Nonlocal and many-particle effects in the microscopic metal theory

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In frames of a reference system approach a variant of microscopic theory of normal metals was suggested and developed. With the aim of equal description both localized and collectivized electrons in metal we developed a method of an optimal one-particle basis $\{\phi_\sigma\}$ construction. It is a direct sum of two orthogonal subspaces – ion core electron states wave functions and delocalized functions. On this base we obtained the Hamiltonian of the electron-nuclear model, that assumes a direct calculation of matrix elements. This Hamiltonian is an obvious generalization of the well-known Bogolyubov's Hamiltonian [1] in his polar model of metal and considers all correlation, hybridization and orthogonalization effects.

The effective Hamiltonian of electron-ion model obtained with the help of reduction procedure (a statistical averaging over ion core electron states). Thus all interactions become nonlocal and many-particle as for ions, as electrons. The influence of nonlocal and orthogonal effects investigated on the formation of the electron-ion interactions. This approach is generalized on the case of binary metallic systems.

We developed some methods for the partition function calculation (over electron variables) in the adiabatic approximation for the electron-ion model with nonlocal interactions. As a result – the effective Hamiltonian obtained for a quasi-atoms system with two-, three- and four-particle interactions. The latest is presented in the form of decomposition of nonlocal electron-ion potential powers and $\mathbf{k}$-components of n-particle static correlation functions of the electron liquid model. We established a good convergence of such decompositions for $n = 2, 3, 4$. Thus was used a local field correction function, which we obtained in frames of the microscopic theory. We calculated the lattice constant for the fcc structure which deviates from experimental data not more than 1%, using a minimization procedure for a metallic Li energy.

1. N.N.Bogolyubov, Izbrannye trudy, vol. 2 (Kiev, Naukova dumka, 1970).