A novel diagrammatic technique for the single-site Anderson model

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A diagrammatic theory around the atomic limit is proposed for the single-impurity Anderson model in which the strongly correlated impurity electrons hybridize with free (uncorrelated) conduction electrons. Using this diagrammatic approach, we prove the existence of a linked cluster theorem for the vacuum diagrams and derive Dyson type of equations for the localized and conduction electrons and corresponding equations for the mixed propagators. The system of equations can be closed by summing the infinite series of ladder diagrams containing irreducible Green's functions. The result allows to discuss resonances associated with the quantum transitions at the impurity site.

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The study of strongly-correlated electron systems has become one of the most active fields of condensed matter physics during the last decade. The properties of these systems cannot be described by Fermi liquid theory. One of the important models of strongly correlated electrons is the single-site or impurity model introduced by Anderson in 1961 [1], which has been intensively discussed in many papers. It is a model for a system of free conduction electrons that interact with the system of a local spin of an electron in the d or f shells of an impurity atom. The impurity electrons are strongly correlated because of the strong on-site Coulomb repulsion and interact with the conduction electrons via exchange and hybridization. Most previous work is based on the method of equations of motion for retarded and advanced Green's functions and a truncating procedure as proposed, for example, by Bogoliubov and Tjablikov [2]. A first attempt to develop a diagrammatic theory for this problem was undertaken by Barabanov in [3]. With introduction of the dynamical mean field theory, the interest in the Anderson impurity model has considerably increased because infinite dimensional lattice models like the Hubbard model can be mapped onto effective impurity models and a self-consistency condition [4, 5].

The Hamiltonian of the model taking only s-like electrons into account is written as

$$\begin{aligned} H &= H_0 + H_{int}, \quad H_0 = H_0^c + H_0^f, \\ H_0^c &= \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k})\; C^+_{\mathbf{k}\sigma} C_{\mathbf{k}\sigma}, \;\; H_0^f = \epsilon_f \sum_{\sigma} f^+_\sigma f_\sigma + U n^f_\uparrow n^f_\downarrow, \\ H_{int} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}\sigma} f^+_\sigma C_{\mathbf{k}\sigma} + V^*_{\mathbf{k}\sigma} C^+_{\mathbf{k}\sigma} f_\sigma \right), \end{aligned} \tag{1}$$

where $n^f_\sigma = f^+_\sigma f_\sigma$, $C_{\mathbf{k}\sigma}(C^+_{\mathbf{k}\sigma})$ and $f_\sigma(f^+_\sigma)$ are the annihilation (creation) operators of conduction and impurity electrons with spin σ, respectively; $\epsilon(\mathbf{k})$ is the kinetic energy of the conduction band states $(\mathbf{k},\sigma)$; ϵ_f is the local energy of f-electrons and N is the number of lattice sites. H_{int} is the hybridization interaction between conduction and localized electrons. Summation over $\mathbf{k}$ will be changed to an integral over the energy $\epsilon(\mathbf{k})$ using the density of states $\rho_0(\epsilon)$ of conduction electrons.

The term in the Hamiltonian involving U describes the on-site Coulomb interaction between two impurity electrons. This term is far too large to be treated by perturbation theory. Therefore, we include it in the non-interacting Hamiltonian H_0. Since this term invalidates Wick's theorem for local electrons, we first of all have to formulate the generalized Wick's theorem (GWT) for local electrons, preserving the ordinary Wick theorem for conduction electrons. Our GWT can be considered as the prescription which allows to determine the irreducible Green's functions or Kubo cumulants. A similar prescription has been used when discussing the properties of the single-band Hubbard model [6, 7, 8].

In interaction representation, the renormalized (Matsubara) Green's functions of conduction and impurity electrons have the form:

$$G(\mathbf{k},\sigma,\tau \mid \mathbf{k}',\sigma',\tau') = -\left\langle \mathrm{T} C_{\mathbf{k}\sigma}(\tau) \overline{C}_{\mathbf{k}'\sigma'}(\tau') U(\beta) \right\rangle^c_0, \tag{2}$$

$$g(\sigma,\tau \mid \sigma',\tau') = -\left\langle \mathrm{T} f_\sigma(\tau) \overline{f}_{\sigma'}(\tau') U(\beta) \right\rangle^c_0. \tag{3}$$

Here τ and τ' stand for the imaginary time with $0 < \tau < \beta$ (β is the inverse temperature) and T is the chronological time ordering operator. The evolution operator $U(\beta)$ is determined by the hybridization interaction H_{int}. The statistical averaging in Eqs. (2) and (3) is carried out with respect to the zero-order density matrix of the conduction and impurity electrons.

The thermodynamic perturbation theory with respect to H_{int} requires an appropriate generalization scheme for the evaluation of statistical averages of the T-products of localized f-electron operators.

In zero-order approximation (negelecting the hy-