Single-site Anderson Model. I Diagrammatic theory

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The diagrammatic theory is proposed for the strongly correlated impurity Anderson model. The strongly correlated impurity electrons are hybridized with free conduction electrons. For this system the new diagrammatic approach is formulated. The linked cluster theorem for vacuum diagrams is proved and the Dyson type equations for electron propagators of both electron subsystems are established, together with such equations for mixed propagators. The approximations based on the summing the infinite series of diagrams are proposed, which close the system of equations and permit the investigation of the system's properties.

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I. INTRODUCTION

The study of strongly-correlated electron systems become in the last decade one of the most active fields of condensed matter physics. The properties of these systems can not 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[1] in the 1961 and discussed intensively in a lot of papers[2−15]. It is a model for a system of free conduction electrons that interact with the system of local spin, treated as just another electrons of d- or f-shells of an impurity atom. The impurity electrons are strongly correlated because of strong Coulomb repulsion and they undergo the exchange and hybridization with conduction electrons. This model has some properties similar to those of Kondo model having more interesting physics[16−18]. It has the application for heavy fermion systems where the local impurity orbital is f - orbital. Investigations of impurity Anderson model have used intensively the methods and results obtained for Kondo model by Nagaoka[18] and other authors[19,20]. All the cited papers are based on the method of equation of motions for retarded and advanced quantum Green's functions proposed by Bogoliubov and Tiablikov[21] and developed in papers[22−24].

The first attempt to develop the diagrammatic theory for this problem was realized in the paper[25]. These authors used the expansion by cumulants for averages of products of Hubbard transfer operators and their algebra.

With introduction of Dynamical Mean Field Theory the interest for Anderson impurity model increases because infinite dimensional lattice models can be mapped onto effective impurity models together with a self-consistency condition[26,27].

The Hamiltonian of the model is written as

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

where $C_{\mathbf{k}\sigma}(C^+_{\mathbf{k}\sigma})$ and $f_\sigma(f^+_\sigma)$ - annihilation (creation) operators of conduction and impurity electrons with spin σ correspondingly. $\epsilon(\mathbf{k})$ is the kinetic energy of the conduction band state $(\mathbf{k},\sigma)$, ϵ_f is the local energy of f - electrons, U - is the on-site Coulomb repulsion of the impurity 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 $\epsilon(\mathbf{k})$ with the density of state $\rho_0(\epsilon)$ of conduction electrons and the matrix elements will be considered as the function of energy $V(\epsilon)$. Because of the hybridization term of the Hamiltonian down and up spins of conduction electrons come and go in the local orbital and there is no appearance of spin flip process. Thus the important parameters of the Anderson model are the band width W, the conduction density of states $\rho(\epsilon)$, the local site energy ϵ_f and the on-site Coulomb interaction U. The electron energies are counted of chemical potential μ of the system: $\epsilon(\mathbf{k}) = \xi(\mathbf{k}) - \mu, \qquad \epsilon_f = \overline{\epsilon}_f - \mu$. There is also an energy parameter $\Gamma(\epsilon)$ associated with the hybridization term

$$\Gamma(\epsilon) = \frac{\pi}{N} \sum_{\mathbf{k}} V^2_{\mathbf{k}} \delta(\epsilon - \epsilon(\mathbf{k})) = \pi V^2(\epsilon) \rho_0(\epsilon). \qquad (2)$$

This function is assumed to be a constant, independent of energy. The term in the Hamiltonian involving U comes from on-site Coulomb interaction between two impurity