Numerical Methods as Exploration Tools for Theoretical Condensed Matter Physics

Siew-Ann CHEONG
Division of Physics and Applied Physics
School of Physical and Mathematical Sciences
Nanyang Technological University

Abstract

It was no accident that out of the five papers I published with Chris as I worked towards my PhD, three reported analytical results. I think this is how Chris likes to think about problems in theoretical condensed matter physics: using various methods to open windows of insight into such problems. Numerical methods were no exception: numerical outputs generated by simple codes would lead me in unexpected ways to exact solutions and scaling relations. In this talk, I would share these three journeys that shaped how I now think as a physicist. First, I would describe a numerical procedure for calculating the many-body fermion density matrix to a block of sites within an infinite chain, in terms of the ground-state expectations of products of projection operators. I then show regularities that appear in the numerical results, when these ground-state expectations are computed in the one-dimensional Fermi sea. Adapting an analytical method in a paper [1] that appeared a few years before we obtained the numerical results, we then worked out an exact formula for the many-body fermion density matrix [2]. This exact formula allowed us to write the eigenvalues of the density matrix in terms of exponentials of pseudo-energies of a non-interacting system of fermions, and thus allowed us to compute the eigenvalues for very large block sizes. Again, numerical regularities appeared when we plot the spectra of different block sizes, which led us to suspect, and thereafter work out a scaling relation for the pseudo-energies [3]. Finally, I would talk about the numerical methods to compute the many-body fermion density matrix of two distant blocks in an infinite chain [4]. To demonstrate the utility of such a density matrix, we worked with the exactly diagonalized ground states of fermion chains with infinite nearest-neighbor repulsion. Again, we discovered numerical regularities in the many-body ground-state wave function. Chris immediately realized that the $P$-particle ground state of a chain of length $L$ with infinite nearest-neighbor repulsion can be mapped to the $P$-particle ground state of a chain of length $L' = L - P$ with zero nearest-neighbor repulsion. I very quickly verified that this mapping is exact, and moved on to write the ground-state expectation of nonlocal operator products (like the two-point function) on the chain with infinite nearest-neighbor repulsion as an intervening particle expansion of ground-state expectations of a series of nonlocal operator products that can be explicitly constructed on the chain with zero nearest-neighbor repulsion [5]. If time permits, I would describe how we used this exact mapping to investigate finite-size effects resulting from different boundary conditions [6].

References


