# RELEVANCE OF THE WIGNER–SEITZ CELL APPROXIMATION FOR THE COULOMB CLUSTERS

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The system of massive charged particles on the compensating uniform background is commonly termed the one-component plasma (OCP). If the volume of such system is confined to a sphere (we treat a finite compensating background) then the limited OCP or Coulomb cluster is formed. Here, the state of a system is defined not only by the Coulomb coupling parameter $\Gamma$ but by the number of particles $N$ as well. The Coulomb clusters encountered in complex plasmas are most extensively studied both theoretically and experimentally [1–3]. It was found that such a system has much more complex structure than that of an infinite OCP, and at high $\Gamma \sim 10^2$, it is in fact a combination of 2D and 3D dust crystal structures. The objective of this study is to test the relevance of the Wigner–Seitz cell approximation for such a complex system, in particular, for the determination of $\Gamma$.

We perform molecular dynamics simulation of the Coulomb clusters. The temperature was controlled by the Langevin thermostat modified to conserve the total momentum of the particles. Fixed are the given damping frequency $\gamma$ and the autocorrelation decay time for the stochastic force $\tau_{\mathrm{st}}$. The simulation was performed for $N$ ranging from 155 to 1075 and $\Gamma$, from 10 to 500. The structure of a cluster is represented by a set of embedded spherical shells. Melting of this system is a combination of 2D and 3D melting demonstrating the regularities, which are almost independent on $N$. Notably, the self-diffusion in this system is intensive not only in the liquidlike but in solidlike states as well. In this connection, the estimation of $\Gamma$ used in the experimental data analysis (e.g., in [4]) is demonstrated to be not reliable. Indeed, estimation of $\Gamma$ from the mean-square deviation of a particle from the center of its cell $\delta r$ based on the Wigner–Seitz cell approximation, $\Gamma = 3(r_d / \delta r)^2$, where $r_d = (3/4\pi n_d)$ and $n_d$ is the dust particles number density, flaws due to the perpetual shifts of the cell center upon the particle thermal jumps, which results in the divergence of $\delta r$ in time. A new method for the determination of $\Gamma$ based on the Wigner–Seitz cell approximation is proposed. It is shown that

$$\Gamma = \frac{3r_d^2}{m^2 \left\langle v^2 \right\rangle^2} \left[ \left\langle a^2 \right\rangle + \gamma \left( \gamma - \frac{2}{\tau_{\mathrm{st}}} \right) \left\langle v^2 \right\rangle \right], \tag{1}$$

where $m$, $v$, and $a$ are the mass, velocity, and acceleration of a particle, respectively. For Eq. (1), the coordinates of the particle cell center are not required. Our simulation points to a good accuracy of (1) for the cluster particles irrespective of their position and the cluster phase state. This proves the relevance of the Wigner–Seitz cell approximation for the Coulomb clusters (as regards $\Gamma$). Relation (1) can be used in the experiments with complex plasma.

## References

[1]. Arp O., Block D., and Piel A. *Phys. Rev. Lett.* **93** (16) 165004-1–165004-4 (2004).

[2]. Bonitz M., Block D., Arp O., Golubnychiy V., Baumgartner H., Ludwig P., Piel A., and Filinov A. *Phys. Rev. Lett.* **96** (7), 075001-1–075001-4 (2006).

[3]. Baumgartner H., Kählert H., Golobnychiy V., Henning C., Käding S., Melzer A., and Bonitz M. *Contrib. Plasma Phys.* **47** (4-5), 281–290 (2007).

[4]. Zhukhovitskii D. I., Naumkin V. N., Khusnulgatin A. I., Molotkov V. I., and Lipaev A. M. *Phys. Rev. E.* **96** (4), 043204-1–043204-10 (2017).