BerkeleyGW GW/BSE quiz for Benasque TDDFT 2018

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1. To calculate bandstructure, we can't just use Kohn-Sham eigenvalues from DFT and need GW for quasiparticle energies because:
a) we don't have the exact exchange-correlation functional
b) Kohn-Sham eigenvalues have no physical meaning at all
c) DFT is not a many-body theory but GW is
d) DFT is only a ground-state theory

2. What does the G stand for in GW?

3. What does the W stand for in GW?

4. Does GW increase the band gap?
a) always
b) sometimes
c) never

5. Which term in the BSE is repulsive?
a) direct
b) exchange
c) kinetic

6. Which term in the BSE is **not** present for triplet excitons?
a) direct
b) exchange
c) kinetic

7. Which property is true of the self-energy operator?
a) Hermitian
b) local
c) energy-independent
d) consistent with space-group symmetry

8. Which condition is **not** needed to have real plane-wave coefficients of the wavefunction?
a) k = Γ only
b) inversion symmetry about the origin
c) time-reversal symmetry

9. Which is **not** a reason for special handling of the q->0 limit in GW?
a) divergent quantities
b) finite limit which is ratio of two divergent quantities
c) proper evaluation of velocity matrix elements
d) rapid variation near q=0 with truncation

10. Which material should **not** be calculated using Coulomb truncation?
a) crystalline pentacene
b) benzene molecule
c) graphene
d) carbon nanotube

11. Why is Coulomb truncation needed in GW/BSE but not generally used in DFT?

12. Which quantity is **not** interpolated in BSE?
a) quasiparticle energies
b) direct term in kernel
c) exchange term in kernel
d) dipole matrix elements

13. Which will likely lead to a bad result in GW?
a) large band gap in DFT
b) small band gap in DFT
c) no gap in DFT (when there should be a gap)
d) strong correlations

14. Which material has the strongest excitonic effects?
a) sodium
b) silicon
c) BN sheet
d) benzene

15. Increasing which of these parameters adds most to the computational expense in GW?
a) bands
b) atoms
c) k-points
d) G-vectors
e) spins