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Quantum mechanical local energy density applied to many-electron systems

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The concept of a local energy density in a many-electron system has been a topic of discussion and debate for over 30 years. Chetty and Martin conducted the initial research in this field in the early 1990s, expanding upon the quantum mechanical stress theorem that Nielsen and Martin had derived in 1985. In the research that they conducted in 1992, Chetty and Martin introduced the idea of local energy density by utilizing the Kohn-Sham formalism within the framework of Density Functional Theory (DFT). They proposed that the kinetic energy density was non-unique, expressible either through the asymmetric operator, $-\frac{1}{2}\psi(\mathbf{r})\nabla^2\psi(\mathbf{r})$, or the symmetric operator, $+\frac{1}{2}|\nabla\psi(\mathbf{r})|^2$. Likewise, they also stated that the Hartree energy density can be represented in two distinct forms: one that incorporates the Coulomb potential, $\frac{1}{2}n(\mathbf{r})V(\mathbf{r})$, and another that involves the square of the electric field, $\frac{1}{8\pi}|\mathbf{E}(\mathbf{r})|^2$.

Subsequent research largely focused on working within a specific choice of energy density formulation and ensuring internal consistency within that gauge to obtain meaningful computational results. It has been demonstrated that local perturbative changes in a real physical system lead to corresponding local variations in the energy density. This establishes a correlation between modifications in the electronic band structure typically described in reciprocal space and variations in the energy density, which is a real-space quantity.

The recent study by Martin, Chetty, and Trinkle (2025) posits that the energy density in a many-electron system may be uniquely characterized. The primary objective of this thesis is to place this assertion on a solid mathematical and physical foundation. By starting from the many-body formulation of the electron problem, we demonstrate that the kinetic energy density is uniquely determined by the asymmetric operator that appears in the Hamiltonian. The Coulomb potential energy density is shown to be uniquely defined within this many-electron framework. It is only when the mean-field Hartree term is separated from the term involving the pair correlation function that one can argue the Hartree energy density is non-unique being expressible either in terms of the Coulomb potential or the square of the electric field. However, we argue that this separation is merely an artefact rather than a fundamental property of the system. Since the many-body formulation fully defines the problem, it naturally leads to a unique local energy density expressed through all the operators present in the Hamiltonian.

From this, we conclude that the local energy density of a many-electron system is uniquely defined and, crucially, experimentally measurable. This implies that the quantum mechanical energy density distribution of a many-electron system is not just a theoretical construct or a computational tool for deriving the total energy uniquely determined within Density Functional Theory via the electron density but rather an intrinsic and physically meaningful attribute of the system.

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