How reliable is the RPA for van der Waals (dispersion) interactions?

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Dispersion forces dominate the long-distance part of the van der Waals interaction, and they occur between any two separated pieces of matter that contain electrons. They can be regarded as a "residual" Coulomb interaction from Coulomb-induced long-distance correlations between charge density fluctuations occurring within each of the charge-neutral interacting fragments. There are analogies of this physics involving other interactions – even the strong interaction between color-neutral nucleons has sometimes been attributed to this type of residual-interaction physics.

The (direct, non-exchange) Random Phase Approximation (dRPA) for the energy of the combined interacting system is most compactly defined by a sum of all ring diagrams of open bubbles, with no ladders. Equivalently it is the Adiabatic Connection-Fluctuation-Dissipation Theorem (ACFFDT) energy, wherein the density-density response χ is evaluated in the Random Phase (Time Dependent Hartree) approximation.

I will discuss some of the obvious serious failings of such a simple theory, and how it nevertheless is a very powerful tool for accurate prediction of dispersion energies of a wide class of condensed-matter systems. Some unpublished numerical results will be given on the cohesive energetics of graphitic systems, one of the most important problems in current nanoscience and nanotechnology.

Some relevant publications:

'Quasi-local-density approximation for a van der Waals energy functional', J.F. Dobson, pp 121-142 in 'Topics in condensed matter physics', Ed. M.P. Das, (N ova Science Publishers, Commack New York 1994, ISBN 1560721804): reproduced in cond-mat/0311371

"Constraint satisfaction in local and gradient susceptibility approximations: application to a van der Waals density functional" John F. Dobson and Bradley P. Dinte, Phys. Rev. Lett. 76, 1780 (1996)

"Toward the Description of van der Waals Interactions within Density Functional Theory", M. Lein, J.F. Dobson and E. K. U. Gross, J. Comp. Chem. **20**, 12 (1999)

"Successful test of a seamless van der Waals density functional", John F. Dobson and Jun Wang, Phys. Rev. Lett. 82, 2123 (1999)

"Energy-optimized, local exchange-correlation kernel for the electron gas, with application to van der Waals forces", John F. Dobson and Jun Wang, Phys. Rev. B 62, 10038 (2000).

"Prediction of dispersion forces: is there a problem?", John F. Dobson, Keith McLennan, Angel Rubio, Jun Wang, Tim Gould, Hung M. Le and Bradley P. Dinte, Australian J. Chem. **54**, 513 (2001

"Correlation energies of inhomogeneous many-electron systems", John F. Dobson, Jun Wang, and Tim Gould , Phys. Rev. B (Rapid Communications) 66, 081108 (2002) (Inhomogeneous STLS theory)

"Effects beyond the random-phase approximation in calculating the interaction between metal films " J. Jung, P. Garcia-Gonzalez, J.F. Dobson, R.W. Godby, Phys. Rev. B 70, 205107 (2004)

"Asymptotics of the dispersion interaction: analytic benchmarks for van der Waals energy functionals", John F. Dobson, Angela White and Angel Rubio, Phys. Rev. Lett. 96, 073201 (2006).

"Enhanced Van der Waals interaction between quasi-one dimensional conducting collinear structures ", Angela White and John. F. Dobson. Phys. Rev. B **77**, 075436 (2008)

"van der Waals dispersion power laws for cleavage, exfoliation and stretching in multi-scale, layered systems" Tim Gould, Evan Gray, and John F. Dobson Phys. Rev. B **79**, 113402 (2009) (arXiv:0809.0736v3)

"Dispersion interaction between crossed conducting wires", John F. Dobson, Timothy Gould and Israel Klich, PRA **80**, 012506 _2009