Fermi-Amaldi Model Project Report

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Abstract

The advantages and limitations of Fermi-Amaldi model has been partly summarized. A simple observation of B3LYP is presented.

1 Advantages

1. The Fermi-Amaldi model hole naturally satisfies the normalization condition.
2. The Fermi-Amaldi potential v_{xc}^{FA} has the correct asymptotic behavior $-1/r$.
3. The Fermi-Amaldi Approximation is exact for one-electron system. In other words, it is self-interaction-free.

There might be other advantages which need to be explored.

2 Limitations and Disadvantages

1. For two systems, A and B, in the limit of infinite separation, we should have $V_{ee}[\rho_A + \rho_B] = V_{ee}[\rho_A] + V_{ee}[\rho_B]$. But in FA approx., $V_{ee}[\rho_A + \rho_B] > V_{ee}[\rho_A] + V_{ee}[\rho_B]$
2. For uniform electron gas systems, E_{xc} should recover LDA. But FA term does not show such property. (this will be mentioned later)
3. The scaling properties of FA term is the same with $J[\rho]$, ($J[\lambda\rho] = \lambda^2 J[\rho]$) but differs from E_{xc}.

3 Observation of B3LYP

Obviously, B3LYP agrees with LDA in UEG-limit perfectly. All three terms with unknown parameters will disappear in UEG-limit. Consider FA hybrid model, say $FA + GGA$, how can we restore LDA?

What linear combinations do you recommend?