

The National Institute of Standards and Technology (NIST) employs several relativistic and quantum mechanical corrections to refine the measured value of the Hartree energy. Here's a breakdown of how these corrections are applied:

1. Relativistic Corrections:

- **Relativistic Local-Density Approximation (RLDA):** In this approach, the non-relativistic local-density approximation (LDA) is modified by substituting the relativistic kinetic-energy operator for its non-relativistic counterpart. This includes using relativistic corrections to the local-density functional, specifically those proposed by MacDonald and Vosko. These corrections account for the effects of special relativity on electron behavior, particularly important for high-energy states or heavy atoms where electron velocities approach a significant fraction of the speed of light. The radial equations solved in RLDA include terms for the Dirac equation's large and small components, adjusting for the spin-orbit coupling effects.
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- **Scalar-Relativistic Local-Density Approximation (ScRLDA):** This is a simplified version of RLDA, which still includes some relativistic effects but in a less computationally intensive manner. It uses the average κ (Dirac's quantum number) to handle relativistic effects without fully solving the Dirac equation, thus providing a middle ground between accuracy and computational efficiency.


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2. Quantum Mechanical Corrections:

- **Hartree-Fock Method:** While not a direct correction to the Hartree energy itself, the Hartree-Fock method is used as a starting point for many quantum mechanical calculations. It involves solving a set of self-consistent one-electron equations where the interaction between electrons is treated in a mean-field approximation. This method inherently includes some quantum mechanical effects like exchange interactions. However, for high-precision work, further corrections beyond Hartree-Fock are necessary.
- **Exchange-Correlation Energy:** Within the LDA framework, the exchange-correlation energy (Exc) is approximated to account for the fact that an electron does not interact with itself and to include electron correlation effects. This energy term is crucial for correcting the total energy in quantum mechanical calculations, providing a more accurate depiction of electron behavior in a many-body system.

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3. Other Corrections Mentioned in Context:

- **Fine-Structure Constant (α):** In discussions about relativistic corrections, the fine-structure constant plays a role in determining the magnitude of these effects. It appears in the formulation of relativistic corrections both in RLDA and in broader quantum electrodynamics (QED) contexts.
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- **Quantum Electrodynamics (QED) Corrections:** For the most precise measurements, corrections from quantum electrodynamics might be considered, including effects like the

Lamb shift, although these are not directly specified for Hartree energy by NIST in the provided context but are relevant for atomic physics calculations.

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These corrections collectively help in providing a more accurate value for the Hartree energy by accounting for the interactions and behaviors of electrons under both quantum mechanical and relativistic frameworks. They are essential for applications in atomic physics, computational chemistry, and wherever precise energy levels are required.