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Classical Density Functional Theory: Representability, Universal Bounds and Local Density Approximation

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We provide upper and lower bounds on the lowest free energy of a classical system with short range interactions at given one-particle density $\rho(x)$ and prove that the lowest free energy at temperature T with a prescribed density profile $\rho(x)$ can be approximated by the local free energy $\int f_T(\rho(x)) dx$, provided that ρ varies slowly over sufficiently large length scales. A quantitative error on the difference is provided in terms of the gradient of the density. Here f_T is the free energy per unit volume of an infinite homogeneous gas of the corresponding uniform density. The proof uses quantitative Ruelle bounds (estimates on the local number of particles in a large system). The talk is based on two recent papers [1, 2].

References

- [1] M. Jex, M. Lewin, P. Madsen: *Classical Density Functional Theory: Representability and Universal Bounds*, Journal of Statistical Physics, vol. 190, no. 4, pp. 73, 2023.
- [2] M. Jex, M. Lewin, P. Madsen: *Classical density functional theory: the local density approximation*, accepted to Reviews in Mathematical Physics, preprint arXiv:2310.18028, 2024.