Electron-electron and electron-ion correlations at arbitrary densities, spin-polarizations and temperatures using pseudo-atom and classical-map approaches.

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Abstract

Density functional theory (DFT) proves that all many-body correlations can be written as effective functionals of the one-body densities; these are known as the exchange-correlation (XC) functionals F_{xc}. Hence, all many-body problems can be reduced to effective one-body problems, if the XC-functionals are known. In dealing with electron-ion systems, standard DFT does NOT reduce the ion-ion correlation problem, but explicitly treats N nuclei in a simulation box as providing an external potential for the electrons treated in DFT, where the electron-electron XC-functional is provided from an external model. Thus, while the e-e many-body problem is reduced to a one-body problem, the ion-ion problem is treated as an N-body problem at great computational cost. Attempts to use an externally supplied ion-ion XC-fucntional F^{ii}_{xc} fail as this functional is extremely non-local. The solution to the problem is to construct the ion-ion XC-functional *in situ* from the ion-ion pair distribution function (PDF) g_{ii}, from classical molecular dynamics (MD) or from equivalent integral equations like the modified hyper-netted chain (MHNC) sum of diagrams coupled to the Ornstein-Zernike (OZ) equation. This enables us to define a rigorous one-body DFT object known as the 'neutral-pseudo atom' (NPA) which, while being a one-body procedure, successfully captures even the covalent bonding structures found in liquid carbon or silicon accurately, and with negligible effort on a laptop.
While the ion-ion functional is made *in situ,* the NPA uses a standard externally provided e-e XC-functional. One can overcome this if the e-e XC-functional could also be made in *situ* from the e-e PDF g_{ee} for the system, calculated *in situ*. This is feasible using the MHNC and the OZ equations (or with MD) if the electrons are classical particles. Hence we construct a *classical map* of the electron system (at zero or finite temperature T) to a statistically equivalent classical Coulomb fluid at an effective classical-fluid temperature T_{cf}. This effective temperature is selected so that the classical Coulomb fluid has the same XC-energy as the quantum fluid for an interacting uniform electron liquid at the same density and spin polarization. This method, where a classical map is used for the electrons, and the e-e and ion-ion PDFs are calculated using the MHNC-OZ integral equations (or MD) is extremely efficient numerically, and quite accurate. Illustrative calculations show that the results obtained from these methods for the energies, PDFs, local-field corrections to response functions etc., agree well with highly computer intensive quatum-Monte-Carlo (QMC) results or MD-DFT Kohn-Sham simulations. Classical-map methods have also been tested

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for two-diemnsional electron layers, thick layers, multi-valleys etc. showing good agreement with QMC data where available. Results for hydrogen in regimes where *both* electrons and ions are quantum particles are easily obtained and discussed here.

Since the classical-map methods use only pair-distribution functions and not wavefunctions, the question of the N-representability of the densities obtained can be raised. A proof of the N-representability of the classical-map densites is given.

1. M. W. C. Dharma-wardana, https://arxiv.org/abs/1906.05941

2. M. W. C. Dharma-wardana, https://arxiv.org/abs/1602.04734

High temperature 3D electron-hole superfluidity in a superlattice

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In principle, bound states of electron-hole pairs in a semiconductor could condense to form a quantum superfluid[1]. Because of the strong electron-hole pairing interactions, one could expect the superfluid transition temperature to be very high. The electrons and holes can be confined to a pair of two-dimensional (2D) layers separated by a thin insulating barrier[2] to prevent electron-hole recombination, and for an insulating barrier only a few atomic layers thick, the electrons and holes in the superfluid bound-pairs feel a very strong Coulomb attraction. This typically can result in very large zero temperature superfluid gaps, $\Delta \sim 600$ K.[3]

However there is a problem in going to 2D, because it introduces a topological mechanism that suppresses superfluidity except at very low temperatures. The low-energy topological excitations do not depend on the strength of the electron-hole coupling. Recently, experimental evidence of an electron-hole superfluid condensate in two sheets of electron- and hole-doped graphene bilayers was reported[4], but the transition temperature was only $T_c \sim 1.5$ K. Such a low T_c is in line with predictions for a 2D Berezinskii-Kosterlitz-Thouless transition temperature[5]. The T_c is very low because it depends only on the density, and screening of the long-ranged Coulomb interaction is known to confine the superfluidity to low densities[3].

We are trying a new strategy to boost the superfluid transition to high temperatures, by generating three-dimensional (3D) superfluidity in a superlattice of alternating electron- and hole-doped semiconductor layers. The superlattice keeps the electrons and holes spatially separated, but leaves them sufficiently close for the electron-hole pairing interaction to be very strong, leading to large 3D superfluid gaps. In 3D, a large superfluid gap is associated with high transition temperatures. For example, the BCS transition temperature in the weak-coupling limit is proportional to the zero-temperature superfluid gap, $T_c \simeq \Delta(T=0)\exp(\gamma)/\pi$, a gap $\Delta(T=0) = 600$ K giving a $T_c = 340$ K.

To carry out full numerical calculations across the complete coupling spectrum from the BCS to the crossover to the BEC regimes using long-ranged screened Coulomb pairing interactions is a challenging task that verges on the impractical. Here we adopt an effective approach to evaluate the transition temperature that incorporates the detailed momentum structure of the electron-hole Coulomb pairing and a large part of the pair fluctuations that become increasingly important in strong coupling, as one moves into the crossover and BEC regimes. Using this approach, we present quantitative results for the properties of an electron-hole superfluid in a superlattice of doped monolayers of transition metal dichalcogenides. We find remarkably high transition temperatures approaching room temperature, and even in the deep BEC regime, the transition temperatures are high.

[1] L. V. Keldysh and Y. V. Kopaev, Sov. Phys. Solid State **6**, 2219 (1965).
[2] Y. E. Lozovik and V. I. Yudson, JETP Lett **22**, 274 (1975).
[3] A. Perali, D. Neilson, and A. R. Hamilton, Phys. Rev. Lett. **110**, 146803 (2013).
[4] G. W. Burg, N. Prasad, K. Kim, T. Taniguchi, K. Watanabe, A. H. MacDonald, L. F. Register, and E. Tutuc, Phys. Rev. Lett. **120**, 177702 (2018).
[5] J. M. Kosterlitz and D. J. Thouless, J. Phys. C: Solid State **6**, 1181 (1973).