Unitary Correlation Operator Method for ^{4}He Droplets

R. Roth, H. Feldmeier, T. Neff (GSI)

The Unitary Correlation Operator Method (UCOM) [1] provides a new concept for the treatment of short–range correlations which are induced by the strong short–range repulsion of particle–particle–interactions. This type of correlations plays a major role in several many–body systems, e.g., molecules, atomic clusters and liquids, nuclei and nuclear matter.

The basic idea of UCOM is to treat the correlations by a unitary operator C which shifts two particles in the uncorrelated state $|\psi\rangle$ away from each other whenever they are so close together that they feel the strong repulsion of the core. In this way short–range repulsive correlations are included in the correlated state $|\widetilde{\psi}\rangle = C \, |\psi\rangle$. The explicit form of C is obtained by the requirement that the exact correlated two–body wave function equals the uncorrelated one at short distances. This is achieved by a transformation of the radial coordinate $\widetilde{r} = R_-(r)$. $R_-(r)$ and it's inverse $R_+(r)$ are called correlation functions.

Equivalently one can use the correlation operator C to define correlated operators, e.g., the correlated Hamiltonian $\widetilde{H} = C^\dagger \, H \, C$. They contain, however, many–body operators up to rank N, the total particle number of the system. For a Hamiltonian composed of the kinetic energy T and a two–body potential V one gets

$$\widetilde{H} = C^\dagger T C + C^\dagger V C = T + \widetilde{H}^{[2]} + \widetilde{H}^{[3]} + \cdots + \widetilde{H}^{[N]}.$$

$\widetilde{H}^{[2]}$, for example, is the two–body part of the correlated kinetic energy plus that of the correlated potential. Low order approximations of this expansion are expected to be good if the range of the correlations is small compared to the distance between the particles. In this case the probality is small that more than two particles are at the same time within the range of the short–range correlations and the neglect of three–body and higher operators is a successful approximation. It has been shown in ref. [1] that the two–body approximation works very well for nuclear few–body systems with simple central NN–potentials.

The situation is not so favorable in the case of ^{4}He droplets. Here the core radius $\sigma = 2.556\,\text{Å}$ of the Lennard–Jones–potential $V_{LJ}(r) = 4\,\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ ($\epsilon = 10.22\,\text{K}$) is not much smaller than the distance $d \approx 3.6\,\text{Å}$ between the particles (in liquid ^{4}He). One therefore expects three–body and higher terms not to be negligible. All expressions up to two–body order are known analytically [1], beyond this one has to implement further approximations. To study the possibility to describe the higher order contributions with density–dependent correlation functions we look at small clusters of bosonic ^{4}He atoms with $N = 3, \cdots, 10$ for which 'exact' many–body calculations are available [2].

First of all we look at the binding energy of ^{4}He droplets in a variational scheme. Since in the ground state (Bose–Einstein–condensate) all particles are in the same quantum state the N–body trial state is assumed to be the N–fold product of a Gaussian single–particle state with a variable width which is varied to minimize the energy. The correlation function is parametrized by

$$R_+(r) = r + \alpha\xi \, \left(\frac{r}{\beta\xi}\right)^\eta \exp[-\exp(r/\beta\xi)].$$

The calculation of the energy in two–body approximation ($\rightarrow$ diamonds) for correlator parameters α, β, η that map a two–body trial onto the exact $E = 0$ solution ($\xi = 1$) shows agreement up tp $N = 5$ but an increasing overbinding for higher particle numbers, when compared to 'exact' calculations [2] ($\rightarrow$ open gray squares). This indicates that contributions beyond two–body order are relevant. To cure this overbinding one may in a first step try to reduce the strength of the correlator using the scale factor ξ. A value of $\xi = 0.957$, which is only 4.3% below the value for the two–body case, has to be chosen in order to match the energy of the $N = 10$ droplet ($\rightarrow$ black triangles). This leads to an underbinding for lower particle numbers, the $N = 3$ droplet is not bound at all.

These results show, that it is not possible to describe the energies for all particle numbers with one fixed state–independent correlator in two–body approximation. To get an effective description of higher order contributions in two–body approximation we implement a *state–dependent* correlator by introducing a global linear density–dependence into the scaling parameter $\xi(\rho) = 1 - \gamma\rho$. For low densities the optimal two–body correlator derived from the two–body system should be suitable and for high densities a reduction of the correlator strength is expected. The slope γ of the density–dependence is again fixed by the energy of the $N = 10$ system. The energies for this density–dependent correlator ($\rightarrow$ black squares) are in very good agreement with reference [2] for all particle numbers under consideration.

Apparently it is possible to include the effects of higher order contributions by an effective density–dependent correlator in two–body approximation. Up to now the density–dependence is fixed in a phenomenological way, but it may be possible to derive it from the known properties of the higher order contributions. Thus we could go beyond the two–body approximation without loosing practicability.

[1] H. Feldmeier, T. Neff, R. Roth, J. Schnack; Nucl. Phys. A 632 (1998) 61
[2] E.W. Schmid, J. Schwager, et al.; Physica 31 (1965) 1143