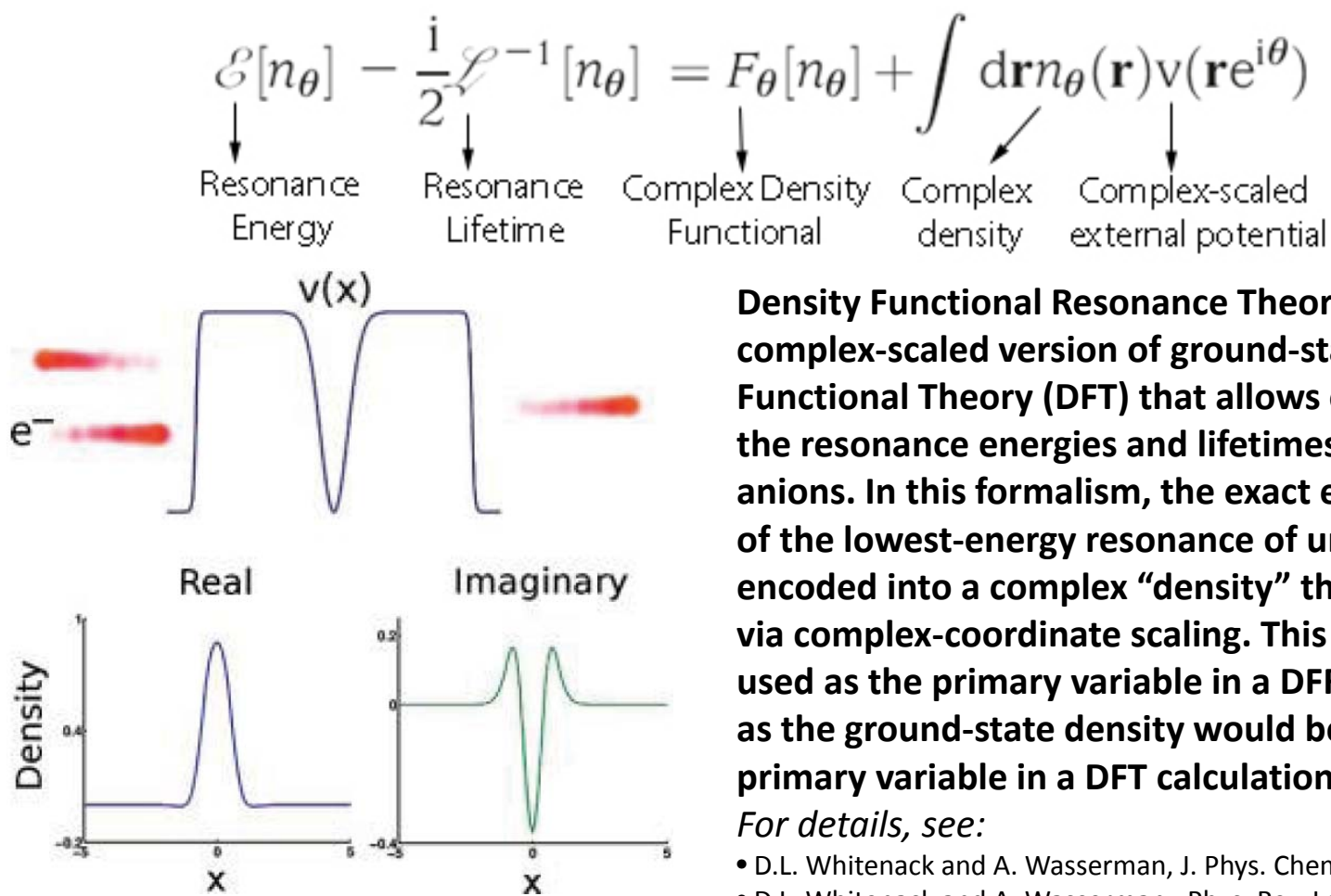# Density Functional Resonance Theory of Metastable Negative Ions

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$$\mathcal{E}[n_\theta] - \frac{i}{2}\mathscr{L}^{-1}[n_\theta] = F_\theta[n_\theta] + \int d\mathbf{r}\, n_\theta(\mathbf{r}) v(\mathbf{r}e^{i\theta})$$

Resonance Energy · Resonance Lifetime · Complex Density Functional · Complex density · Complex-scaled external potential

v(x)

e⁻

Real   Imaginary

Density

X   X

Density Functional Resonance Theory (DFRT) is a complex-scaled version of ground-state Density Functional Theory (DFT) that allows one to calculate the resonance energies and lifetimes of meta-stable anions. In this formalism, the exact energy and lifetime of the lowest-energy resonance of unbound systems is encoded into a complex "density" that can be obtained via complex-coordinate scaling. This complex density is used as the primary variable in a DFRT calculation just as the ground-state density would be used as the primary variable in a DFT calculation.

For details, see:

• D.L. Whitenack and A. Wasserman, J. Phys. Chem. Lett. **1**, 407 (2010).
• D.L. Whitenack and A. Wasserman, Phys. Rev. Lett. (accepted) (2011).