

Abstract for an Invited Paper
for the MAR08 Meeting of
The American Physical Society

Theory of Orbital Magnetization and its Generalization to Interacting Systems¹

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Recently, a new formula for the orbital magnetization was proposed. In this talk, I will review the original derivation of the formula based on the semi-classical wave-packet dynamics, as well as a general derivation based on the standard perturbation theory of quantum mechanics. The quantum derivation clarifies the origin of the novel aspects of the semi-classical derivation, such as the Berry phase correction to the density of states. It is valid for general systems including insulators with or without a Chern number, metals at zero or finite temperatures. More importantly, we are able to combine the quantum derivation with the exact current and spin density functional theory (SCDFT), proving the validity of the formula for interacting systems. With this development, the new magnetization formula, in combination with the recent advances in the construction of optimized effective potential for SCDFT, will turn out to be a powerful practical tool for the study of systems that have long defied traditional ab-initio methods.

[1] J. Shi, G. Vignale, D. Xiao and Q. Niu, Phys. Rev. Lett. 99, 197202 (2007).

[2] Z. Wang, P. Zhang and J. Shi, Phys. Rev. B 76, 094406 (2007).

[3] D. Xiao, J. Shi and Q. Niu, Phys. Rev. Lett., 95, 137204 (2005).

¹Supported by NSF of China, NSF, DOE and Welch Foundation.