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A DQMC study of cohesion energy of small Li clusters based on an RVB nodal structure[1] DANIEL NISSENBAUM, Northeastern University, LEONARDO SPANU, UC Davis and SISSA, Italy, CLAUDIO ATTACCALITE, SISSA, Italy, BERNARDO BARBIELLINI, ARUN BANSIL, Northeastern University — We have carried out a diffusion Quantum Monte Carlo study (DQMC) of the cohesion energy of small (2, 4, and 8 atom) Li clusters based on Resonating Valence Bond (RVB) wavefunctions, and compared the results to the corresponding values obtained via wavefunctions utilizing a typical Hartree-Fock (HF) nodal structure (Jastrow-Slater wavefunctions). The RVB wavefunction allows more flexibility in the nodal structure than the HF wavefunction, and yields some improvement in the cohesion energy of Li_2, with comparable gain for the larger clusters. Interestingly, the variance of the local energy for the variationally optimized (VQMC) RVB wavefunction is found to be significantly smaller than for the VQMC-optimized Jastrow-Slater wavefunction, resulting in faster convergence of the DQMC calculations. This would make the RVB wavefunction a promising candidate for investigating larger and more complicated clusters.

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