Monte Carlo hyperspherical description of cluster excited states

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Though a variety of approaches can be used to calculate ground state properties, widely applicable methods for the calculation of excited state energies and wave functions of many-body systems are still lacking. For example, Monte Carlo (MC) methods such as the variational Monte Carlo (VMC) method, the diffusion quantum Monte Carlo (DMC) method, and the Green's function Monte Carlo (GFMC) method show a favorable scaling of the computational effort with the number of particles when used to calculate ground state properties, but they cannot readily be extended to calculate excited state properties. This talk outlines a new approach to treating excited states of many-body systems by combining MC methods with the adiabatic hyperspherical description. Application of this new approach to helium clusters, and also heavier rare gas clusters, will be presented.

Bosonic helium systems — i.e. liquid bulk ^{4}He, two-dimensional ^{4}He films, and finite size ^{4}He$_N$ clusters — have been studied extensively. ^{4}He$_N$ clusters, which are investigated here, offer a wealth of interesting physics by virtue of its weak van der Waals attraction, and its light atomic mass. Numerous theoretical calculations have determined the existence, size, and energetics of small ^{4}He$_N$ clusters in their ground state. However, only comparatively few predictions — mostly for the ^{4}He trimer and tetramer, and for larger clusters with $N = 20$ or more atoms — for excited state behavior exist. Here, we report on excited state calculations for ^{4}He$_N$ clusters with up to $N = 10$ atoms, which thus narrow the gap between small cluster and "large cluster" treatments. Our MC calculations predict the number of $J = 0$ (rotationless angular momentum) bound states for ^{4}He$_N$ clusters, and also the ^{4}He + ^{4}He$_{N-1}$ elastic scattering lengths.

The $J = 0$ many-body Schrödinger equation for the nuclear coordinates is solved numerically by combining Monte Carlo methods with the adiabatic hyperspherical approximation. Adopting the adiabatic approximation is motivated by the following two main arguments. First, the separation into one radial coordinate, the hyperradius R, and $(3N - 1)$ angular coordinates, collectively denoted by Ω, results in an effective one-dimensional potential curve $U(R)$, which in turn allows the approximate calculation of excited states. Second, the effective one-dimensional curve allows us to use our intuition to interpret the size of the system, as well as showing the regions where transitions occur between one geometrical configuration and another. As an example, Fig. 1 shows the lowest adiabatic potential curves $U(R)$ for ^{4}He$_N$ clusters with $N = 3 - 10$, together with the lowest radial wave functions, and the ground state energies. Excited state energies can be readily calculated by solving the one-dimensional Schrödinger equation in the R coordinate for a collective particle with effective mass that feels the interaction potential $U(R)$.

The characteristics of weakly bound helium clusters are compared with those for spin-polarized tritium clusters, in the following denoted by $(T\uparrow)_N$. It turns out that spin-
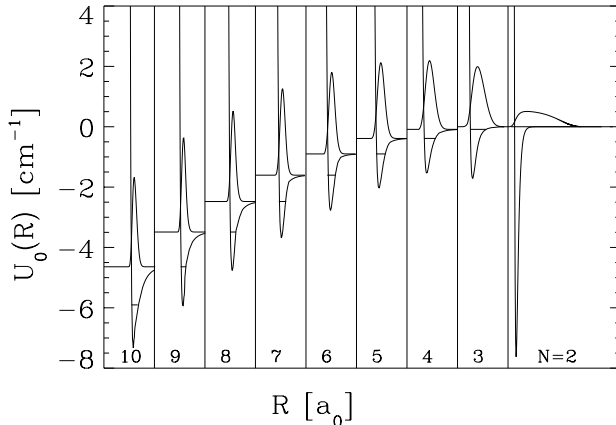
Figure 1: Effective potential curves $U_0(R)$, wave functions $F_{00}^{BO}(R)$, and ground state energies E_0 for He_N clusters with $N = 3$ through 10 together with the two-body He-He potential, the exact dimer ground state wave function, and the He dimer ground state energy. The hyperspherical radius R (R is identical to the interparticle distance r_{12} for the He dimer) has a logarithmic scale; for the $N = 3$ through 10 plots, $R \in [3\ a_0, 150\ a_0]$, while for the $N = 2$ plot, $R \in [3\ a_0, 1200\ a_0]$. Note that $U_0(R)$ of the cluster with N atoms approaches the ground state energy E_0 of the next smaller cluster with $N - 1$ atoms for large R ($1a_0 = 0.529\text{Å}$). This figure is taken from Ref. [1].

polarized tritium clusters are even more weakly bound than helium clusters. Of particular interest is furthermore the lowest quartet state of the tritium trimer, which we predict to be a Borromean or halo state. We also predict a Feshbach resonance for two high-field seeking $|F, m_F\rangle = |0, 0\rangle$ tritium atoms (F denotes the total angular momentum, and m_F the magnetic quantum number of this state), which could lead to unexpected physics when manipulating $(T\uparrow)_N$ cluster formation through an external magnetic field.

To illustrate the highly quantum (sometimes referred to as "liquid-like") behavior of ^4He_N clusters further, we contrast the behavior of ^4He_N clusters to that of heavier rare gas clusters, i.e., bosonic neon and argon clusters. These heavier rare gas clusters exhibit a manifold of geometrically and energetically distinct isomers, each of which shows non-negligible zero point energy. These isomers can be identified in the adiabatic hyperspherical potential curves. Comparison with adiabatic potential curves for ^4He_N clusters underlines the unique behavior of helium clusters.

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References: [1] D. Blume and C. H. Greene, J. Chem. Phys. **112**, 8053 (2000)