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## The $GW$ approach to spectral, ground-state and transport properties

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The  $GW$  approximation is the first-order term in an expansion of the self-energy operator  $\Sigma$  in powers of the dynamically screened electron-electron interaction,  $W$ . It may be thought of as exact exchange (the Hartree-Fock exchange operator), together with an partial inclusion of correlation diagrams through dynamical screening of the Coulomb interaction. From  $\Sigma$ , the one-electron Green's function  $G$  may be calculated, from which various spectral and ground-state properties are available. For transport properties (as well as certain other excited-state properties), the two-electron Green's function is required, which may also be formulated at the same level of approximation as  $GW$ .

I shall start with a brief review of key applications of  $GW$  to spectral properties such as quasiparticle energies and lifetimes for added electrons or holes, including some recent work on metallic clusters [1].

In applying  $GW$  to the ground-state total energy, the choice of whether  $G$  and/or  $W$  are made to be consistent with the Green's function that arises *from*  $\Sigma$  is particularly important:  $G_0W_0$ ,  $GW_0$  and fully self-consistent  $GW$ , where  $G_0$  generally indicates the LDA Green's function. I shall present results for finite and infinite systems at all three levels of self-consistency. These include converged results resulting from the incorporation of self-consistency and  $GW$  total-energy techniques into our general-purpose GWST "space-time" supercell code suite [2], which interfaces with pseudopotential plane-wave DFT calculations as its input. This allows the extension of the  $GW$  total-energy approach from high-symmetry test systems [3] to general systems, and opens the possibility of applications to systems whose energetics is not described sufficiently reliably within the usual DFT-based approaches.

I shall also describe our recent formulation [4] of the conductance of a junction between two nanowires in a form which permits the inclusion of electronic correlation effects in a  $GW$ -like framework.

[1] "Image States in Metal Clusters", Patrick Rinke, Kris Delaney, P. García-González and R.W. Godby, submitted

[2] "Space-time method for *ab initio* calculations of self-energies and dielectric response functions of solids", H. N. Rojas, R. W. Godby and R. J. Needs, Phys. Rev. Lett. **74** 1827 (1995)

[3] "Many-body  $GW$  calculations of ground-state properties: quasi-2D electron systems and van der Waals forces", P. García-González and R. W. Godby, Phys. Rev. Lett. **88** 056406 (2002)

[4] "Conductance and polarization in quantum junctions", P. Bokes and R.W. Godby, Phys. Rev. B **69** 245420 (2004)

Further details at <http://www-users.york.ac.uk/~rwg3/>.