INCOMMENSURATE CHARGE DENSITY WAVE WITH QUANTUM LATTICE FLUCTUATIONS

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We discuss how quantum lattice fluctuations can destroy a CDW. Usually, CDW are treated within the adiabatic approximation (i.e mean field approximation). However, the validity of this approximation, which neglects the quantum lattice fluctuations, remains uncontrolled. We analyse this problem in one dimensional models. The main result that we have obtained is that *incommensurate CDW with a strictly gapless Fröhlich mode are necessary destroyed by the quantum fluctuations.* Our approach can also be used for the commensurate case, specially for the half-filled band case, which is important for conducting polymers as it will be reported in ref. [1]. It has been previously (see reference in ref.[3], this proceeding) shown that within the adiabatic approximation, incommensurate CDW are of two types:

1) "analytic CDW". For small enough electron-phonon coupling, the CDW has a strictly gapless Fröhlich mode (phason) and is conducting by the coherent displacement of the CDW associated with its periodic lattice distortion (PLD) under the action of an electric field. Let us note that no strictly gapless phason mode has ever been observed in real compounds (eg the blue bronzes of molybdenium).

2) "non-analytic CDW". For electron-phonon coupling larger than a critical value (which belongs to the physical range!), in the absence of any defects or impurities, the CDW is intrinsically pinned to the lattice. The gap of the phason mode is non-zero. The CDW can be interpreted as incommensurate arrays of ordered and localized bipolarons (ref.[2]). The earlier numerical observations are now supported by a rigorous result valid at any dimension (see [3]). Such CDW are "defectible" by localized defects of the bipolaronic structure (ref.[2]).

We start with the mean-field Holstein hamiltonian (eq.3 in ref.[3]), with the same notations), which becomes using the equality $\langle u_i \rangle = -\frac{k}{2}\langle n_i \rangle$:

$$(1) \qquad H_{MF} = -\frac{1}{2}\sum_{\langle i,j\rangle\sigma} c_{i,\sigma}^{+}c_{i,\sigma} + \frac{k}{2}\sum_i n_i\langle u_i\rangle + \frac{1}{2}\sum_n ((u_n-\langle u_n\rangle)^2 + \frac{\gamma^2}{4}p_n^2) + \frac{1}{2}\sum_i \langle u_i\rangle^2$$

k and γ are the electron-phonon coupling and the quantum lattice parameter respectively both in reduced units. The problem of finding the ground-state and the excited state of (1), is the same as for solving the adiabatic hamiltonian (γ=0). Accurate numerical calculations yields the mean lattice distortion $\langle u_i \rangle$ and the electronic wave functions for the ground-state. These lattice distortion can be written using a 2π-periodic hull function g(x) as:

$$(2) \qquad \langle u_i \rangle = g(2\pi i\zeta)$$

where ζ is the number of pairs of electron per site. Fig.1 shows g(x) calculated with two different couplings k for a loop with 21 electron pairs over 55 sites. For this band filling ζ=21/55, the transition of breaking of analyticity occurs at $k=k_c(\zeta)\approx 1.57$. For $k<k_c$, the CDW is "analytic. For $k>k_c$, the CDW is non-analytic. In the second regime, some examples for the shape $\{b_i\}$ of the bipolarons (defined by eq.4 in ref.3) are shown fig.2 for a system 21/55.

For large k, this bipolaron becomes localized on a single site. It extends when decreasing k and its size diverge at k_c. Let us note on fig.2, the evolution of the localization

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when k varies. In addition to the ground-state, there exist infinitely many other eigenstates corresponding to the bipolaronic configurations.

fig.1

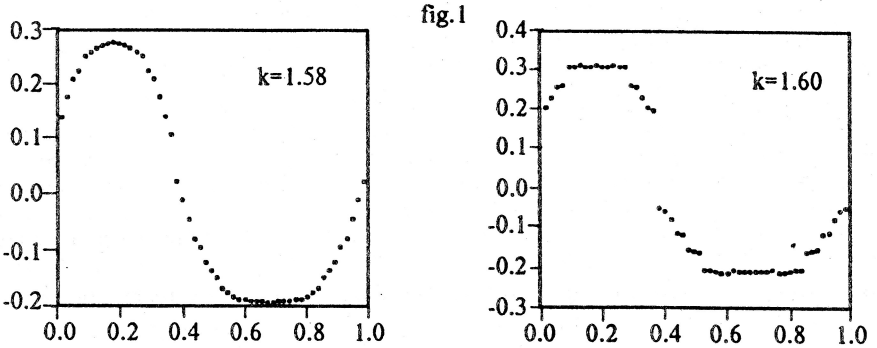
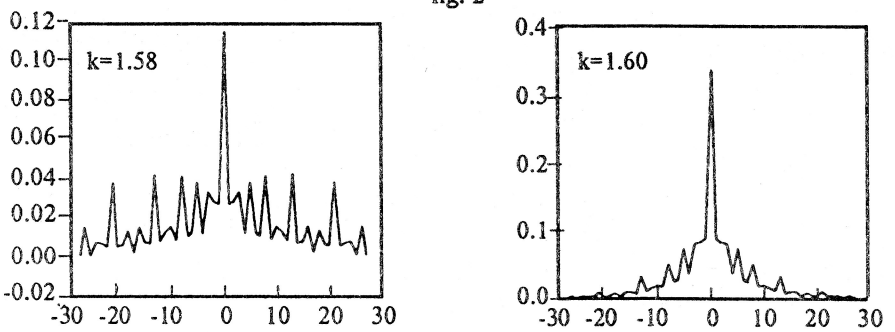
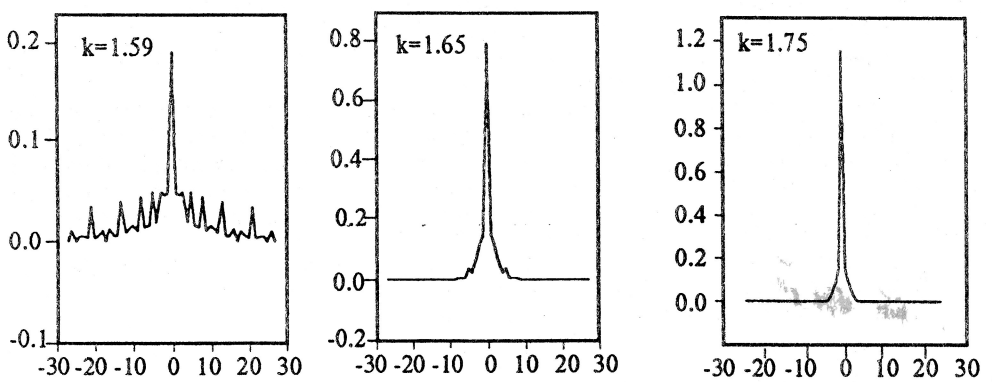


fig. 2





Let us now discuss the validity of the mean-field (i.e. adiabatic) approximation. For any metastable configuration $\{\langle u_i \rangle\}$, the corresponding mean-field approximation quantum state is exactly given by eq.5 ref.[3]. To be good approximations for the eigenstates of the initial hamiltonian (1) in ref.[3], a necessary condition is the orthogonality of these states. For γ small and fixed, it can be shown analytically that the overlaps $\langle \Psi_1 | \Psi_2 \rangle$ and $\langle \Psi_1 | H | \Psi_2 \rangle$ (which can

be calculated explicitely) between any couple of different mean-field eigenstates $|\Psi_1\rangle$ and $|\Psi_2\rangle$ sharply drop to zero as soon as k is slightly larger than k_c. Therefore, for small γ, and $k>k_c$ the bipolaronic states are quite good eigenstates of the quantum Holstein hamiltonian.

When k approaches k_c from above, these overlaps $\langle\Psi_1|\Psi_2\rangle$ become close to unity for many couples of metastable states which only differs locally by a finite number of defects. *Consequently, the validity of the mean field approximation necessarily breaks down* for some $k_c^*(\zeta,\gamma)$ slightly above $k_c(\zeta)$ whatever γ be small (but non zero). More precisely, the exact knowledge of these overlaps can be used for example, for estimating numerically the quantum correction to the energy of the discommensurations of a commensurate CDW due to its tunnelling through the lattice. The trying eigenstate for a tunelling discommensuration is a linear combination of the mean-field eigenstates corresponding to a discommensuration located successively in each unit cell. The total energy of this quantum discommensuration is then the sum of a positive potential (classical) energy (see curve (1) on fig.3) and of a negative quantum energy $-\Delta E_Q$ (see curve (2) on fig.3). *It becomes always negative when k is smaller than the critical coupling $k_c^*(\zeta,\gamma)$ corresponding to strong overlaps.* In physical terms, this quantum instability essentially originates from the softening of the lattice pinning mode (i.e. the phason mode) of the bipolarons due to the increasing of their size. The same result holds both for advanced and retarded quantum discommensurations which proves that the commensurate CDW becomes unstable.

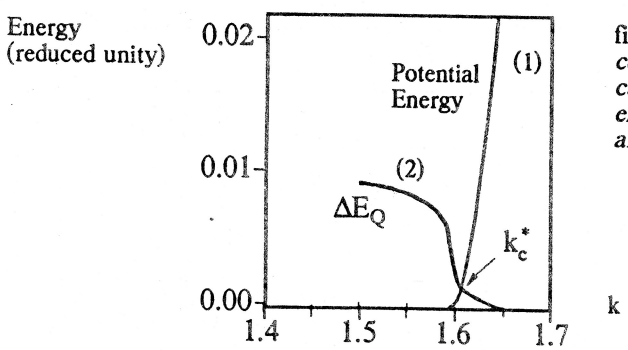


fig.3: *Energy of the defect for a commensurate system 21/55. The curve 1 is the sum of the potential energy of a retarded defect, plus an advanced defect.*

When ζ goes to an irrational number ζ, the classical energy of a discommensuration goes to zero while the quantum correction does not when the CDW is gapless. We find $k_c(\zeta)=k_c^*(\zeta,0)<k_c^*(\zeta,\gamma)$. In principle, the same method can be extended to models in 2 and more dimensions for analysing the tunnelling energy of any kind of localized defects in the bipolaronic structures. We expect the same result: CDW with strictly gapless Fröhlich modes are always unstable against quantum lattice fluctuations.

In summary, we have essentially proven here that in the case of a zero (or sufficiently small) phason gap, the validity of the adiabatic approximation breaks down and then the CDW are unstable against quantum phase fluctuations. Therefore, it is clear that the estimation of the defect energies shown here hold only for bipolaronic CDW which are stable. For unstable CDW, the mean-field eigenstates become too bad approximations for the eigenstates of the initial hamiltonian to be used as a base for expanding the genuine eigenstates. As pointed out in ref [3], the "antiadiabatic effect" (inducing probably superconductivity) have to be taken into account in this regime where CDW are destroyed by quantum lattice fluctuations. A better understanding of these features are currently under development.

[1] P. QUEMERAIS, J.L. RAIMBAULT, D.K. CAMPBELL and S. AUBRY, in preparation.
[2] P. QUEMERAIS, Thèse de Doctorat *" Une nouvelle approche pour l'étude des composés à onde de densité de charge. Conséquences de la brisure d'analyticité"*, Université de Nantes 1987, France.
[3] S. AUBRY, P. QUEMERAIS and J.L. RAIMBAULT, this proceeding