Quantum chemistry with Clifford and Green

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In this talk I will present the latest results of two ongoing projects.

First, I will discuss an original approach to study periodic Coulomb systems. The main idea is to isolate a supercell, containing several unit cells, from the periodic structure and modify its topology to that of a Clifford Torus. While an ordinary torus is curved, a Clifford torus is flat. Therefore the supercell can be represented on it without deformation. Like an ordinary torus, a Clifford torus has no boundaries which makes the extrapolation of the results to the thermodynamic limit smooth. I will show how we have successfully applied our strategy to the calculation of Madelung constants and Wigner crystals [1] [2] [3]

Second, I will discuss an approach based on many-body Green's functions that uses a multi-channel Dyson equation that couples different many-body Green's functions. I will mainly focus on the multi-channel Dyson equation that couples the one-body Green's function to the three-body Green's function to model photoemission spectral functions. Unlike the standard (single-channel) Dyson equation the multi-channel Dyson equation puts quasi-particle and satellite excitations on an equal footing. I will show how this can lead to an improved description of spectral functions [4].

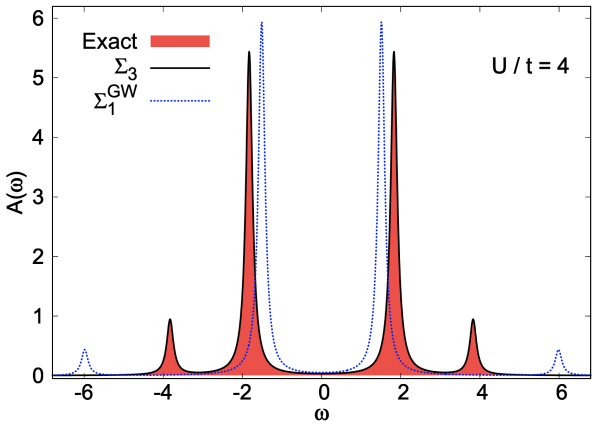

Figure 1. Spectral function of the Hubbard dimer with 2 electrons. Exact result (red filled); the multichannel Dyson equation (black solid line); GW (blue dotted line).

Keywords: periodic systems, Clifford torus, Green function.

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