

L6: Mean-Field Methods and Density Functional Theory II

February 17, 2025

Density in Real space

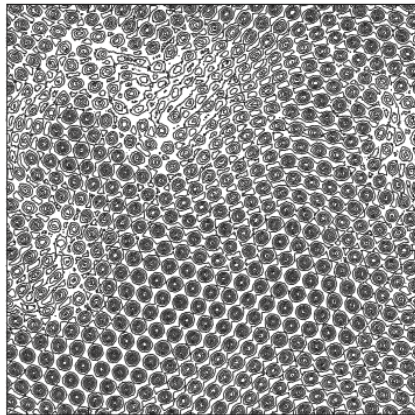


Figure 5.1. A contour plot of the spatial density in a realization of a 2D Wigner crystal as computed with path-integral Monte Carlo at a surface density of $3.2 \times 10^{12} \text{ cm}^{-2}$ ($r_s = 60$) and temperature 16 K (10^{-4} Ry). For the definition of the model, see Sec. 3.1. The disorder results from the initial conditions of the Monte Carlo random walk. The spatial boundary conditions frustrate the formation of a perfect crystal.

Momentum Distribution HEG

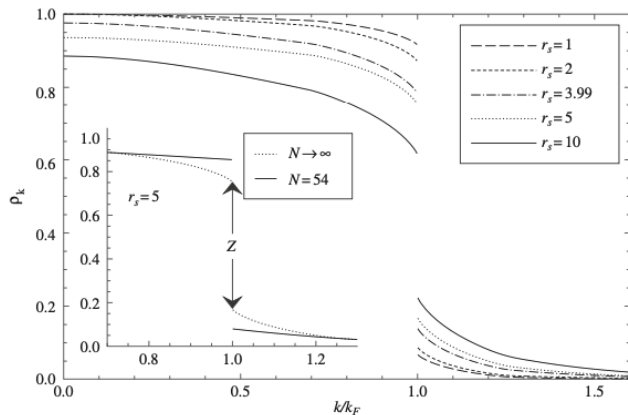


Figure 5.2. The momentum distribution of the unpolarized 3D homogeneous electron gas (Sec. 3.1) calculated in QMC for various densities r_s . The inset shows the extrapolation at $r_s = 5$ from a system of $N = 54$ electrons to the thermodynamic limit [231]. The jump at the Fermi surface Z , the quasi-particle strength, is the renormalization factor, see Sec. 7.5.

Momentum Distribution Na

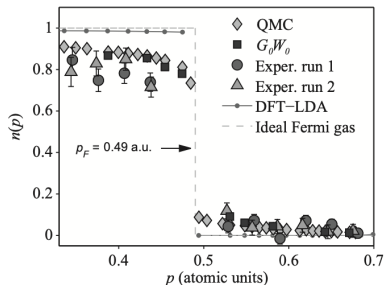


Figure 11.7. The momentum distribution function $\rho(\mathbf{k})$ of sodium (in the figure denoted $n(p)$). Shown are results of experiment, QMC with Slater–Jastrow wavefunctions, G_0W_0 , and LDA calculations. The step function is the free-electron gas result. (From [230].)

Pair Correlation Function HEG

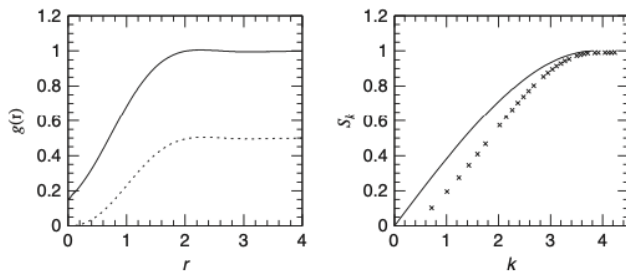


Figure 5.3. The pair correlation function (left panel) of the 3D homogeneous electron gas at $r_s = 2$. The upper curve is the total, the lower curve for parallel spins. The derivative at $r = 0$ is related to the cusp condition on the many-body wavefunction, see Sec. 6.1. The right panel shows the total spin-independent structure factor. The solid curve is for non-interacting electrons. Note that its value at $k = 0$ is $N/2$, as in Eq. (5.18).

Pair Correlation Function Wigner Crystal

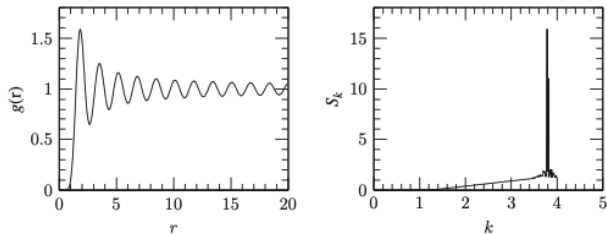


Figure 5.4. The pair correlation function (left panel) of a Wigner crystal in 2D at $r_s = 60$. The right panel shows the corresponding structure factor; the peak shows ordering at the first reciprocal lattice vector.

Analytic Structure of time correlation Functions

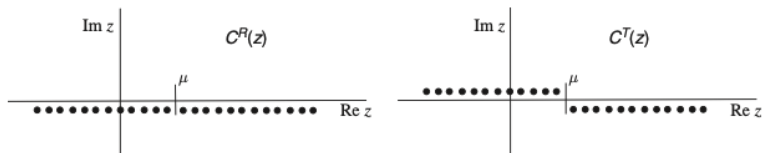


Figure 5.5. Analytic structure of correlation functions as a function of complex frequency z . As explained after Eq. (5.31), μ is the chemical potential for adding or removing one or more particles, and zero for an excitation with no change in particle number. Left: Poles for a retarded correlation function, such as a causal response function discussed in Sec. 5.5. The poles at frequencies z , corresponding for example to excitation energies of the N -electron system, are displaced into the lower half-plane by the infinitesimal $\text{Im } z = -\eta$. This form follows from the requirement of causality and it leads to the Kramers–Kronig relations, Eq. (5.53). Right: The structure of the time-ordered correlation function $C^T(z)$ at zero temperature in the complex plane, with two branch cuts (see Sec. C.5) on the real axis. For frequencies $\text{Re}(z) < \mu$, the poles are displaced into the upper plane by $+i\eta$. Hence, for example, when C is a one-particle Green’s function, $\text{Im } z = \eta > 0$ denotes energies for which particles can be removed. For addition of particles at real frequency $\text{Re } z > \mu$, the imaginary part $\text{Im } z = -\eta$.

Si Loss and Absorption Spectra

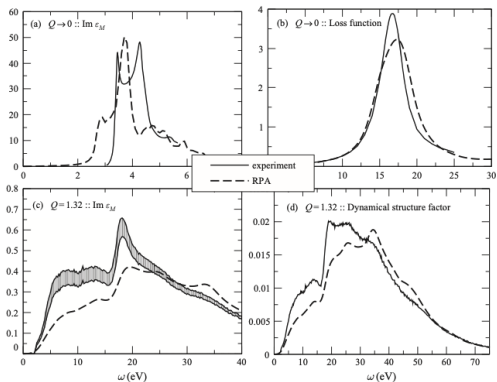


Figure 5.6. Electronic spectra of bulk silicon. Figure by Francesco Sottile, with data of the upper-right and the two lower panels taken from [242–244]. Left panels: $\text{Im } \epsilon_M(\omega)$ (corresponding to absorption when $Q \rightarrow 0$, where the experiment is from [245]). Upper right: Loss function in 1/eV. Lower right: Dynamic structure factor in 1/eV. Top panels are for vanishing momentum transfer, bottom panels for $|Q| = 1.32$ a.u. The result for $\epsilon_M(Q)$ at large Q has been obtained from the measured $\text{Im } \frac{1}{\epsilon_M}$ using the KK relation Eq. (5.53), which explains the error bar. $\text{Im } \epsilon_M$ and $-\text{Im } \frac{1}{\epsilon_M}$ are similar for large momentum transfer, but very different for small momentum transfer, where the long-range part of the Coulomb interaction plays an important role.