Electronic Properties of Warm Dense Matter studied using the Density Matrix Quantum Monte Carlo Method

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Although the behaviour of electrons in solids at room temperature has been studied for decades, much less is known about electrons in warm dense matter. Perturbative approaches are stymied by the lack of a small expansion parameter; computational approaches have been relatively little explored; and it is difficult to obtain accurate experimental data for comparison. Most quantum mechanical simulations of warm dense matter use thermal density functional theory (DFT), but whether this is as miraculously successful as ground-state DFT remains uncertain. Until very recently, we did not even have an accurate knowledge of the finite-temperature equivalent of the local density approximation.

Over the past few years, we have been developing and using a variety of new quantum Monte Carlo (QMC) methods (density matrix QMC at Imperial College [1, 2]; configuration and permutation blocking path-integral QMC at Kiel [3, 4, 5]) to investigate warm dense matter from first principles. This has allowed us to map the phase diagram of the warm dense electron gas and construct the first accurate parametrization of the temperature- and density-dependent exchange-correlation free energy in the local density approximation [6, 7]. We are now beginning to apply density matrix QMC to real solids, hoping to provide accurate benchmarks for thermal DFT.

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