# THE COMPOSITE OPERATOR METHOD FOR IMPURITY MODELS*

A. Avella, F. Mancini

Dipartimento di Fisica E.R. Caianiello, Unità INFM di Salerno
Università degli Studi di Salerno, 84081 Baronissi (SA), Italy

and R. Hayn

Institut für Festkörper- und Werkstofforschung (IFW)
Dresden, 01171 Dresden, Germany

*(Received July 10, 2002)*

An energy-scale-dependent approximation, that allows to resolve low energy features embedded in a high energy background, is reviewed. The Kondo and Anderson models are studied and fully self-consistently resolved as significative examples. A Kondo-like peak is obtained at low enough temperatures. The method is shown to be capable to reproduce the exact results with very low numerical effort and it is applicable for any value of the external parameters.

PACS numbers: 75.50.Ee, 75.30.Et, 75.25.+z, 75.50.–y

The theoretical analysis of the physical properties of some materials, like transition-metal oxides [1] and heavy fermion compounds [2], requires the correct description of more energy scales at once. The impurity systems are the simpler ones presenting two or more relevant scales of energy and could be considered a natural testing ground for analytical schemes willing to capture this fundamental aspect of physics.

Projection methods [3,4] usually capture quite faithfully the high energy physics of strongly correlated systems, whereas slave-boson techniques [5] are capable to describe low energy features with an high degree of confidence. Unfortunately, neither of the two classes of approximation schemes can obtain both energy regimes simultaneously. As a matter of fact, the quest for an approximation scheme capable to describe various energy scales at once is still open. Quite recently [6,7], we have shown how the composite

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

operator method (COM) [4] could be effectively used to resolve coherent low energy features embedded in a high energy background. This method, whose general formulation has been reviewed in Ref. [8], belongs to the class of projection approaches [3,4] that are founded on the conviction that an analysis in terms of the bare fields might be inadequate for a system dominated by strong interactions. In fact, these latter generate new fields, composite operators (CO), and one has to move the attention to them. The CO do not satisfy canonical (anti)commutation relations and their properties must be self-consistently determined. The propagators of the CO can be computed by means of the equations of motion (EM) method [3,4]. By truncating the infinite chain of EM and by projecting the sources on the basis composed by the fields generated by the EM, one obtains an approximation satisfying the conservation of the spectral moments. Both in the projection coefficients of the approximate EM and in the thermal averaged (anti)commutators of the fields, present as inhomogeneous terms in the EM for the propagators, unknown correlators of higher order fields appear. These correlators should be computed self-consistently. A central point of the COM [4] is to recognize the presence of such correlators not as an accident, as all the other approximation schemes do, but as a necessity and an occasion to force the solution to obey all the symmetry constraints (*i.e.*, Pauli principle and Ward–Takahashi identities). In particular, we exploit their presence in order to fix the proper Hilbert space (*i.e.*, the Hilbert space where symmetry relations among operators are also satisfied by thermal averages).

If we want to catch the low energy scales present in the impurity models (which, according to the previous prescription, would require a bigger and bigger number of moments) we need to individuate an effective operatorial basis containing fields directly describing the low energy excitations as shown in Refs. [6, 7]. Actually, we propose the following procedure to solve single-impurity models. Within the composite operators appearing in the hierarchy of the equations of motion, we identify the one (hereafter the *Kondo operator*) describing the conduction electrons dressed by the spin fluctuations of the impurities. The high energy dynamics of the Kondo operator, and of the other higher order operators appearing at the same level of time differentiation, is taken into account by means of the mode-coupling approximation [9] (*i.e.*, the self-consistent Born approximation) that very well describes the high energy part of the spectra, which is quite incoherent. The bosonic propagators entering the mode-coupling procedure are determined either by the atomic approximation, in absence of charge fluctuations, or by further decoupling in terms of the impurity electron propagators. This is widely justified by the fact we need them only to describe the high energy regime. The low energy dynamics of the Kondo operator is described, nonperturbatively, by projecting its source on all and only the original electronic

operators (*i.e.*, by means of a simple quasi-particle theory). This step is possible as the mode-coupling approximation fails to give the correct weight of the Kondo operator [6, 7]. The low energy parameters (*i.e.*, the projection coefficients) are fixed by requiring that the low energy weight of the Kondo operator satisfies the correct sum rule.

To better illustrate the above described procedure for single-impurity models we will report, as relevant examples, the solution of the Kondo and Anderson models [10].

The Kondo model is described by the following Hamiltonian

$$H = \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger(\boldsymbol{k}) \cdot \left[ \delta_{\boldsymbol{k}\boldsymbol{k}'}\, \varepsilon_{\rm c}(\boldsymbol{k}) + 2 J_{\rm K} \frac{1}{N} \vec{\sigma}\, \vec{n}^d \right] c(\boldsymbol{k}')\,, \tag{1}$$

where $c(\boldsymbol{k})$ denotes the conduction electron operator in spinorial notation, and $\vec{n}^d$ represents the spin operator at the impurity site, $\varepsilon_{\rm c}(\boldsymbol{k})$ and $J_{\rm K}$ are the conduction electron energy and the Kondo coupling, respectively, $N$ is the number of sites, $\vec{\sigma}$ are the Pauli matrices. We have $\mathrm{i}\partial_t c(\boldsymbol{k}) = \varepsilon_{\rm c}(\boldsymbol{k})\, c(\boldsymbol{k}) + 2 J_{\rm K}\, \vec{\sigma} \cdot \vec{n}^d\, c_0$, where $c_0$ is the electron at the impurity site.

In this case the Kondo operator is just $\psi_2 = \vec{\sigma} \cdot \vec{n}^d\, c_0$ and its weight is $I_{22} = \langle\{\psi_2, \psi_2^\dagger\}\rangle = 3 + 4\langle c_0\, \psi_2^\dagger\rangle$. According to the scheme described above, we split the field $\psi_2$ in low $\psi_2^{\rm L}$ and high $\psi_2^{\rm H}$ energy components. The propagator of the latter is computed in the mode-coupling approximation, which absorbs a weight equals to 3. In the low energy regime, we assume the following dynamics for the field $\psi_2$: $\mathrm{i}\frac{\partial}{\partial t}\psi_2^{\rm L} = \aleph\, c_0$. By projecting we get $\aleph = J_{\rm K}\, I_{22}^{\rm L}$, where $I_{22}^{\rm L}$ is the low energy weight. This latter is computed self-consistently by means of the following sum rule $I_{22}^{\rm L}(T) = I_{22}(T) - I_{22}^{\rm H}(T)$, where $I_{22}^{\rm H}(T) = I_{22}[T, I_{22}^{\rm L}(T) = 0]$. The spectral weight of $\psi_2$ is reported in the upper panel of Fig. 1. Our results are in quantitative agreement with the well known exact solution [10]. For temperatures lower than the Kondo one $T_{\rm K}$ (which is quantitatively well reproduced: for $J_{\rm K} = 0.1$ we have $T_{\rm K} = 0.0058$) the Kondo peak is clearly visible. In the inset it is shown as it shrinks on increasing the temperature. Finally, at temperatures higher than the Kondo one only a high energy incoherent background is left: the well defined singlet excitation mode no longer exists.

The Anderson model is defined by the Hamiltonian

$$H = \frac{1}{N} \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} + \varepsilon_f f^\dagger f + U n_{f\downarrow} n_{f\uparrow} + \frac{V}{\sqrt{N}} \sum_{\boldsymbol{k}} (c_{\boldsymbol{k}}^\dagger f + f^\dagger c_{\boldsymbol{k}})\,, \tag{2}$$

where $f$ are the electrons in the impurity level ($\varepsilon_f$), $n_{f\sigma}$ is the charge density operator of spin $\sigma$ for the $f$-electrons, $V$ is the strength of the hybridization between the valence band and the impurity level and $U$ is the Coulomb repulsion at the impurity site. This latter splits the field $f$ in the Hubbard

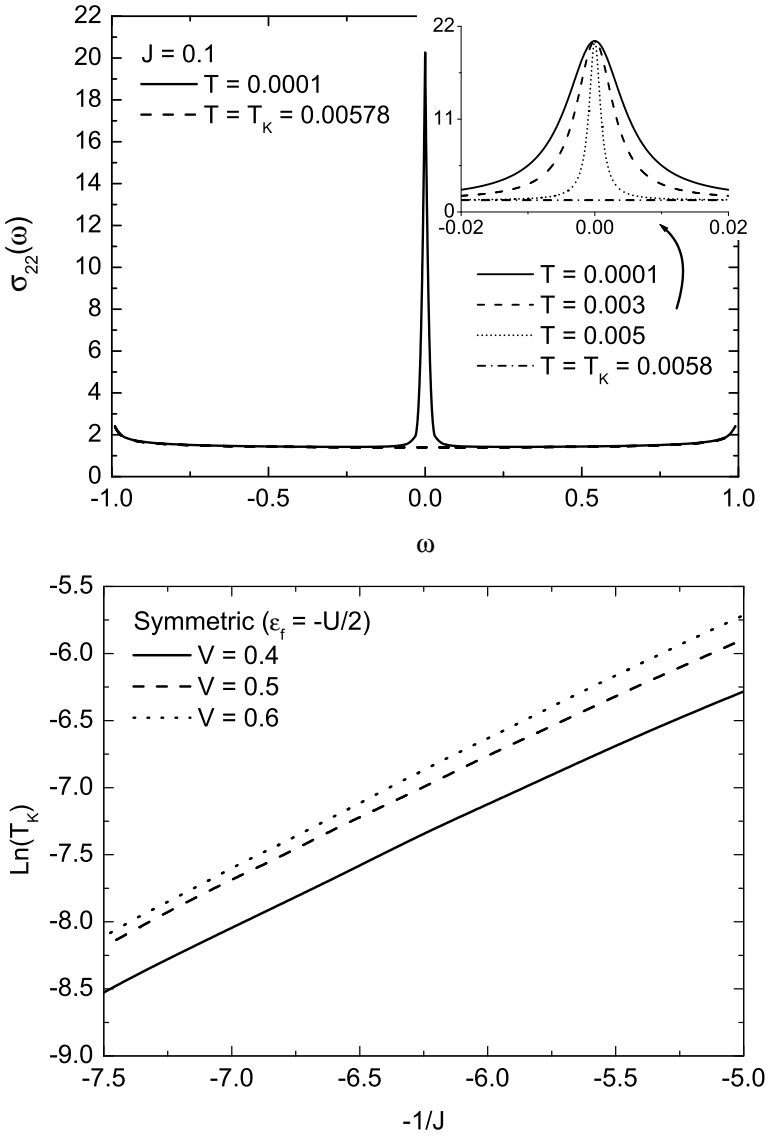


Fig. 1. The spectral weight of the Kondo operator ($\sigma_{22}(\omega)$) for the Kondo model is reported for $T = 0.0001$ and $T = T_{\mathrm{K}} = 0.0058$ for $J_{\mathrm{K}} = 0.1$, in the inset is shown how the peak shrinks with the temperature (upper panel); the Kondo-temperature for the Anderson model in the symmetric case is reported as a function of the exchange coupling $J$ (lower panel).

operators $\xi = (1 - f^\dagger f)f$ and $\eta = (f^\dagger f)f$. The equations of motion of $\xi$ and $\eta$ introduce the fluctuation field $\pi = \frac{1}{2}(1 - n_f)c_0 + \frac{1}{2}\vec{\sigma} \cdot \vec{n}_f c_0 + \left(c_0^\dagger \xi\right) \eta$ corresponding to the coupling of the valence band to density, spin and pair impurity fluctuations.

According to the general prescription, the Kondo operator is taken as $\psi_2 = \frac{1}{2}\vec{\sigma} \cdot \vec{n}_f c_0$ with a weight $I_{22} = \frac{3}{4}(\langle n_f \rangle - 2\langle n_{f\downarrow} n_{f\uparrow} \rangle) + \langle c_0 \, \psi_2^\dagger \rangle$. We split the field $\psi_2$ in low $\psi_2^{\mathrm{L}}$ and high $\psi_2^{\mathrm{H}}$ energy components. The propagator of the latter is computed in the mode-coupling approximation, which absorbs a weight equals to $\frac{3}{4}(\langle n_f \rangle - 2\langle n_{f\downarrow} n_{f\uparrow} \rangle)$. We make the following Ansatz at low energy $\mathrm{i}\partial_t \psi_2^{\mathrm{L}} = \kappa_1 c_0 + \kappa_2 \xi + \kappa_3 \eta$. The coefficients $\kappa_i$ are determined by projection and contains the low energy weight of $\psi_2$ which will be computed by means of the same equation stated for the Kondo model. A Kondo peak is obtained with the correct dependence on the model parameters [10]. In the lower panel of Fig. 1, the natural logarithm of the Kondo temperature $\ln T_{\mathrm{K}}$ is reported as a function of $-1/J$ in the symmetric case ($\varepsilon_f = -U/2$) and for various value of $V$. $T_{\mathrm{K}}$ becomes exponentially small for small values of $J = V^2(1/|\varepsilon_f| + 1/|\varepsilon_f + U|)$ in agreement with the exact theoretical formula [10] $T_{\mathrm{K}} \propto \exp(-1/J)$. The linear behavior shows the correct exponential dependence which is not possible to obtain perturbatively.

In conclusion, we have reported a recently developed energy-scale-dependent approach [6,7] and shown that it is capable to reproduce in a reasonable way both high- and low- energy features of known exact solutions of impurity models. The advantages of the proposed procedure reside in the very low numerical effort required and in the possibility to use it to study systems (*e.g.*, the impurity lattice models) where exact methods (*e.g.*, Bethe Ansatz, RG, ...) cannot be applied.

## REFERENCES

[1] M. Imada, A. Fujimori, Y. Tokura, *Rev. Mod. Phys.* **70**, 1039 (1998).

[2] O. Gunnarsson, K. Schönhammer, *Many Body Formulation of Spectra of Mixed Valence Systems*, vol. 10, Elsevier Science, 1987.

[3] H. Mori, *Progr. Theor. Phys.* **33**, 423 (1965); *Progr. Theor. Phys.* **34**, 399 (1965). D.J. Rowe, *Rev. Mod. Phys.* **40**, 153 (1968). L.M. Roth, *Phys. Rev.* **184**, 451 (1969). P. Fulde, *Electron Correlations in Molecules and Solids*, Springer-Verlag, 1995.

[4] F. Mancini, S. Marra, H. Matsumoto, *Physica C* **244**, 49 (1995); *Physica C* **250**, 184 (1995); *Physica C* **252**, 361 (1995); A. Avella, F. Mancini, R. Münzner, *Phys. Rev.* **B63**, 245117 (2001); V. Fiorentino, F. Mancini, E. Zasinas, A. Barabanov, *Phys. Rev.* **B64**, 214515, (2001).

[5] S.E. Barnes, *J. Phys. F* **6**, 1375, (1976).

[6] D. Villani, E. Lange, A. Avella, G. Kotliar, *Phys. Rev. Lett.* **85**, 804 (2000).

[7] A. Avella, R. Hayn, F. Mancini, *Energy-scale-dependent analysis of the single-impurity Anderson model*, Preprint University of Salerno, 2002.

[8] F. Mancini, A. Avella, `cond-mat/0006377`.

[9] J. Bosse, W. Götze, M. Lücke, *Phys. Rev.* **17**, 434 (1978).

[10] A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge University Press, Cambridge 1997.