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Mott-Hubbard Type Transition and Thermodynamic Properties in Nanoscale Clusters ARMEN KOCHARIAN, California State University, Northridge, CA 91330-8268, GAYANATH FERNANDO, University of Connecticut, Storrs CT 06269, JAMES DAVENPORT, Brookhaven National Laboratory, Upton NY 11973 — Thermodynamic and magnetic properties of clusters of various geometries, sizes, etc. are calculated using exact diagonalization and quantum Monte Carlo simulations. Studies of electron correlations in clusters, with respect to the interaction strength U, number of electrons n, temperature T and magnetic field h are fundamental for understanding the nature of ferromagnetism. Small clusters contain also important technical features necessary for monitoring the Mott-Hubbard (MH) transition in thermodynamic systems in higher dimensions. Grand canonical ensemble approach for the two site Hubbard cluster gives insight into the nature of MH transition at half filling ($n = 1$) with respect to variations of U, h and T. At $n = 1$ the developed "pseudo gap" at infinitesimal temperature decreases with increasing T. This pseudo gap in the spectrum disappears at characteristic T_c similar to MH critical temperature. A four peak structure in the density of states at finite U indicates the existence of a pseudo gap at $n = 1$, quarter $n = 1/2$ and three $n = 3/2$ fillings at relatively low T. The differences between the spin and charge energy gaps for finite clusters are also analyzed. A comparison of the exact results for the two atomic cluster with those calculated from quantum Monte Carlo shows reasonable agreement in a wide range of T and h.

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