

Correlation energy of the uniform quantized electron gas

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Abstract

The electrons of atoms and molecules form a uniform gas of electrons. Here we consider an inhomogeneous gas of interacting electrons in a neutralizing background. This is a crude model for the conduction electrons of metals that are present in an external periodic varying potential from the atoms of a regular lattice. On the basis of Feynman's path integral we consider this as a problem of classical statistical mechanics in four dimensions.

With the path integral the free fermion gas of non-interacting electrons can be identified with an ideal classical gas mixture of polymers where exchange effects are taken into account by combining single particles (polymers) into larger ideal gas molecules, about half of which for fermions have negative densities.

Since polymers are linked together into larger molecules, they will be correlated. When integrated together with the Coulomb interaction, this gives the well known exchange energy. We consider temperature $T = 0$.

The Coulomb interaction modifies the pair correlation function for the electrons. This again will change the free energy (ground state energy) to make it somewhat lower. This change is the correlation energy, which is a non-local quantity for which various methods have been used to try to obtain useful approximations. From the statistical mechanical viewpoint we find that it must correspond to the Casimir energy or van der Waals energy with electrostatic Coulomb interaction. By further study of it we find that its basic version happens to coincide with the well known RPA (random phase approximation).

It turns out that the RPA gives a correlation energy clearly too large in magnitude. In an effort to improve upon that we use methods and properties known from the statistical mechanics of classical fluids. In this respect we replace the Coulomb interaction with an effective one, which is the former modified at short distances. The modification contains a free parameter to be determined by some condition. One such condition that we have investigated, was to put it on the pair correlation function, mainly to reflect that particles (fermions) with the equal spins can not overlap. Improved results were obtained, but various problems appeared to make results somewhat unclear.

Thus in another work we noticed that thermodynamic self-consistency could be utilized, a method that had given some very accurate results for classical fluids. With this method the equation of state (like the free energy) is obtained in two independent ways from the correlation function, in the present case (at $T = 0$) these two ways are via the charging principle and via the compressibility, to determine a free parameter. With this improved and stable results were obtained, depending somewhat upon the functional form of the assumed smooth modification of the potential. One of the forms gave very accurate results when compared with results from previous computer simulations.

We find that the method sketched here, can be valid for nonuniform systems too, like the electron gas of molecules, and it may be extended to this situation by extending quantum computations to incorporate the above type of modifications to the RPA.

References:

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