EXACT SOLUTION OF THE TWO-SITE CORRELATED KONDO LATTICE MODEL*

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The correlated Kondo lattice model simultaneously describes the interaction of itinerant conduction electrons with localized magnetic moments as well as with other electrons in the conduction band. As a limiting case a two-site cluster with $S = 1/2$ is studied. By analytical calculations we were able to find the exact expression for the energy poles and spectral weights of the one-particle Green's function and all contributing correlation functions.

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1. Motivation

The recent success in growing diluted magnetic semiconductors (DMS) which show remarkably high Curie temperatures has led to a renewed interest in models originally proposed by Zener [1]. As pointed out by several authors, a strong but finite intra-atomic exchange interaction J between the doped magnetic ions and the itinerant conduction carriers dominates the magnetic behavior of these materials [2,3]. Therefore, a Hamiltonian like the correlated Kondo lattice model (CKLM)

$$\mathcal{H} = \sum_{i,j} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - J \sum_{i} \boldsymbol{\sigma}_i \cdot \boldsymbol{S}_i \,, \tag{1}$$

where additionally a Hubbard-like Coulomb interaction U within the single conduction band is incorporated, has to be studied to understand and predict magnetic properties of DMS.

There is the possibility to reduce (1) to an RKKY-like interaction. However, since J is rather large in the considered class of materials (a typical value is $J = -0.3$ eV, corresponding to $\beta N_0 \approx -1.2$ eV) this perturbational

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approach is mostly insufficient [4]. On the other hand the CKLM is not exactly soluble and there is the necessity to perform convincing approximations. If these are not perturbational in nature, as *e.g.* for the various kinds of decoupling techniques [5], then the difficulty of a clear justification emerges. Limiting cases are a powerful tool to weaken this shortcoming. Their exact solution offers the possibility to test approximations.

When intending a description of DMS another point needs to be considered. The usage of a model like (1) implies the assumption of homogeneously distributed dopants. However, Monte Carlo simulations of Timm *et al.* [6] demonstrated that this assumption is rather questionable. On the contrary their calculations show that the defects in GaAs, both the Mn dopants ($x = 5\%$) and the anti-site As atoms ($p = 0.3$ holes per Mn), form clusters, an effect which noticeable influences magnetic properties.

With this contribution we provide the analytical solution of a two-site cluster described by the Hamiltonian

$$\begin{aligned}\bar{\mathcal{H}} &= \sum_{\alpha=1}^{2}\sum_{\sigma=\uparrow,\downarrow}\left\{T_0\hat{n}_{\alpha\sigma} + \frac{U}{2}\hat{n}_{\alpha\sigma}\hat{n}_{\alpha-\sigma} - \frac{J}{2}\left(z_\sigma S_\alpha^z\hat{n}_{\alpha\sigma} + S_\alpha^\sigma c_{\alpha-\sigma}^\dagger c_{\alpha\sigma}\right)\right\} \\ &+ \tilde{T}\sum_{\sigma=\uparrow,\downarrow}\left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}\right), \qquad (2)\end{aligned}$$

where $S^\uparrow \equiv S^+, S^\downarrow \equiv S^-$ and $z_\uparrow \equiv +1, z_\downarrow \equiv -1$. On the one hand this cluster is an exactly soluble limiting case of the CKLM (1) and, therefore, allows the test of approximations in the above mentioned sense. On the other hand it may serve together with the atomic-limit result (special case $\tilde{T} = 0$) as the major component of a disorder-driven treatment of the CKLM.

2. Calculation and results

Despite the finiteness of the cluster and the simplicity of the Hamiltonian (2) an exact solution of the one-particle Green's function $\langle\langle c_{i\sigma}; c_{j\sigma}^\dagger\rangle\rangle_E$ is rather tricky. Limiting ourselves to $S = 1/2$, we are probably at the edge of what can be done analytically. Just from considering the Hilbert-space dimensions one can easily determine the number of imaginable one-electron excitation processes to be 896. Neglecting all symmetries the number of Green's function contributing to a closed system of equations of motion is with 1040 even slightly higher, a minor drawback of this approach.

All these equations of motion can be combined in a single large equation, consisting of a coefficient matrix formed by the model parameters $\tilde{T}, T_0, U, J$, a column-vector of all participating Green's functions and a column-vector of all inhomogeneities. An analytical solution requires the simplification of this matrix to blocks of a manageable size. This can only be achieved by a clever combination of corresponding Green's functions.

First of all, symmetries are a crucial tool to find such correspondents. The usage of the symmetry with respect to the two cluster sites splits the problem into two parts which only differ in the sign of $\tilde{T}$. Also particle-hole symmetry reduces the effort by a factor of 2. Secondly, special sub-cases give a deeper insight into helpful combinations. If the conduction band is assumed to be empty, then the Green's functions (despite of the operator for the excess electron) consist of spin operators only, and their treatment can be studied. After solving this situation the problem of arbitrary band occupation can be divided into 4 density classes. A two-site Hubbard model provides the rules for the correct combination of Green's functions with respect to the electron Fermi operators only.

With such a procedure the reduction of the large coefficient matrix to blocks of the size 3×3 is possible. There are four types of such blocks. Their determinantal polynomial is, respectively,

$$0 = (\hat{E}_0 - \tilde{T} + 2a)(\hat{E}_0^2 - 4a^2 - 2a\tilde{T} - \tilde{T}^2)\,, \tag{3}$$

$$0 = (\hat{E}_I + U)(\hat{E}_I - 2a)(\hat{E}_I + 2a)\,, \tag{4}$$

$$0 = \hat{E}_{II}^3 - \hat{E}_{II}^2 U - 4\hat{E}_{II}\left(a^2 + \tilde{T}^2\right) + 4a^2 U\,, \tag{5}$$

$$0 = \hat{E}_{III}^3 - \hat{E}_{III}^2(4a + U) - 4\hat{E}_{III}\left(3a^2 + \tilde{T}^2 - aU\right) + 4a\left(4\tilde{T}^2 + 3aU\right), \tag{6}$$

with $a = \frac{1}{4}J$. The subindex at the energies $\hat{E}$ numbers the equations. The factorization of Eqs. (5) and (6) requires the use of Cardano's formulas.

The simplification of the mentioned matrix equation allows its inversion, leading to an analytical result for all contributing Green's functions. Their principle structure is

$$G(E) = \sum_{k=1}^{102} \frac{\alpha_k}{E - E_k + i\,0^+}\,. \tag{7}$$

A common feature is the set of 102 energy poles, 27 of which are given by

$$E_k = T_0 - \tfrac{1}{4}J - \hat{E}_{xi} - \hat{E}_{0j}\,, \qquad \text{for } x = I, II, III, \qquad i, j = 1, 2, 3 \tag{8}$$

where $\hat{E}_{xi}(\hat{E}_{0j})$ is the ith (jth) root of the corresponding cubic Eqs. (3)–(6). Other 27 energy poles can be obtained by replacing $\tilde{T}$ for $-\tilde{T}$ (site symmetry). Since with $E_k = T_0 + f(\tilde{T}, J, U)$ also $\bar{E}_k = U + T_0 - f(-\tilde{T}, J, U)$ is an energy pole (particle-hole symmetry) the number of poles doubles again. Poles that stem from $E_k = T_0 - J\frac{\hbar}{4} + U - \hat{E}_{0j}$ are double degenerate.

The total number of 102 excitation energies expresses the richness of the limiting case. Compared to the 8 poles of the Hubbard cluster the additional exchange interaction J leads to a much finer structure of the spectrum.

The spectral weights α_k of the Green's functions are determined by the correlation functions due to inhomogeneities of the equations of motion. Almost all of them can be calculated by applying the spectral theorem to the obtained set of Green's functions. The remaining set of expectation values is used to couple the cluster to a larger lattice. This procedure gives again a set of equations, now for the correlation functions. The system has been solved, too. Even so the analytical expressions are too lengthy to be given here [7], Fig. 1 provides an impression of the spectral-weight distribution for a representative set of parameters.

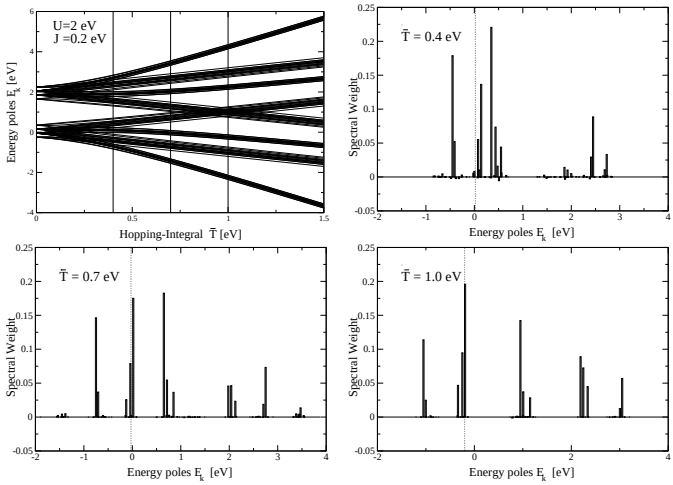

Fig. 1. All 102 one-particle excitations of the two-site cluster. Top left: dependence of energy poles of $\langle\langle c_{i\sigma}; c^{\dagger}_{j\sigma}\rangle\rangle_E$ on the parameter $\tilde{T}$. Others: distribution of the spectral weight for three representative values of $\tilde{T}$, calculated for $T = 500\,\mathrm{K}$.

The sum of all mentioned ingredients makes the cluster solution valuable for an understanding of the CKLM, its applications and approximations.

REFERENCES

[1] C. Zener, *Phys. Rev.* **81**, 440 (1951).

[2] H. Akai, *Phys. Rev. Lett.* **81**, 3002 (1998).

[3] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, D. Ferrand, *Science* **287**, 1019 (2000).

[4] J. König, J. Schliemann, T. Jungwirth, A. MacDonald, *Physica E* **12**, 379 (2002).

[5] W. Nolting, S. Rex, S. Mathi Jaya, *J. Phys. Condens. Matter* **9**, 1301 (1997).

[6] C. Timm, F. Schäfer, F. von Oppen, `cond-mat/0201411`.

[7] Details in: T. Hickel, *Exact Statements on the Correlated Kondo Lattice Model*, diploma thesis, Department of Physics, Humboldt-Universität zu Berlin, 2001.