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Recursive Method for Calculating T-Matrix of Electron Scattering on Arbitrary Many-Particle Clusters in Strongly Correlated Systems

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The generalized recursive method for calculating the T-matrix of electron scattering on arbitrary many-particle clusters for determining the Green's function of the strongly correlated system is developed. This approach is extended to the studying electronic spectra in both direct (Wannier) and reciprocal (Bloch) representations with taking into account the influence of atomic and magnetic correlations arising in the system at a temperature of 0 K. The one-band Hubbard model, the correlated random field approximation, and the one-site coherent potential approximation for the effective Hamiltonian of system are also used in this approach. The spectral density in reciprocal space is calculated in the same way (the same scheme) as in direct space, using the appropriate expressions for the effective Green's function, which includes contributions from all crystal sublattices. Calculation of the small parameter of the cluster expansion of the Green's function in direct and reciprocal representations shows its smallness for different parameters of b.c.c alloys. This ensures the convergence of obtained recursive formulas for T-matrix of scattering on many-particle clusters and the applicability of pairwise approximation for T-matrix. It should be noted that to calculate the configuration-averaged Green's function it is necessary to use at least the pairwise approximation of T-matrix for describing the influence of the cluster environment of each atom on the redistribution of charge and spin densities on atoms, as well as atomic and magnetic correlations. In addition, the possibility of nanoclusters formation and their influence on the magnetic state was investigated in the b.c.c. alloy with strong electron correlations. The calculation of electronic spectra in the reciprocal (as in direct) representation showed the high sensitivity to the changes in the characteristics and composition of the b.c.c. alloy including the nanoclusters formation as well as to the change of resulting short-range atomic and magnetic orders. This method could be useful to analyze experimental data obtained, for example, in positron spectroscopy to study electronic structure, defects, chemical composition, and various correlations in systems.

Key words: Green's function for strongly correlated alloys, recursive expression for T-matrix, arbitrary many-particle clusters, short-range atomic and magnetic ordering.

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