Thermodynamics of Debue systems in weakly and moderately coupled regimes

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For reducing inaccuracy of the traditional Debye-Hückel theory for evaluating thermodynamic properties of strongly coupled OCP the Debye-Hückel plus hole (DHH) approximation had been evolved. The term “Debye-Hückel plus hole” is conventionally associated with the work by Nordholm [1], although similar arguments were used earlier by Gryaznov and Iosilevskiy [2]. Below we apply DHH approximation to the model Yukawa system. The main idea behind the DHH approximation is that the exponential particle density *n* must be truncated close to a test particle so as not to become negative upon linearization: *n*{0, *r* ≤ *h*; *n*0(1-*Qφ*/*T*), *r* > *h*}. The neutralizing background follows Boltzmann distribution everywhere and can be linearized: *nb**nb*0(1+*eφ*/*T*). Matching the solution of the Poisson equation for the potential *φ* at the hole boundary *r* = *h* and using boundary conditions, we obtain an equation for determination of the hole radius

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where *x* = *kbh*, *kb*= , *κ* = *akb*, *a* = (3/4π*n*0)1/3, Γ = *Q*2/*aT* and *Q* is the particle charge.

The internal energy per particle in units of *T* in the DHH approximation is



which yields

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In the case of OCP (*κ* = 0) it becomes



and coincides with those obtained in [1,2]. In the strongly coupled regime Γ >> 1, the DHH approximation yields the correct scaling *u* ~ Γ, but the coefficient of proportionality is too low (0.750 instead of 0.899).

Comparison with results of MD simulations of *u* [3] in regime *κ* ≤ 1 shows that the DHH approximation is rather accurate up to Γ/Γ*m* ~ 10−2 (Γ*m* is the coupling parameter at which fluid-solid phase transition occurs). In this regime, typical deviations of DHH from MD simulations do not exceed few percent. For stronger coupling, DHH systematically overestimates the (negative) internal energy. As fluid-solid phase transition is approached, the difference between DHH and MD simulations amounts to ~ 15% at *κ* = 0, and reduces to ~ 10% at *κ* = 1. In the regime *κ* > 1 the qualitative picture remains the same. The DHH approximation provides good accuracy up to Γ/Γ*m* ~ 10-2. Here the difference between DHH and MD results does not normally exceed ~ 1%. For stronger coupling, DHH is again systematically overestimating *u.* On approaching the fluid-solid transition the inaccuracy of DHH is ~ 5% for *κ* = 2.0. As *κ* increases, *u* ~ −Γ*κ*/2 and DHH becomes virtually more and more accurate. Already for *κ* = 5.0 one can hardly observe any difference between DHH and MD simulations.

References

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