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(G*) Preserving the Hermiticity of the One-body Density Matrix for a Non-interacting Fermi Gas

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The one-body density matrix (ODM) for a d-dimensional non-interacting Fermi gas can be approximately obtained in the semiclassical regime through different $\hbar$-expansion techniques. One would expect any method of approximating the ODM should yield equivalent density matrices which are both Hermitian and idempotent to any order in $\hbar$. The method of Grammaticos and Voros does ensure these properties for any order of $\hbar$. Meanwhile, the Kirzhnits and Wigner-Kirkwood methods do not yield these properties when truncated, which would suggest these methods provide non-physical ODM's. Here we show explicitly, for arbitrary $d \geq 1$-dimensions through an appropriate change into symmetric coordinates, that each of the methods are not only identical but also Hermitian and idempotent. This change of variables resolves the inconsistencies between the various methods discussed in previous literature. We show that the non-Hermitian and non-idempotent behaviour of the Kirzhnits and Wigner-Kirkwood methods is an artifact of performing a non-symmetric truncation to the semiclassical $\hbar$-expansions.

Keyword-1

Semiclassical

Keyword-2

Density functional theory

Keyword-3

Ultracold Fermi gas

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