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An asymptotically exact mean-field approach for Hubbard X-operators

A C Hewson† and A L Wasserman‡§

† Department of Mathematics, Imperial College, London SW2 2BZ, UK

‡ School of Mathematical and Physical Sciences, University of Sussex, Brighton BN1 9QH, UK

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Abstract. We consider a systematic projection method for terminating the Green function equations of motion for Hubbard X-operators. This gives a set of mean fields that depend on the operators chosen. When applied to lowest order in the N-fold-degenerate $U \rightarrow \infty$ Anderson model an expression for the one-electron Green function is obtained that is exact for $N = 1$ and in the limit $N \rightarrow \infty$. This approach avoids the necessity of introducing auxiliary fields, such as constraint fields or slave bosons, to obtain asymptotically exact mean fields in the large-N limit and has general applicability in similar strongly correlated problems.

Mean-field theories that are asymptotically exact in the limit of large degeneracy N have been developed in recent years for magnetic impurity models such as the Coqblin–Schrieffer model and the $U \rightarrow \infty$ degenerate Anderson model. (For recent reviews see Newns and Read (1987), Bickers (1987).) The Hamiltonians for these models are most conveniently expressed in terms of Hubbard X-operators $X_{pq} = |p\rangle\langle q|$ where $|p\rangle$ and $\langle q|$ are impurity-state ket and bra operators. Because these operators satisfy the commutator relations

$$[X_{pq}, X_{rs}]_{\pm} = \delta_{qr} X_{ps} \pm \delta_{sp} X_{rq}$$

and not Bose or Fermi commutator relations, the standard many-body techniques, such as perturbation theory in terms of Feynman diagrams, are not applicable. Representations have therefore been sought in terms of auxiliary (slave) Bose or Fermi operators which restore some familiar aspects of many-body methods.

Such representations are possible, in general, provided a constraint is imposed on the total occupancy of the Bose of Fermi particles, which is accomplished by introducing a constraint field. Making the saddle point approximations for the constraint and auxiliary Bose fields yields a mean- field solution that is asymptotically exact as $N \rightarrow \infty$ and at low temperatures (Read and Newns 1983). When Gaussian fluctuations to these mean fields are taken into account, corrections to order $1/N$ are obtained (Read 1985). This flexible approach has been generalised to the periodic Anderson model to describe heavy fermions and has more recently been applied to the Hubbard model in exploring the possibility of strong-correlation mechanisms for high-T_c superconductivity.

§ Permanent address: Department of Physics, Oregon State University, Corrallis, Oregon 97331, USA.

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However, the method is not without limitations. It breaks down at higher temperatures as the constraint field becomes simply a Lagrange multiplier in the saddle point approximation, and is then insufficient to suppress thermal fluctuations which violate the constraint. Moreover, improvements beyond Gaussian fluctuations in the Boson field seem to be prohibitively difficult. Neither is it clear that the approximations at the Gaussian level are sufficient for describing models for which the regime of physical interest corresponds to $N = 2$.

An alternative approach to the slave Boson method is to work directly with the Hubbard X-operators and use Brillouin–Wigner perturbation theory (see, for example, Keiter and Morandi 1984). Here the perturbation terms can be summed systematically in a $1/N$ expansion, or self-consistently as in the non-crossing approximation (NCA) (see, for example, Bickers 1987). Results are now not limited to the low-temperature regime as there is no longer violation of an operator constraint. The chief disadvantage of these methods is the complexity that arises when they are generalised to many sites or to lattice problems. They also lack the physically intuitive appeal of the mean-field approach which corresponds to a simple renormalisation of the Fermi liquid picture.

Here we consider a method of generating mean fields directly for the Hubbard operators from which we might hope to gain the intuitive advantages of mean fields without the limitations imposed by the requirement of a constraint field in the slave Boson method. The method is based on a truncation of the equations of motion for X-operators which generate elementary excitations. For example, an exact single-particle excitation operator Ω where $[H, \Omega]_- = \omega_{ex}\Omega$, with ω_{ex} the excitation energy and H the Hamiltonian, can be expressed as a linear combination of operators A_λ in a complete set $\{A_\lambda\} = C$. An approximation to this excitation can be made by using just a subset, C', of these. In the equations of motion for the elements of C', operators will appear that are not contained in C'. These need not be neglected entirely but can be takens into account by projecting them back onto the set C' by using a suitably defined inner product. For a pair of operators A and B we use the inner product $\{A, B\} = \langle [B, A^+]_\pm \rangle$ where $\langle\ \rangle$ indicates a thermal expectation value with respect to the Hamiltonian H. The anti-commutator is used if both A and B are Fermi-like, i.e., correspond to the creation or annihilation of an odd number of fermions. An operator outside the set $C' = \{A_{\lambda'}\}$ can be replaced by its projection onto the set C' according to

$$A \rightarrow \sum_{\lambda'} \frac{(A, A_{\lambda'})}{(A_{\lambda'}, A_{\lambda'})} A_{\lambda'}.$$

This provides a systematic way of terminatiing the equations of motion and can be applied to thermal or double-time Green functions (Goryachev *et al* 1982). This approach has been previously applied to the non-degenerate Anderson model (Bowen 1975, 1978). It is similar to the memory function method (Moriya 1965) but with a different definition for the inner product. Here we apply it to the $U \rightarrow \infty$, N-fold-degenerate Anderson model and show that it leads to an exact mean-field result in the limit $N \rightarrow \infty$.

The Hamiltonian for the N-fold-degenerate $U \rightarrow \infty$ Anderson model is

$$H = \sum_{k,m} \varepsilon_k c^+_{km} c_{km} + E_0 X_{00} + \sum_m E_1 X_{mm} + \sum_{k,m} (V_k X_{m0} c_{km} + V^*_k c^+_{km} X_{0m})$$

where c^+_{km} (c_{km}) create (annihilate) conduction band states with total z component of angular momentum m about the impurity site. The X-operators are constructed from the state $|0\rangle$, which is the state corresponding to a non-magnetic configuration, and the

states $|m\rangle$, which correspond to one extra localised electron with total z component of angular momentum m. Examples of operators that generate an excitation in which a single particle is annihilated are X_{0m}, c_{km} $c_{km}X_{00}$ and $X_{m0}c^{+}_{km}c_{km}$. We base the lowest-order approximation on retaining the minimal set $\{X_{0m}, c_{km}\}$ which does not involve any particle–hole pairs.

In developing the equations of motion we require the commutator

$$[X_{0m}, H]_{-} = \sum_{k,m'} V_k(\delta_{mm'}X_{00}c_{km} + X_{m'm}c_{km'}) + \varepsilon_f X_{0m} \tag{1}$$

where $e_f = E_1 - E_0$. If the first term on the right-hand side is projected onto the state c_{km} we obtain term

$$\sum_k V_k\langle X_{00} + X_{mm}\rangle c_{km}$$

which corresponds to an intuitive decoupling of the terms in (1). However, in projecting onto X_{0m}, the remaining operator of the minimal set, we obtain the additional term

$$-\sum_{k,m'} [V_k(1 - \delta_{mm'})/\langle X_{00} + X_{mm}\rangle]\langle X_{m'0}c_{km'}\rangle X_{0m}.$$

This term, which does not correspond to an obvious decoupling of (1), can be absorbed as a renormalisation of the f level to give

$$\tilde{\varepsilon}_f = \varepsilon_f - \sum_{k,m'} \frac{V_k(1 - \delta_{mm'})}{\langle X_{00} + X_{mm}\rangle}\langle X_{m'0}c_{km'}\rangle. \tag{2}$$

Applying this scheme to calculate the double-time thermal Green function $\langle\langle X_{0m}; X_{m0}\rangle\rangle = G^{f}_{m}(\omega)$, we find

$$G^{f}_{m}(\omega) = D_m\left(\omega - \tilde{\varepsilon}_f - \sum_k \frac{|V_k|^2 D_m}{(\omega - \varepsilon_k)}\right)^{-1} \tag{3}$$

where $D_m = \langle X_{00} + X_{mm}\rangle$. This Green function is of the same form as in the non-interacting ($U = 0$) Anderson model but with a renormalised f level and a renormalised resonance width $\tilde{\Delta} = D_m\Delta$ where

$$\Delta = \pi \sum_k |V_k|^2 \delta(\omega - \varepsilon_k).$$

The self-consistent equation for the correlation function $\langle X_{m'0}c_{km'}\rangle$ that appears in (2) leads to the self-consistent equation for $\tilde{\varepsilon}_f$ at $T = 0$

$$\tilde{\varepsilon}_f = \varepsilon_f - [(N - 1)\Delta/\pi] \ln(\sqrt{\tilde{\varepsilon}_f^2 + \tilde{\Delta}^2}/D) \tag{4}$$

where $2D$ is the width of a conduction band that is taken to be constant and half-filled.

There are two limits in which the spectral density of the Green function $G^{f}_{m}(\omega)$ has a single resonance. These are the case $N = 1$ and the case $N \to \infty$. The case $N = 1$ is trivial for then, as is evident from (2), $D_m = 1$ so $\tilde{\Delta} = \Delta$ and $\tilde{\varepsilon}_f = \varepsilon_f$. If the $N \to \infty$ limit is taken in the usual way so that $N\Delta$ is finite then, to leading order in $1/N$, $D_m \to \langle X_{00}\rangle = (1 - n_f)$, where n_f is the total occupation of the impurity f level and ε_f is given by

$$\tilde{\varepsilon}_f = \varepsilon_f - (N\Delta/\pi) \ln(\tilde{\varepsilon}_f/D). \tag{5}$$

If $\tilde{\varepsilon}_f = T_A$ is the solution of (5) with $\varepsilon_f > 0$ then $G^{f}_{m}(\omega) = (1 - n_f)/(\omega - T_A)$ with the

corresponding spectral density $\rho^{\mathrm{f}}_m(\omega) = (1 - n_{\mathrm{f}})\delta(\omega - T_{\mathrm{A}})$. These results satisfy the sum rules on the spectral density in the large-N limit at $T = 0$:

$$\int_{-\infty}^{0} \mathrm{d}\omega\, \rho^{\mathrm{f}}_m(\omega) = 0 \qquad \int_{0}^{\infty} \mathrm{d}\omega\, \rho^{\mathrm{f}}_m(\omega) = (1 - n_{\mathrm{f}}) \tag{6}$$

identically. As a consequence, these sum rules cannot be used to determine n_{f}. The f-level occupation can, however, be deduced from the Friedel sum rule in the large-N limit,

$$n_{\mathrm{f}} = \frac{1}{\pi} \lim_{N\to\infty} \mathrm{Im}(\ln G^{\mathrm{f}}_m(\omega + \mathrm{i}0^+)) \tag{7}$$

giving

$$n_{\mathrm{f}} = (N\Delta/\pi T_{\mathrm{A}})(1 + N\Delta/\pi T_{\mathrm{A}})^{-1} \tag{8}$$

which is the leading-order large-N result. These results are, of course, all well known. The new feture is that they have been derived from a mean-field theory deduced from the systematic application of a projection method for Hubbard X-operators without introduction of auxiliary Bose or constraint fields. The mean field is exact for $N = 1$ as well as for $N \to \infty$.

At this lowest level of approximation the spectral density deduced for $G^{\mathrm{f}}_m(\omega)$ corresponds to a single resonance. This is not appropriate in the Kondo regime where $\varepsilon_{\mathrm{f}} < 0$, for small values of N (other than $N = 1$). For we know that when $\varepsilon_{\mathrm{f}} < 0$ the spectral density has, in general, two resonances; a narrow one just above the Fermi level (Kondo resonance) and another of width Δ near the original f-level position ε_{f}. However, on enlarging the basis set of operators C', the projection method provides a hierarchy of approximations. We are currently examining the effect of expanding the minimal basis C' to include operators corresponding to a single electron–hole pair.

In summary, we have established that it is possible to describe asymptotically exact mean fields for Hubbard X-operators without invoking slave Bosons or constraint fields. Higher-order approximations can be generated in a systematic way. We have demonstrated the method for the degenerate $U \to \infty$ Anderson model. But the generality of the approach suggests its applicability to other strong-correlation problems such as the Hubbard model and the periodic Anderson model.

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References

Bickers N E 1987 *Rev. Mod. Phys.* **59** 845
Bowen S P 1975 *J. Math. Phys.* **16** 620
—— 1978 *Phys. Rev.* B **18** 3400
Goryachev E G, Kuzmin E V and Ovchinnikov S G 1982 *J. Phys. C: Solid State Phys.* **15** 1481
Keiter H and Morandi G 1984 *Phys. Rep.* **109** 227
Moriya T 1965 *Prog. Theor. Phys.* **34** 329
Newns D M and Read N 1987 *Adv. Phys.* **36** 799
Read N 1985 *J. Phys. C: Solid State Phys.* **18** 2651
Read N and Newns D M 1983 *J. Phys. C: Solid State Phys.* **16** 3273