Strong-coupling approach to ground-state properties of the Anderson lattice-model

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A Slave-Boson perturbational approach to ground-state properties of the $U \to \infty$ periodic Anderson model is derived as an expansion around the Atomic Limit ($V = 0$). In the case of zero temperature any constraint-integral or limiting procedure can be avoided, a gauge-symmetry broken Mean-Field phase is not involved. Physical quantities like the wave vector $k$ dependent Green’s function obey a direct representation in Feynman-skeleton diagrams in $k$-space. A self-consistent $1/N$-expansion is derived, and its relation to the limit of infinite spatial dimension $d \to \infty$ is pointed out.

Although being under consideration for long, the strong-coupling-perturbation theory for electronic properties of High-$T_c$ Superconductors and Heavy-Fermion Systems poses major difficulties, since it apparently cannot be based on a linked-cluster expansion with small (i.e. one- and two-particle) vertices. A perturbation series in e.g. the hybridisation of the periodic Anderson model either involves (Hubbard-) cumulants [12] or other kinds of vertices with an arbitrary number of legs [3], or the linked-cluster theorem is lost in an unconventional diagrammatic expansion which uses small vertices [11,13]. In the following it is shown that a Feynman-type expansion around the Atomic Limit may become available if the problem is restricted to the case of zero temperature.

We consider the periodic SU($N$) Anderson model with interaction $U \to \infty$ of localised $f$-electrons in auxiliary particle (‘Slave Boson’) representation, $H = H_0 + H_V$ with

$$H_0 = \sum_{k,m} \varepsilon_k c_{km}^\dagger c_{km} + \sum_{\mu,m} \varepsilon_f s_{\mu m}^\dagger s_{\mu m},$$

$$H_V = \frac{1}{\sqrt{N L}} \sum_{\mu,k,m} \left( V_k e^{-i k R_\mu} s_{\mu m}^\dagger b_{\mu} c_{km} + h.c. \right).$$

Bosons $b_{\mu}$ and Fermions $s_{\mu m}$ with spin $m$ on $N_L$ lattice sites $R_\mu$ are subject to operator constraints $Q_\mu = 1$ for conserved ‘charges’ $Q_\mu = b_{\mu}^\dagger b_{\mu} + \sum_m s_{\mu m}^\dagger s_{\mu m}$. Consider a grand canonical ‘$Q$-ensemble’ with chemical potential $\lambda$ for the total ‘charge’ $\hat{Q} = \sum_\mu Q_\mu$, that is $H \to K = H - \lambda \hat{Q}$. The constraints are faithfully represented by

$$\langle Q_\mu \rangle^\lambda = 1, \quad \mu = 1, \ldots, N_L$$

$$\Delta Q_\mu^2 = \langle Q_\mu^2 \rangle^\lambda - (\langle Q_\mu \rangle^\lambda)^2 = 0, \quad \mu = 1, \ldots, N_L$$

with expectation values in the ‘$Q$-ensemble’. Due to the lattice symmetry of the Hamiltonian $K$ the density $\langle Q_\mu \rangle^\lambda = \langle \hat{Q} \rangle^\lambda / N_L$ is site-independent, and Eqs.(3) are fulfilled for a suitably chosen $\lambda = \lambda(T)$. Also is the local fluctuation $\Delta Q_\mu^2$ site-independent, but for finite temperature it is $> 0$. In the limit $T \to 0$, however, fluctuations of conserved quantities $Q_\mu$ vanish, and Eqs.(3) are strictly fulfilled if a unique ground state is assumed. The latter has to be confirmed explicitly by calculation of $\Delta Q_\mu^2$ at $T \to 0$, since in principle it cannot be ruled out that $K$ takes a degenerate ground state with fixed $\hat{Q} = N_L$, i.e. an invariant (reducible) subspace of the lattice symmetry containing states which obey an inhomogeneous distribution of $\hat{Q}$ on the lattice with $\Delta Q_\mu^2 > 0$, whereas $\langle Q_\mu \rangle^\lambda = 1$.

The retarded one-particle Green’s function $F_{k,m}(\omega)$ for $f$-electrons is given by the analytic continuation $\omega \to \omega + i 0_+$. These propagators obey a skeleton Feynman-diagram expansion in $k$-space with respect to $V_k$, using the vertices shown in Fig. 3 and renormalised Matsubara Green’s functions for auxiliary Fermions (dashed line)

$$G_{k,m}^F(i\omega_l) = \frac{i}{\omega_l - \varepsilon_f + \lambda - \Sigma_{k,m}^F(i\omega_l)}^{-1},$$

auxiliary Bosons (wavy line) $D_k(i\nu_l) = (i\nu_l - \lambda - \Pi_k(i\nu_l))^{-1}$, and the conduction electrons (continuous line) $G_{k,m}^c(i\omega_l) = (i\omega_l - \varepsilon_k - \Sigma_{k,m}^c(i\omega_l))^{-1}$, with standard diagram rules.

A diagrammatic large-$N$ expansion scheme [14] is now easily applied to the lattice model: In Fig. 3 a $\Phi$-derivable self-consistent approximation is shown, which contains all diagrams to the $f$-Green’s function Eq.(4) up to order $(1/N)^1$. (Note that $F_{k,m}$ is written as a

![FIG. 1. Vertices for correlated hybridisation events $\sim V$ in $k$-space.](image-url)
Also due to the local repulsion the simplest gauge-invariant approximation would be massively violated in this case [9]. Accordingly Bose condensation ('spurious Bose condensation'), since the constraint Eqs. (4) simultaneously breakdown of gauge symmetry here (no 'spurious Bose condensation').

In order (1/N) theory the self-consistency equations for the lattice model were iterated numerically at finite T below the Kondo energy T_K while adjusting λ to fulfill Eq. (3). A pseudo gap tends to appear in the Abrikosov-Suhl resonance in the local f-spectrum $\frac{1}{N_L} \sum_q (-\frac{1}{\pi} \text{Im} F_k(\omega))$. However, to be able to extrapolate to T → 0 much lower temperatures have to be reached [14]. Note that $G_{\text{SIAM}}^{(0)}$ needs not be determined here, in contrast to known strong-coupling approaches applied in the Local Approximation [15,16].

In conclusion it has been demonstrated that restriction to the case of zero temperature opens the way to a Feynman-type strong-coupling-perturbation approach to physical Green’s functions of the periodic U → ∞ Anderson model. Since the excluded-volume problem does not show up here, Φ-derivable self-consistent approximations are formulated conveniently in terms of skeleton diagrams in k-space. To order (1/N) the skeleton expansion is proven equivalent to the Local Approximation. In higher orders non-local effects will appear through vertex corrections.

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