The effective interatomic pair potential of Na and its asymptotic form are computed from first principles using the pseudopotential method taking into account successively the exchange-correlation effects, the density of orthogonal holes, and shifts in the energies of the internal electronic levels. The potential obtained was used to estimate the role of long range action in stabilization of the stable crystalline modification.

In a preceding work [1], following step-by-step Harrison's program [2], we obtained a nonlocal pseudopotential (PP) for metallic Na. Using this PP, we calculated the values of such quantities as the equilibrium volume, total energy, dispersion law for electrons and phonons, as well as the equilibrium crystal structure. In addition, using the same approximations, we calculated the effective interatomic pair potential

\[ V_{\text{eff}}(R) = \frac{2Z^*}{\pi^2} \int \frac{q^2 F(q) \sin(qR)}{qR} dq, \]

where \( Z^* \) and \( \Omega_0 \) are the effective valence and atomic volume, respectively, while \( F(q) \) is the form factor [1]. This potential is a result of the mutual compensation of the direct Coulomb potential (first term) and the indirect interaction through the conduction electrons (second term). This potential is an oscillating and long-range function (Fig. 1). Since calculations of the energy of metallic structures are usually carried out in the reciprocal space [2, 3], the role of long-range action, following from the form of the potential, is not analyzed in this case.

In this paper we carry out calculations in the direct space in order to estimate the role of distant spheres in the stabilization of the stable crystal modification and we present an analysis of the formation of the total energy from contributions of various origin. The idea for this analysis follows from the work by Harrison [2] and Brovman-Kagan [3], but here it is carried out in a different manner.

The contributions of distant spheres to stabilization of a crystal structure turn out to be nonvanishing and elimination of the contribution of any sphere (even such distance spheres as the 100th) can change the theoretically predicted crystalline modification. This is related to the small difference in the energies of the main crystalline modifications. Space does not permit presenting the results of the calculation of contributions from all coordination spheres examined in this work, so that in Table 1 only several particular cases are presented.

It should be noted that it is not possible to make comparisons with respect to energies of different crystalline structures taking into account the same number of coordination spheres due to the different packing densities and splitting of the coordination spheres (hcp structure). This is clearly evident from the first line of Table 1, which presents the comparative data for three structures taking into account the first 50 coordination spheres. The stable structure in this case will turn out to be the most densely packed structure and least symmetrical (fcc), for which the overall number of atoms inside the interaction sphere is a maximum. It makes sense to compare different structures with an identical magnitude of
the radius of interaction or identical number of atoms inside the interaction sphere. These two methods complement one another, since in the first case, the number of interacting atoms may turn out to be different, while in the second, the interaction radius may be different. The second line of Table 1 compares the energies of different crystalline structure with an identical interaction radius: 17.8835 atomic units. An identical interaction radius (in this case 17.8835 atomic units) ends up in the fcc at the sixth, bcc at the seventh, and hcp at the ninth spheres and encompasses a different number of atoms. For this radius of interaction, the stable structure turned out to be the hcp structure, but at the first several tens of coordination spheres, this will not happen. Here, in comparing the energy structures, one more factor is included: it is not always possible to find simultaneously in the three structures atoms that are located at identical distances. Finally, it is also possible to compare crystal structures with an identical number of atoms in the interaction sphere. As is evident (third and fourth lines in Table 1), the same number of atoms corresponds to a different interaction radius and, as a result of this, the stable structures are different (in one case, the hcp structure, and in the other, the fcc).

We believe that the comparison that makes most physical sense is a comparison of the energy structures according to equal interaction radius with equal or nearly equal number of atoms. At the same time, it should be noted that the comparison of energy structures of metallic phases, often presented in estimates, taking into account the interaction at the first several coordination spheres, is unjustified, since the cutoff of the interaction radius can be made only based on comparing the contribution of the next coordination sphere taken into account to the difference in the energies of the crystalline modifications. The last number is on the order of $10^{-5}$ Ry/ion. Examples of the contribution to the energy of different coordination spheres, per ion, are presented in Table 1. Comparison of these quantities confirms the previous conclusion that even the contributions of such distant spheres as the 50, 60, and 70th spheres are still important in choosing the equilibrium crystalline modification.

If we examine the contributions of the direct and indirect interactions to the formation of the equilibrium structure, then it will turn out (detailed numbers are not presented here due to the cumbersomeness) that the appearance of the least energy for the hcp modification is due precisely to the contribution of the indirect interaction. In other words, the stabilization of this structure is due to the energy band structure.

The equilibrium energy properties of a metallic crystal arise from the mutual compensation of large, opposite in sign, contributions to the total energy (such as, e.g., the direct and indirect interactions). This is evident in greater detail in Table 2, where the different contributions to the total energy of metallic Na in the equilibrium state are presented. Since the direct and indirect interactions damp quite slowly, the numbers are presented for a quite distant (50th) sphere. As can be seen, the electrostatic energy ($E_{el} = -0.506980$ Ry/ion) is made of two large contributions: the unscreened Coulomb interaction and the interaction of ions with the uniform distribution of conduction electrons (background energy). The first of these contributions is structurally dependent, while the second depends only on