QUANTUM FLUCTUATIONS OF CDW IN THE HOLSTEIN MODEL: A VARIATIONAL RESCALING APPROACH

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The usual mean-field treatment of the Peierls instability leading to Charge Density Wave (CDW) formation relies on the adiabatic approximation. This amounts to neglect the kinetic energy of the ions and is strictly valid in the limit of zero phonon frequency. Quantum fluctuations are known to destabilize the CDW ground state for large enough frequencies (see Refs 1-4 and contributions by S. Aubry , P. Quémerais and C. Bourbonnais, this issue). Up to now no satisfying treatment exists which spans the full range of electron-phonon coupling and phonon frequency.

We present here a variational calculation for the simplest one-dimensional electron-phonon problem, the molecular crystal (or Holstein model)[5]. The method interpolates between the adiabatic and the anti-adiabatic (phonon frequency much larger than the bandwidth) limits. In addition we show that the phonon frequencies are renormalized in the intermediate coupling regime. The results are successfully compared to the Monte-Carlo simulations of Hirsch and Fradkin[1] for the half-filled band case.

The basic Hamiltonian of the model is

$$H = \sum_i h\omega_0 \left(a_i^+ a_i + \frac{1}{2}\right) + g \sum_{i\sigma} c_{i\sigma}^+ c_{i\sigma} \left(a_i^+ + a_i\right) - T \sum_{\langle ij\rangle \sigma} c_{i\sigma}^+ c_{j\sigma} \tag{1}$$

where a_i^+, a_i and c_i^+, c_i are creation and annihilation for, respectively, dispersionless phonons and electrons of spin σ. Omitting the spin degree of freedom yields a particular model of "spinless fermions". Defining $k = 2g / (T\hbar\omega_0)^{1/2}$ and $\gamma = \hbar\omega_0 / T$ as the parameters of the model, one can write a reduced Hamiltonian $\hat{H} = H / 2T$ as

$$\hat{H} = \frac{1}{2} \sum_i \left(u_i^2 + \frac{\gamma^2}{4} p_i^2\right) + \frac{k}{2} \sum_i n_i u_i - \frac{1}{2} \sum_{\langle ij\rangle \sigma} c_{i\sigma}^+ c_{j\sigma} \tag{2}$$

where $n_i = \sum c_{i\sigma}^+ c_{i\sigma}$ is the charge density at site i. k is related to the usual electron-phonon coupling constant l by $k^2 = 4\lambda$. The scaled coordinates and momenta are defined as

$$u_i = \frac{\sqrt{\gamma}}{2} (a_i + a_i^+) \quad ; \quad p_i = \frac{i}{\sqrt{\gamma}} (a_i^+ - a_i) \tag{3}$$

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In the adiabatic limit ($\gamma = 0$) (2) yields the adiabatic Hamiltonian H_{ad} (see Ref. 4 for more details)

$$H_{ad} = \frac{1}{2}\sum_i u_i^2 + \frac{k}{2}\sum_i n_i u_i - \frac{1}{2}\sum_{\langle ij\rangle\sigma} c^+_{i\sigma} c_{j\sigma} \tag{4}$$

where the u_i 's represent the classical (periodic) Peierls deformation. The equilibrium deformation u_i^{ad} (k) is obtained after minimizing the electronic ground state energy of (4) (Ref. 4). We successively perform on (2) three canonical transformations U_1, U_2, U_3 yielding the Hamiltonian $\tilde{H} = U_3U_2U_1HU_1^{-1}U_2^{-1}U_3^{-1}$ and obtain an effective electronic Hamiltonian after averaging in the phonon vacuum $|0\rangle_{ph}$. U_1, U_2, U_3 are given by

$$U_1 = e^{i\sum_i p_i u'_i} \quad ; \quad U_2 = e^{-i\frac{k}{2}\delta\sum_i p_i n_i} \quad ; \quad U_3 = e^{r\sum_i (a_i a_i + a_i^+ a_i^+)} \tag{5}$$

U_1 displaces the lattice coordinates by u'_i (adiabatic limit). U_2 is a modified small polaron transformation which solves exactly the problem for infinite γ (anti-adiabatic limit), provided one takes $\delta = 1$. It correlates to an amount proportional to δ the lattice fluctuations to the charge fluctuations. Finally U_3 is a two-phonon "squeeze" transformation, equivalent to a phonon softening. It increases the fluctuations of the u_i's (due to the electron band motion) and decreases the fluctuations of the p_i's (see Ref.6 for more details). Taking for sake of simplicity the spinless case, the resulting effective Hamiltonian is $H_{eff} = {}_{ph}\langle 0|\tilde{H}|0\rangle_{ph}$

$$\begin{aligned} H_{eff} = N\left[\frac{\gamma}{2}\cosh 4r - \frac{k^2}{8}(2\delta - \delta^2)\, n_0\right] & \\ + \rho\left[\frac{1}{2\rho}\sum_i u'^2_i + \frac{k}{2\rho}(1-\delta)\sum_i n_i u'_i - \frac{1}{2}\sum_{\langle ij\rangle} c_i^+ c_j\right] & \end{aligned} \tag{6}$$

In the first bracket the first terms represents the increase of zero-point energy due to the phonon transformation U_3, the second term the polaronic binding energy (n_0 is the average electron density). The second bracket is identical to the adiabatic Hamiltonian (4), with the band parameter renormalized by a polaronic narrowing factor

$$\rho = \exp\left(-\frac{k^2}{4\gamma}\delta^2 e^{-4r}\right) \tag{7}$$

More precisely, E_{ad} (k) being the ground state energy of (4), the ground state energy of (6) is obtained as follows

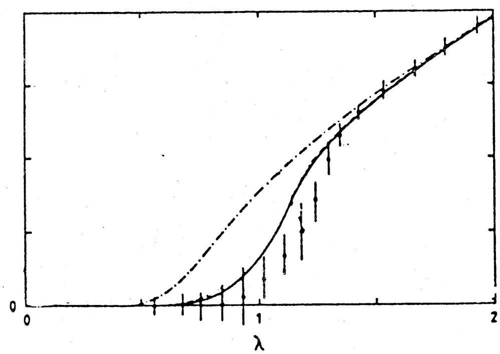
$$E_0(\delta, r) = \frac{\gamma}{2}\cosh 4r - \frac{k^2}{8}(2\delta - \delta^2)\, n_0 + \rho\, E_{ad}(\tilde{k}) \tag{8}$$

where $\tilde{k} = k\,(1 - \delta) / \sqrt{\rho}$ is a renormalized coupling constant . On the other hand the net lattice deformation u_i is given as a function of the equilibrium adiabatic deformation u_i^{ad} (k) by $u_i = \sqrt{\rho}\ / (1 - \rho)\ u_i^{ad}(\tilde{k})$.

The variational solution is obtained by minimizing (8) with respect to δ and r. One expects physically, and verify numerically, that $\tilde{k} < k$ and $u_i < u_i^{ad}(k)$. The u_i^{ad} 's are found either analytically (in weak coupling k<<1) or numerically. In the half-filled band case ($n_0 = 1/2$) one has $u_i = (-1)^i u_0$ and

$$E_{ad} = \frac{u_0^2}{2} - \frac{1}{\pi}\int_0^{\pi/2} dq\,(\cos^2 q + \frac{k^2}{4} u_0^2)^{1/2} \qquad 1 = \frac{k^2}{\pi}\int_0^{\pi/2} dq\,(\cos^2 q + \frac{k^2}{4} u_0^2)^{-1/2} \tag{9}$$

The figure shows the agreement with Monte-Carlo calculations (vertical bars) for the particular value $\gamma = 1.1$. The dashed-dotted line is the mean-field value for u_0 (arbitrary units), the full line is our solution (see more details in Ref. 7).



References.

1. J. E. Hirsch and E. Fradkin, Phys. Rev. B **27**, 4302 (1983).
2. C. Bourbonnais and L. G. Caron, Synthetic Metals, **27**, A27 (1988).
3. J. Voit and H. J. Schulz, Phys. Rev. B**37**, 10068 (1988).
4. S. Aubry and P. Quémerais, in *Low-Dimensional Electronic Properties of Molybdenum Bronzes and Oxides* 295-405 Ed. C. Schlenker, Kluwer Academic Publishers Group (1989).
5. T. Holstein, Ann. Phys. (N. Y.) **8**, 325 (1959); **8**, 343 (1959).
6. D. Feinberg, F. de Pasquale and S. Ciuchi,to be published, Int. Journal of Mod. Phys.B.
7. H. Zheng, D. Feinberg and M. Avignon, Phys. Rev. B**39**, 9405 (1989).