Hubbard-like models with more than two species

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1 Hubbard model for electrons or two cold atom species

The standard Hubbard model for spin up and down fermions is given by:

$$H \; = -t \sum_{\langle i,j \rangle} (a^\dagger_\uparrow(j) a_\uparrow(i) \; + \; a^\dagger_\downarrow(j) a_\downarrow(i)) \; + \; U \; \sum_i a^\dagger_\uparrow(i) a_\uparrow(i) a^\dagger_\downarrow(i) a_\downarrow(i), \qquad (1)$$

where $\langle i, j \rangle$ are nearest-neighbor sites on the lattice, and t is the kinetic term and U is the on-site interaction. This can be shortened to

$$H \; = -t \sum_{\langle i,j \rangle, \sigma} a^\dagger_\sigma(j) a_\sigma(i)) \; + \; U \sum_{i, \sigma <> \sigma'} a^\dagger_\sigma(i) a^(_\sigma i) a'^\dagger_\sigma(i) a'_\sigma(i), \qquad (2)$$

where the sum over σ is over all the spins (here and up and down) of the fermions and the on-site interaction involves two different spins σ and σ' (for fermions there are no on-site interactions possible for the same spin).

This model in 2D away from half-filling is often used to try to simulate high T_c. In this case U is typically large and repulsive, with $U/t \approx 10$. It can also be used to study dilute Fermi gases (particularly near unitarity in 3D), in this case the interaction strength is tunable in both theory and experiment. A particular choice of attractive $U/t < 0$ gives unitarity, essentially a zero-energy bound state in the two-particle system (1 up and 1 down). Many calculations of the unitary Fermi gas have been performed both in the continuum and using this lattice model.[2] To reliably mimic cold atom systems the simulation must be run in the dilute limit, many fewer particles than lattice sites.

The same model can be used to simulate pure neutron matter at very low density, similar to what should exist in the inner crust of the neutron star.[4, 5] The attractive Hubbard model has no sign problem for any filling, but the superfluid correlations are very strong. At zero temperature there is a smooth transition from BCS (weak pairing) to BEC (bound dimers of up and down particles).

2 More Species

In both cold atom physics and particularly in nuclear physics, it may be useful to generalize this fermion model to more than two species. For example it may be possible to mimic atomic nuclei using such a model. This is the lowest-order term in 'pionless effective field theory', often used to study models of nuclei, particularly light ones.

In this case the Hamiltonian is:

$$H_m^0 \;= -t \sum_{\langle i,j\rangle,\sigma} a_\sigma^\dagger(j) a_\sigma(i) \;+\; \sum_{i,\sigma<\sigma'} U_{\sigma,\sigma'}\; a_\sigma^\dagger(i) a_\sigma(i) a_{\sigma'}^\dagger(i) a_{\sigma'}(i). \qquad (3)$$

For nuclei the sum over spins runs over four types ($\uparrow$ *neutron*, $\downarrow$ *neutron*, $\uparrow$ *proton*, $\downarrow$ *proton*). Each spin has a kinetic term as for the two-component species, and each pair of species can interact if two different species of particle are on the same lattice site. In principle each pair of species can have a different interaction strength that labeled $U_{\sigma,\sigma'}$. People have discussed and sometimes even measured these types of systems in cold atom experiments.

For sufficiently attractive two body interactions the Hamiltonian H_m in the continuum is not bounded from below. The attraction of three particles on a site can overwhelm the two-body physics and produce an extremely strongly-bound three-particle cluster. To avoid this in effective field theory one uses a three-body repulsive term, again in principle it can depend upon the labels of the three particles of species involved. The full Hamiltonian is then:

$$H_m \;=\; H_m^0 + \sum_{i,\sigma<\sigma'<\sigma''} V_{\sigma,\sigma',\sigma''}\; a_\sigma^\dagger(i) a_\sigma(i) a_{\sigma'}^\dagger(i) a_{\sigma'}(i) a_{\sigma''}^\dagger(i) a_{\sigma''}(i). \qquad (4)$$

For sufficiently repulsive three-particle terms V the continuum Hamiltonian is bounded from below. The ground-state of N fermions with an infinite number of species problem is the same as the ground state of the many-boson problem with the same Hamiltonian. If we tune the three-body problem to a weakly bound trimer by adjusting the two-body problem to a zero-energy bound state and then adjusting V to get a weakly bound three-body system, many properties of the system can be solved for different particle number.[1] These properties are universal in the sense they do not depend upon details of the two-body interaction if we are in the dilute limit. Unitary bosons have been studied experimentally in cold atom experiments.

For bosons the energy simply decreases monotonically with the number of particles for the case where the trimers are weakly bound. Hence N-body ground-state clusters are always bound states (they do not separate into smaller clusters). For many particles the system saturates and there is an equilibrium density at zero temperature. One can then study two- and three-particle contacts (the probability of two- or three- particles being at one site), the condensate fraction, the scaled energy (energy per particle in an N-particle cluster compared to energy per particle in the three-body bound state), etc.

For three- or four species this may well not happen. It is not clear that an eight particle system with four species will not be higher in energy than two isolated four-particle systems. Variational calculations find that 4 4-particle clusters (alpha particles) are lower in energy than a 16 nucleon system with 8 neutrons and 8 protons.[3] This is definitely what happens for two-species, two dimers interact with a repulsive interation. The phase diagram of these systems at zero (and finite) temperature is quite interesting. At low enough densities they may well isolate into clusters where the number of particles per clusters is equal to the number of species. This will produce a cloud of composite fermions (3-species) or bosons (4-species). As the density is increased the clusters will overlap and a ground-state with interesting properties should emerge. Some kind of superfluidity is likely, either a simple two-species pairing or some kind of more exotic superfulidity. We are trying to investigate these systems now using Quantum Monte Carlo. They all have sign problems, so some kind of approximation (variational, fixed node, etc.) is required.

There is also a lot of interesting dynamics on all these systems, some of which has already been studied experimentally.

References

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