Week 3: Logic Questions

April 18, 2020

1. Given the RG Theorem for densities, does it imply a theorem for current densities? Explain.
2. In KS-TDDFT, the exact TDKS potential reproduces the exact $n(\mathbf{r},\, t)$. Doesn't this violate RG, as two potentials (both $v(\mathbf{r},\, t)$ and $v_s(\mathbf{r},\, t)$) produce the same $n(\mathbf{r},\, t)$? Explain.
3. For non-interacting fermions, can you find more than one $v_s(\mathbf{r},\, t)$ that yields a given $n(\mathbf{r},\, t)$? Explain.
4. For non-degenerate ground states, which of the following are purely functionals of the ground state density: $\chi_s,\, f_{xc},\, \chi$?
5. Explain how to extract $f_{xc}(\omega = 0)$ exactly from the exact ground state E_{xc}.
6. What two conditions must $n(\mathbf{r},\, t)$ satisfy if it comes from an initial wavefunction $\Psi(\mathbf{r}_1 ... \mathbf{r}_N)$?
7. For a single-particle wavefunction $\phi(\mathbf{r},\, t) = e^{i\alpha(\mathbf{r},\, t)}\sqrt{n(\mathbf{r},\, t)}$, derive formulas for the KS potential.
8. Does $\chi(\omega)$ contain excitations beyond single excitations? If not, how do you know? If so, what does that mean for f_{xc}?
9. Since E_{xc} is determined by $\chi^{\lambda}(\omega)$ via the ACFD formula, I could start from $f_{xc} = 0$, get E_{xc}^{RPA} for the uniform gas, feed f_{xc}^{RPA} into χ, get a new E_{xc}, and repeat. Will I converge to the exact E_{xc}^{unif}? Explain.
10. Power is defined as $\frac{dE}{dt}$. What great simplification occurs in calculating power in TDKS? *Hint: Think Newton's Third Law.*