

New developments in the transcorrelated method for multicomponent quantum gases

Chris Bradly^a, Matija Čufar^a and Joachim Brand^a

^a*Dodd-Walls Centre for Photonics and Quantum Technology,*

New Zealand Institute of Advanced Studies and Centre for Theoretical Chemistry and Physics,

Massey University, Auckland 0632, New Zealand

Effective treatment of particle correlation is one of the most important aspects of quantum many-body methods. One approach is to define a Jastrow ansatz that factors the wavefunction into a regular part and a singular part that contains the correlation information. The transcorrelated method takes this one step further and incorporates the correlation factor into a similarity transformation of the Hamiltonian that acts on a regular wavefunction. The transformed Hamiltonian is generally non-Hermitian but the smoothness of the wavefunction is improved. This is beneficial for numerical techniques where convergence in a finite basis is faster compared to bare or renormalised lattice methods. The transcorrelated method has long been used for electron systems and was recently applied to the strongly-interacting Fermi gas in one and three dimensions [1, 2].

We report new results in which we extend the transcorrelated method to a general system of multiple components with arbitrary masses to form a broader framework for studying cold atom physics. We discuss applications of our methods to few atom systems that are achievable in experimental setups with optical tweezer dipole traps, as well as further applications to liquid droplets and heavy impurities in quantum gases. In particular we use the transcorrelated method together with the full configuration interaction quantum Monte Carlo (FCIQMC) algorithm [3].

[1] P. Jeszenszki, H. Luo, A. Alavi, and J. Brand, *Phys. Rev. A* **98**, 053627 (2018).

[2] P. Jeszenszki, U. Ebling, H. Luo, A. Alavi, and J. Brand, *Phys. Rev. Research* **2**, 043270 (2020).

[3] Rimu.jl, <https://github.com/joachimbrand/Rimu.jl>