in Fig. 3 the result for $\Delta_c/2$. Evidently for larger hopping parameter $\Delta_c/\Delta_{qp} < 2$.

III. THE SQUARE AND SIMPLE CUBIC LATTICES

In two or more spatial dimensions it is believed that the Kondo lattice model has a true quantum phase transition at some $(J/t)_c$, between a gapped spin-liquid phase and a small $J$ magnetically ordered gapless phase. For the square lattice quantum Monte Carlo simulations provide strong indications of a transition at $(t/J)_c \simeq 0.69$, while a bond-operator mean-field theory gives $(t/J)_c = 0.664, 0.546$ for the square and simple cubic lattices, respectively. A previous series study has given $(t/J)_c \simeq 0.7, 0.5$ respectively. These latter estimates are relatively imprecise, and it seemed worthwhile to investigate this using longer series.

We have derived dimer series for the square lattice for the following quantities: ground state energy $E_0$, antiferromagnetic spin susceptibilities for both local and conduction spins ($\chi_l$ and $\chi_c$), and the triplet spin excitation spectrum (all to order 12), and the one-hole (“quasiparticle”) excitation spectrum (to order 11). This adds two non-zero terms to the results of Ref. 8. The excitation series are new. In addition we have computed, for the first time, Ising expansions for the ground state energy and for the staggered magnetizations (for both local and itinerant spins) to order 13. Series, to the same order, have been derived for the simple cubic lattice for all of the same quantities, except for the excitations, where we have only computed the minimum gap rather than the full spectrum. The dimer series for ground state energy $E_0$, antiferromagnetic spin susceptibilities for both local and conduction spins ($\chi_l$ and $\chi_c$), and the minimum triplet spin gap are given in Table I. Our results agree completely with those of Ref. 8 for the square lattice but disagree for the simple cubic lattice susceptibilities beyond the 4th term. We are unable to resolve this, but we confident that our results are correct.

We first show, in Figure 4, our estimate of the ground state energy, as a function of $t$, obtained from both dimer and Ising expansions. Both series converge well for small $t$, but the Ising expansion has better convergence for larger $t$. There are no previously reported data for $E_0$. There is no evidence of any anomaly in $E_0$ at the supposed phase transition point, nor would we expect this.

The most direct way of identifying any critical point $(t/J)_c$ is from poles of Dlog Padé approximants. However
the series are irregular (Table I) and, perhaps not surprisingly, this yields no consistent results. However if we know, or assume, the value of the critical exponent $\gamma$ then biased estimates of the critical point can be obtained from direct Padé approximants to the series for $\chi^{1/\gamma}$, which should have a simple pole. Here we expect the transition for the square lattice to be of the same universality class as the $d = 3$ classical Heisenberg model with $\gamma \approx 1.4$, and for the simple cubic lattice to be in the $d = 4$ universality class, with $\gamma = 1.0$. In Table II we show estimates of $\rho_c^2 (x = t/J)$ obtained in this way. As can be seen, a number of consistent estimates of the pole are obtained, particularly for the series for the conduction electron susceptibility. We might reasonably estimate for the square lattice $(t/J)_c = 0.68 \pm 0.02$, and for the simple cubic lattice $(t/J)_c = 0.46 \pm 0.01$, where the error are subjective confidence limits. These correspond to $(J/t)_c = 1.48, 2.15$ for the 2D and 3D case, values which are consistent with previous estimates.

An alternative approach is to evaluate the staggered magnetization and susceptibility directly via integrated differential approximants and to look at the behaviour as a function of $t/J$. The staggered magnetizations shown in Figure 5 are obtained from an Ising expansions, starting from an antiferromagnetically ordered state. These are relatively constant for $t/J > 1$, but drop sharply to zero around $t/J \sim 0.6 - 0.7$ in 2D and $t/J \sim 0.5$ in 3D, confirming the existence of a transition to a magnetically disordered phase. The error limits are rather large, and it is not possible
FIG. 7: The triplet spin excitation spectrum (a) and quasiparticle excitation spectrum (b) for the square lattice. The open points with errorbars are variational Monte Carlo results for a $6 \times 6$ lattice.

FIG. 8: The triplet spin gap $\Delta_s/J$ and quasiparticle gap $\Delta_{qp}/J$ for the square lattice (a) and for simple cubic lattice (b) obtained from different orders of integrated differential approximants. The points are the results of a Quantum Monte Carlo study.

Next we consider the spin triplet and 1-hole (quasiparticle) excitations. Figure 7(a) shows the full spin triplet dispersion curve for $t/J = 0.25$, both in the Kondo phase, for 2D. For comparison we also show variational Monte Carlo results of Wang et al. The lowest spin excitation is at $(\pi, \pi)$, and the spin gap clearly decreases as $t$ increases.

In Figure 7(b) we show the dispersion relation for the 1-hole excitation, again for $t/J = 0.25$, 0.4, both in the Kondo phase, for 2D. For comparison we also show variational Monte Carlo results of Wang et al. The lowest spin excitation is at $(\pi, \pi)$, and the spin gap clearly decreases as $t$ increases.

Series have also been computed directly for the spin gap and quasiparticle gap, for both 2D and 3D cases. Analysis to determine the transition point with high precision in this way. Our magnetization curves in 2D are very similar to the Quantum Monte Carlo results, although our conduction electron magnetization is much smaller. We show the QMC results for comparison. In Figure 6 we show curves of the inverse susceptibilities, in the Kondo phase, obtained from dimer expansions. Again there is clear evidence for a transition, but it is difficult to locate precisely. Our best estimates from these figures would be $t/J \simeq 0.75 \pm 0.10$ in 2D and $t/J \simeq 0.50 \pm 0.05$ in 3D, less precise but quite consistent with the direct Padé approximant estimates.
is shown in Figure 8. The data clearly show the spin gap decreasing to zero at a critical point \((t/J)_c\), the position being consistent with our estimates above. For the square lattice our results are in excellent agreement with the QMC results. For the 3D lattice we are unaware of any previous results for either energy gap.

IV. SUMMARY AND DISCUSSION

We have used linked cluster series methods in a comprehensive study of zero-temperature properties of the Kondo lattice model at half-filling, for the linear chain, square lattice, and simple cubic lattice. Our work significantly extends a previous series study\(^8\) for the ground state energy and susceptibility, and presents new series results for the magnetization, spin and quasiparticle dispersion relations, and energy gaps. Wherever possible we have compared our results with calculations by other methods and, in general, find excellent agreement.

Our analysis supports the existence of a quantum critical point in the 2D and 3D cases, separating a Kondo spin-liquid phase (large \(J\)) from an ordered phase. Our estimates for the critical point are \((t/J)_c = 0.68 \pm 0.02, 0.46 \pm 0.01\) in 2D and 3D respectively. These results are from direct Padé approximants to the series for \(\chi^{1/\gamma}\), and hence are biassed by, but not particularly sensitive to, the choice of \(\gamma\). The critical point estimate in 2D agrees very well with previous estimates, while in 3D we find a slightly higher value of \((J/t)_c\), 2.17, compared with 1.833 from mean-field.

We have not yet analysed the data for the frustrated close-packed triangular and face-centered cubic lattices, or for the body-centered cubic lattice, which we also have computed. Nor have we explored the possible existence of bound states, or the region away from half-filling. Recent developments in series methods\(^8\) make this possible, and we intend to pursue these directions, as well as others, in future work.

Appendix

The dimer series of ground state energy for 1D KLM are:

\[
E_0/NJ = -3/4 - 2/3\lambda^2 - 14/45\lambda^4 + 0.71146854791\lambda^6 + 0.19256921565\lambda^8 \\
-2.8528410569\lambda^{10} + 2.2809484235\lambda^{12} + 12.882850521\lambda^{14} - 30.44698097\lambda^{16} \\
-43.303667770\lambda^{18} + 270.26259775\lambda^{20} + O(\lambda^{22})
\] (9)

The triplet spin excitation spectrum for 1D KLM are

\[
\Delta_s(k) / J = 1 - \frac{8\lambda^2}{3} + \frac{2356\lambda^4}{135} - 181.93078\lambda^6 + 2152.5066\lambda^8 - 27691.038\lambda^{10} + 329428.5445\lambda^{12} \\
-2.5917002\lambda^{14} - 2.75912\lambda^{16} + 2.232929\lambda^{18} + \left(4\lambda^2 - \frac{272\lambda^4}{9} + 305.675\lambda^6 - 4076.18\lambda^8 \\
+55158.531287\lambda^{10} - 694363.1\lambda^{12} + 6.4442\lambda^{14} + 2.20385\lambda^{16} - 3.67419\lambda^{18}\right)\cos(k) \\
+\left(\frac{308\lambda^4}{27} - 203.122\lambda^6 + 3199.476135\lambda^8 - 50109.7\lambda^{10} + 729779.9656\lambda^{12} - 8.92778\lambda^{14} \\
+5.42326\lambda^{16} + 1.72156\lambda^{18}\right)\cos(2k) + \left(71.0803\lambda^6 - 1809.21\lambda^8 + 35912.6434\lambda^{10} \\
-640789.\lambda^{12} + 1.0026\lambda^{14} - 1.22082\lambda^{16} + 4.1027\lambda^{18}\right)\cos(3k) + \left(521.4000489\lambda^8 \\
-17575.\lambda^{10} + 416938.0779\lambda^{12} - 8.34562\lambda^{14} + 1.40949\lambda^{16} - 1.77087\lambda^{18}\right)\cos(4k) \\
+\left(4305.106\lambda^{10} - 178962.\lambda^{12} + 4.91952\lambda^{14} - 1.09405\lambda^{16} + 2.00128\lambda^{18}\right)\cos(5k) \\
+\left(38024.843\lambda^{12} - 1.87593\lambda^{14} + 5.85515\lambda^{16} - 1.43507\lambda^{18}\right)\cos(6k) \\
+\left(351790.5722\lambda^{14} - 2.06559\lambda^{16} + 7.00211\lambda^{18}\right)\cos(7k) \\
+\left(3.36497\lambda^{16} - 2.17486\lambda^{18}\right)\cos(8k) + 3.30089\lambda^{18}\cos(9k)
\] (10)
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TABLE I: Series coefficients for dimer expansions for the ground energy per site $E_0/JN$, the minimum triplet spin gap $\Delta_s/J$, and the antiferromagnetic spin susceptibilities for both local and conduction spins ($\chi_l$ and $\chi_c$). Nonzero coefficients ($t/J$) up to order $n = 12$ for square lattice and simple cubic lattice are listed.

| $n$ | $E_0/JN$ | $\Delta_s/J$ | $\chi_c$ | $\chi_l$ |
|-----|----------|-------------|----------|----------|
|     |          | square lattice |          |          |
| 0   | -7.500000000×10$^{-1}$ | 1.000000000 | 5.000000000×10$^{-1}$ | 5.000000000×10$^{-1}$ |
| 2   | -1.333333333 | -1.333333333×10$^1$ | 1.777777778 | 6.518518519 |
| 4   | -8.888888889×10$^{-2}$ | 1.611851852 | 4.632888889 | 3.850916872×10$^1$ |
| 6   | 4.234873600 | -2.640795767×10$^2$ | 6.236968731 | 4.067531551×10$^1$ |
| 8   | -1.519899530×10$^1$ | -1.072124632×10$^5$ | 4.340134129 | 6.687413797×10$^1$ |
| 10  | 8.900723089×10$^{-1}$ | 5.495699137 | 1.004232541 | 1.823289007×10$^3$ |
| 12  | 3.109971534×10$^2$ | -1.561259011×10$^8$ | -6.384897515 | -4.654864554×10$^3$ |
|     |          | simple cubic lattice |          |          |
| 0   | -7.500000000×10$^{-1}$ | 1.000000000 | 5.000000000×10$^{-1}$ | 5.000000000×10$^{-1}$ |
| 2   | -2.000000000 | -2.000000000×10$^1$ | 2.666666667 | 9.777777778 |
| 4   | 6.666666667×10$^{-1}$ | 3.063111111×10$^2$ | 1.291555556 | 8.443753086×10$^1$ |
| 6   | 7.834807760 | 1.060237771×10$^3$ | 5.13287514×10$^1$ | 2.399390035×10$^2$ |
| 8   | -7.114791245×10$^1$ | -2.760658123×10$^5$ | 3.510946982 | 1.684586835×10$^3$ |
| 10  | 3.498368486×10$^2$ | 3.860398011×10$^6$ | 1.354232378×10$^3$ | 2.11247537×10$^4$ |
| 12  | -1.603723348×10$^2$ | 5.557190900×10$^8$ | 2.79715237×10$^3$ | -2.514875289×10$^4$ |

* w.zheng@unsw.edu.au; http://www.phys.unsw.edu.au/~zwh
† j.oitmaa@unsw.edu.au

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TABLE II: Estimates of $x_c^2 = (t/J)_c^2$ from poles of $[N, D]$ Padé approximants to the series for $\chi_{c,l}^{1/\gamma}$. The index $c, l$ denotes the series for conduction electron, localized spin respectively.

| Lattice Type          | Approximant   | $x_c^2$  | Approximant   | $x_c^2$  |
|-----------------------|---------------|----------|---------------|----------|
| Square Lattice        | [2, 3]$_c$    | 0.45378  | [3, 3]$_c$    | 0.46298  |
| $\gamma = 1.4$        | [3, 3]$_l$    | 0.46990  | [2, 4]$_c$    | 0.46350  |
| Estimate $x_c^2 = 0.46 \pm 0.02$, $(t/J)_c = 0.68 \pm 0.02$ |               |          |               |          |
| Simple Cubic Lattice  | [1, 1]$_c$    | 0.20647  | [0, 2]$_c$    | 0.20888  |
| $\gamma = 1.0$        | [2, 2]$_c$    | 0.21660  | [2, 2]$_l$    | 0.21637  |
|                        | [1, 3]$_c$    | 0.22094  | [3, 2]$_c$    | 0.19300  |
|                        | [2, 3]$_c$    | 0.20601  | [4, 2]$_c$    | 0.19480  |
|                        | [3, 3]$_c$    | 0.20798  | [3, 3]$_l$    | 0.20078  |
|                        | [2, 4]$_c$    | 0.20809  |               |          |
| Estimate $x_c^2 = 0.21 \pm 0.01$, $(t/J)_c = 0.46 \pm 0.01$ |               |          |               |          |