Correlations in low-dimensional electronic systems

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Theory of electron-pair correlations.

We have developed very accurate scattering and Fermi-hypernetted-chain methods for the calculation of spin-resolved pair distribution functions in the homogeneous electron gas (EG). These methods provide precise knowledge of the ground-state energy and are thus extremely powerful for a quantitative prediction of the phase diagram and quantum critical points.

We have recently predicted the paramagnetic-to-ferromagnetic (Bloch) quantum phase transition in a two-dimensional (2D) EG to occur at a value of the Wigner-Seitz density parameter r_s of about 25, in close agreement with state-of-the-art Quantum Monte Carlo simulation results (see Fig. 1).

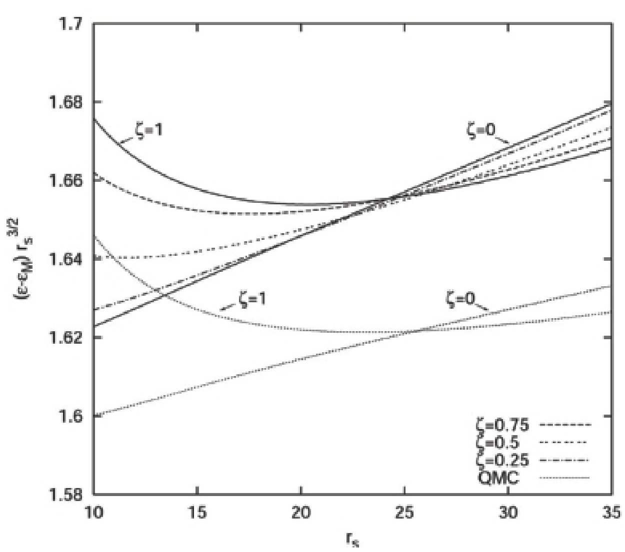
Microscopic many-body calculations of Landau Fermi-liquid parameters

Landau's theory of normal Fermi liquids is a physically appealing method designed to deal with the intermediate density regime of an EG where perturbation theory cannot be applied. The basic idea of Landau's theory is that the low-lying excitations of a system of interacting Fermions with repulsive interactions can be constructed starting from the low-lying states of a noninteracting Fermi gas by adiabatically switching-on the interaction between particles. This procedure allows one to establish a one-to-one correspondence between the eigenstates of the ideal system and the approximate eigenstates of the interacting one. Landau called such single-particle excitations of an interacting Fermi liquid "quasiparticles" (QP's). One of the implications of Landau's theory is that the QP mass m* is renormalized by electron-electron interactions. In essence, the moving QP tends to drag part of the electronic medium along with it producing an extra current. The QP effective mass is a measurable quantity. The most direct way to determine m* would be a measurement of the low-temperature heat capacity $C_V(T)$. It is in fact remarkable that electron-electron interaction effects enter $C_V(T)$ only through m*. These experiments are challenging and have not yet been realized with high precision. An alternative tool to access experimentally the QP effective mass is to analyze quantum Shubnikov-de Haas oscillations of the magnetoresistance.

Motivated by a large number of recent magnetotransport studies (see Ref. [3] and references therein) we have recently revisited [4] the problem of the microscopic calculation of the many-body effective mass enhancement in a paramagnetic 2D EG.

Our systematic study is based on a generalized "GW" approximation which makes use of the many-body local fields and takes advantage of the results of the most recent Quantum Monte Carlo calculations of the static charge- and spin-response of the 2D EG. We have reported extensive calculations for the many-body effective mass enhancement m*/m over a broad range of electron densities (see Fig. 2).

Fig. 1
Magnetic phase diagram of the 2D EG. The ground-state energy of the 2D EG (in Rydbergs, referred to the Madelung energy $e_M = -2.2122/r_s$ and multiplied by $r_s^{3/2}$) is shown as a function of r_s for states of different spin-polarization z [1]. The full lines show the theoretical results for the paramagnetic state and the ferromagnetic state, while the dots report Quantum Monte Carlo (QMC) data from Attaccalite et al. [2].



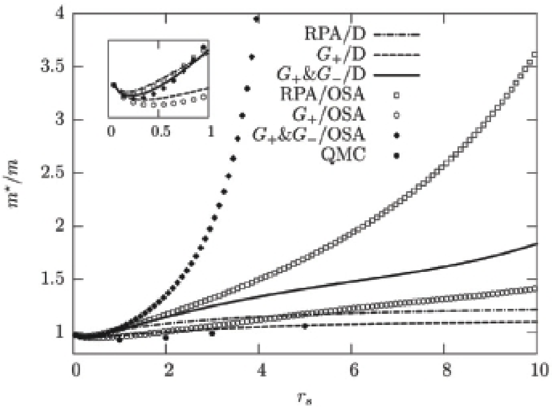


Fig. 2

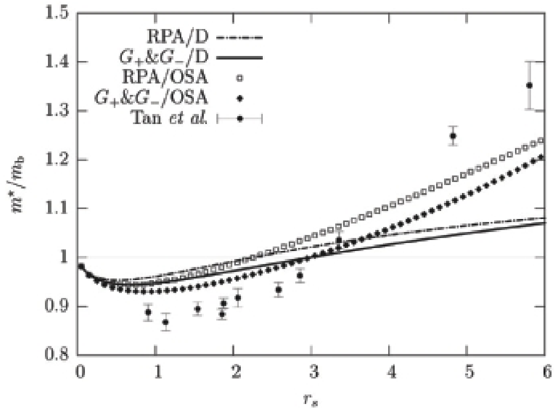


Fig. 3

Fig. 2
Effective mass enhancement in the 2D EG as a function of r_s for 0 £ r_s £ 10. The inset shows an enlargement of the results for r_s £ 1. The lines show the results from the Dyson scheme, while the symbols (except for the dots) are from the OSA. The QMC data (dots) are from Ref. [5]. The labels "RPA", "G_+" and "G_+&G_-" refer to three possible choices for short-range correlations.

Fig. 3
Effective mass enhancement for a 2D EG confined in a GaAs/AlGaAs triangular quantum well of the type used in Ref. [3]. The experimental results (Tan et al.) are from Ref. [3].

In this respect we have critically examined the relative merits of the on-shell approximation (OSA), applicable in weak-coupling situations, *versus* the actual self-consistent solution of the Dyson equation. We have proven that there must be a critical value of r_s for which the effective mass determined within the OSA diverges. A recent paper by Zhang and Das Sarma [6] infers from this fact a true divergence of the effective mass within the Random Phase Approximation. In our view, however, this must be considered an artifact of the OSA, as discussed in detail in Ref. [4]: thus the problem of the 2D metal-insulator transition has been re-opened. Finally we have also shown that our numerical results for a quasi-2D EG, free of any adjustable fitting parameters, are in good qualitative agreement with the recent measurements by Tan *et al.* [3] in a GaAs/AlGaAs heterojunction-insulated gate field-effect transistor of exceedingly high quality (see Fig. 3).

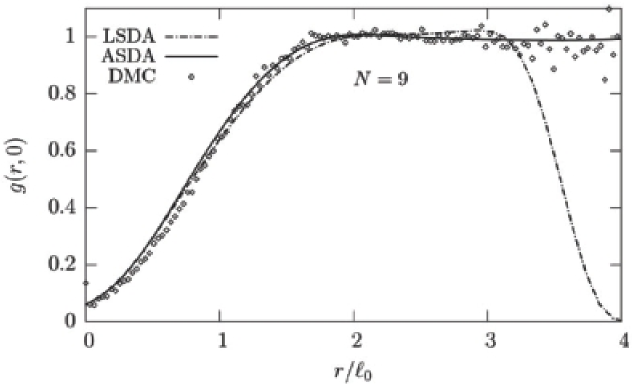
Ground-state densities and pair correlation functions in parabolic quantum dots

For a number of years there has been a growing interest in studying finite quantum systems under external confinement, such as ultracold atomic or molecular gases inside magnetic or optical traps [7] and electrons in quantum dots [8]. The confinement introduces a new length scale and induces novel physical behaviors relative to the corresponding infinitely extended model system. In particular, in a quantum dot the properties of a homogeneous electron gas are profoundly modified by the emergence of effects that are commonly associated with electrons in atoms. A well-known example is the presence of a shell structure in the energy to add electrons to a quantum dot [9].

With regard to the spatial structure of the electronic system, the analogue of 2D Wigner crystallization has been shown in a path-integral Monte Carlo study [10] to occur in two distinct stages inside a circularly symmetric parabolic quantum dot. Radial ordering of the electrons into shells occurs first and is followed by orientational ordering through freezing of intershell rotations. Short-range order in the electronic structure at lower coupling strength is described by the pair distribution function g(**r**,**r'**) giving the spin-averaged probability of finding two electrons at positions **r** and **r'**. Some properties of this function and of its extension to describe spin-resolved pair correlations have been reported for a circular quantum dot in a Diffusion Monte Carlo study by Pederiva *et al.* [11].

In Ref. [12] we have reported an extensive study of ground-state densities and pair distribution functions for electrons confined in 2D quantum dots over a broad range of coupling strength l and electron number N. We have used spin-density-functional theory [13] to determine spin densities that have been compared with Diffusion Monte Carlo data. This accurate knowledge of one-body properties has then been used to construct and test a local approximation for the electron-pair correlations. We have found very satisfactory agreement between this local scheme

Fig. 4
Spin-summed pair distribution function g(r,0) as a function of r/l_0 (l_0 is the harmonic oscillator length) for a partially spin-polarized quantum dot with N=9 electrons at coupling strength $\lambda = l_0/a_B = 1.89$ (a_B being the effective Bohr radius for GaAs). The results of the local spin-density approximation (LSDA) and of the average spin-density approximation (ASDA) [12] are compared with Diffusion Monte Carlo data [11].



and the available Diffusion Monte Carlo data (Fig. 4), thus providing a detailed picture of two-body correlations in a coupling-strength regime preceding the formation of Wigner-like electron ordering. Fig. 5 shows how with increasing coupling strength the system with N=6 electrons acquires the (1,5) structure consisting of one electron at the center of the trap and a surrounding ring of five electrons. Fig. 6 shows that, whereas the paramagnetic ground state at weak coupling does not possess radial structure, the ferromagnetic ground state at $\lambda = 10$ and 12 exhibits a main first-neighbor peak in g(r,0) followed by secondary structures.

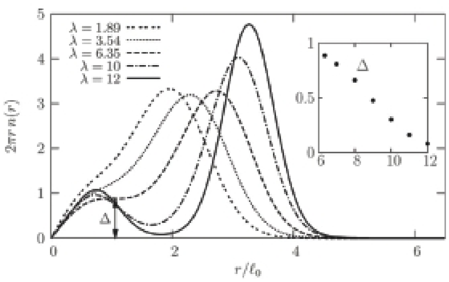


Fig. 5

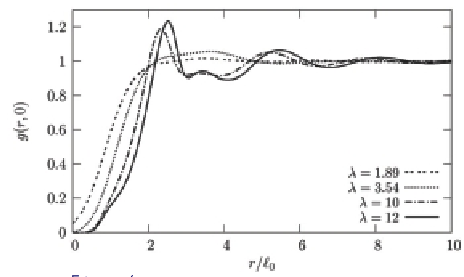


Fig. 6

Fig. 5
Probability density $2\pi r n(r)$ (in units of l_0^{-1}) as a function of r/l_0 for a quantum dot with N=6 electrons at varying λ. The profiles shown are for the ferromagnetic state which is the ground-state of the quantum dot for $\lambda \geq 6.35$. The inset shows the height Δ of the minimum (in units of l_0^{-1}) as a function of λ.

Fig. 6
Spin-summed pair distribution function g(r,0) as a function of r/l_0 for a quantum dot with N=6 electrons in its ground state at various λ. The curves for $\lambda = 1.89$ and 3.54 refer to the paramagnetic state, while those for $\lambda = 10$ and 12 refer to the ferromagnetic state.

References

[1] R. Asgari, B. Davoudi, and M.P. Tosi, Solid State Commun. 131, 301 (2004).
[2] C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G. Bachelet, Phys. Rev. Lett. 88, 256601 (2002).
[3] Y.-W. Tan, J. Zhu, H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. 94, 016405 (2005).
[4] R. Asgari, B. Davoudi, M. Polini, G. F. Giuliani, M. P. Tosi, and G. Vignale, Phys. Rev. B 71, 045323 (2005).
[5] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B 50, 1684 (1994).
[6] Y. Zhang and S. Das Sarma, Phys. Rev. B 71, 045322 (2005).
[7] See for instance C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, England, 2002); A. Minguzzi, S. Succi, F. Toschi, M. P. Tosi, and P. Vignolo, Phys. Rep. 395, 223 (2004).
[8] L. Jacak, P. Hawrylak, and A. Wójs, *Quantum Dots* (Springer, Berlin, 1998); T. Chakraborty, *Quantum Dots: A Survey of the Properties of Artificial Atoms* (North Holland, Amsterdam, 1999); L. P. Kouwenhoven, D. G. Austing, and S. Tarucha, Rep. Prog. Phys. 64, 701 (2001).
[9] S. M. Reimann and M. Manninen, Rev. Mod. Phys. 74, 1283 (2002).
[10] A. V. Filinov, M. Bonitz, and Yu. E. Lozovik, Phys. Rev. Lett. 86, 3851 (2001).
[11] F. Pederiva, C. J. Umrigar, and E. Lipparini, Phys. Rev. B 62, 8120 (2000); *ibid.* 68, 089901 (2003).
[12] M. Gattobigio, P. Capuzzi, M. Polini, R. Asgari, and M. P. Tosi, cond-mat/0501375.
[13] See for instance R. M. Dreizler and E. K. U. Gross, *Density Functional Theory, An Approach to the Quantum Many-Body Problem* (Springer, Berlin, 1990).