The properities of a charge density wave phase in the anharmonic Holstein-Hubbard model : A variational approach.

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The Holstein-Hubbard model with anharmonic phonons is treated within a variational canonical transformation framework. The non-perturbative nature of this method allows a reliable inclusion of the effects of anharmonicity. An effective electron Hamiltonian is derived, in which importantly the anharmonicity produces relatively large correlated hopping terms. The half-filled $n = 1$ case is studied, in which the ground state is a charge density wave phase. The ground state order parameter and critical temperature dependence on the anharmonicity parameter α is calculated. A reasonable agreement with earlier Quantum Monte Carlo method results is shown.

9.7 cm

13.4 cm

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