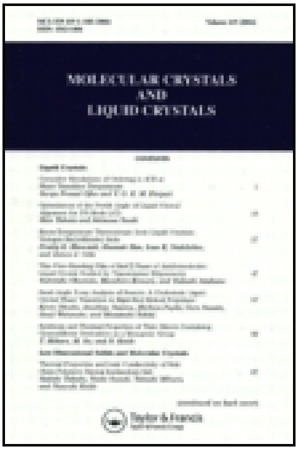

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Effect of Intersite Coulomb Interactions on the Peierls State

M. Avignon [a] & C. Balseiro [b]

[a] LEPES - CNRS, B.P. 166, 38042, Grenoble Cedex, France

[b] Centro Atomico Bariloche, 8400, Bariloche, Argentina

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EFFECT OF INTERSITE COULOMB INTERACTIONS ON THE PEIERLS STATE

M. AVIGNON
LEPES - CNRS, B.P. 166, 38042 Grenoble Cedex, France
C. BALSEIRO
Centro Atomico Bariloche, 8400 Bariloche, Argentina

Abstract We present a real space renormalization group blocking method (RGB) study of the effect of intersite Coulomb repulsion on a dimerized chain (1/4-filled band) in the limit of strong intrasite interaction.

In many one-dimensional conductors, the smallness of the conduction bandwidth has led to consider the role of the Coulomb interactions on the Peierls transition. Controversy still persists on whether on-site interactions may be large[1,2] or small[3] compared with the bandwidth. Recently Mazumdar & Bloch[4] have shown that the magnitude of effective short-range Coulomb interactions depends strongly on band filling and may be large for 1/2-filled and 1/4-filled bands. For strong intra-atomic repulsion $U(U \to \infty)$, the 1/4-filled band system is known[5] to be equivalent to a spinless 1/2-filled band and presents a Peierls instability with wavelength $\lambda = 2a$. This dimerization, as opposed to the $\lambda = 4a$ instability expected if correlations were neglected, can be considered as evidence for strong U. It is known that a number of 1:2 TCNQ salts, e.g. TEA-, DTC-, MEM- $(TCNQ)_2$, with a 1/4-filled band presents dimerized chains of TCNQ. In this situation, it is of interest to study the role of intersite Coulomb repulsion. Nearest neighbor repulsion G is certainly the next dominant interaction to take into account. If sufficiently strong, this interaction also tends to produce a periodicity 2a : a charge ordered state. Hence, interference will occur between the two types of instabilities. In the uniform chain case (t_0, G_0), charge ordering occurs exactly for $G_0/t_0 > 2$ (t_0 being the hopping integral).

We thus consider the corresponding tight-binding spinless hamiltonian with a 1/2-filled band :

$$H = \sum_i t_{i,i+1}(C_i^+ C_{i+1} + C_{i+1}^+ C_i) + \sum_i G_{i,i+1}(n_i - \frac{1}{2})(n_{i+1} - \frac{1}{2}) \quad (1)$$

where $t_{i,i+1}$ takes alternatively different values t_1° and t_2°, and $G_{i,i+1}$ the values G_1°, G_2°.

The renormalization group blocking method (RGB) has been previously applied to the uniform case[6] of (1) (analog of the Heisenberg - Ising chain) and reproduces correctly the exact critical value $(G/t)^* = 2$. Fields[7] has considered the dimerized Heisenberg chain which corresponds to the critical case $G_1/t_1 = G_2/t_2 = 2$. The method has also been applied to the Hubbard[8,9] and extended Hubbard[10] models. The ground state energy and the amplitude of the local moment are well-reproduced, indicating that RGB gives reliable information about the transition.

We present results concerning the ground state energy as function of the dimerization. Calculations of correlation functions and charge ordering parameters will be published elsewhere[11].

REAL SPACE RENORMALIZATION GROUP BLOCKING METHOD

The RGB method consists of dividing the system into blocks of N_s sites. The hamiltonian for an isolated block is solved exactly and one selects from the eigenstates a certain number of states to define a reduced basis on which the hamiltonian is projected. The basis is chosen in order to preserve the form of the hamiltonian with renormalized parameters $\tilde{t}_1$, $\tilde{t}_2$, $\tilde{G}_1$ and $\tilde{G}_2$. The procedure is repeated until a fixed point is reached. We have considered $N_s = 3$ and to reproduce the 1/2-filled band one has to consider blocks of m = 1 and m = 2 electrons. The basis consists of the ground state of m = 1 and m = 2 subspaces, respectively as the new vacuum $|0>$ and the new one-particle states $C^{+/}|0>$.

A constant term $C^{(n)}$ is generated at each step. It gives the ground state energy per site E_G :

$$E_G = \lim_{n\to\infty} \frac{C^{(n)}}{N_s^{\,n}}$$

For G = 0 (XY dimer chain), $t_1/t_2 = 1$ is an unstable fixed point, and $t_1/t_2 = \infty$ (equivalently $t_1/t_2 = 0$) a stable fixed point as it should be.

With Coulomb interactions G_1°, G_2°, when $t_2^\circ/t_1^\circ < 1$, t_2/t_1 still renormalizes to zero, t_1^∞ being either finite or zero. When $G_1^\circ = G_2^\circ = G^\circ$, the recursion relation still gives an unstable fixed point $(G^\circ/t^\circ)^*$ which increases as Δ increases ($\Delta = (t_1^\circ - t_2^\circ/t_o)$.

If the initial parameters are such that $G^\circ/t^\circ < (G^\circ/t^\circ)^*$, we find that $t_1 \to t_1^\infty$, $G_1 \to G_1^\infty$ while $t_2 \to 0$ and $G_2 \to 0$. The fixed point hamiltonian corresponds to independent molecules, and the system is semiconductor because of the dimerization.

If $G^\circ/t_o > (G^\circ/t_o)^*$, one reaches a situation where t_1 and t_2 both renormalizes to zero, and $G_1 \to G_1^\infty$, $G_2 \to G_2^\infty \neq G_1^\infty$. The fixed point hamiltonian becomes that of an interacting system without hopping and alternating G_1^∞ and G_2^∞. The ground state corresponds to charge ordering with dimerization.

The equilibrium value of the dimerization Δ_o can be calculated from the ground state energy, adding the elastic energy term. The energy difference $\Delta E = E_G(\Delta) - E_G(o)$ is plotted in Figure 1 for different values of G°/t_o ($G^\circ/t_o = 0,1,2,3$). The dimerization first increases with G° (curves a,b,c) while as G° increases still further (curve d) the dimerization tends to decrease. Note that for $G^\circ/t_o > 2$, the critical value $(G^\circ/t_o)^*$ that separates the two behaviours of the system is crossed as Δ increases.

It is important to mention that in order to get more reliable results for $E_G(\Delta)$, one should also take into account that G_1°, G_2° are also function of the dimerization ; $G_1^\circ - G_2^\circ$ should also increase as Δ increase.

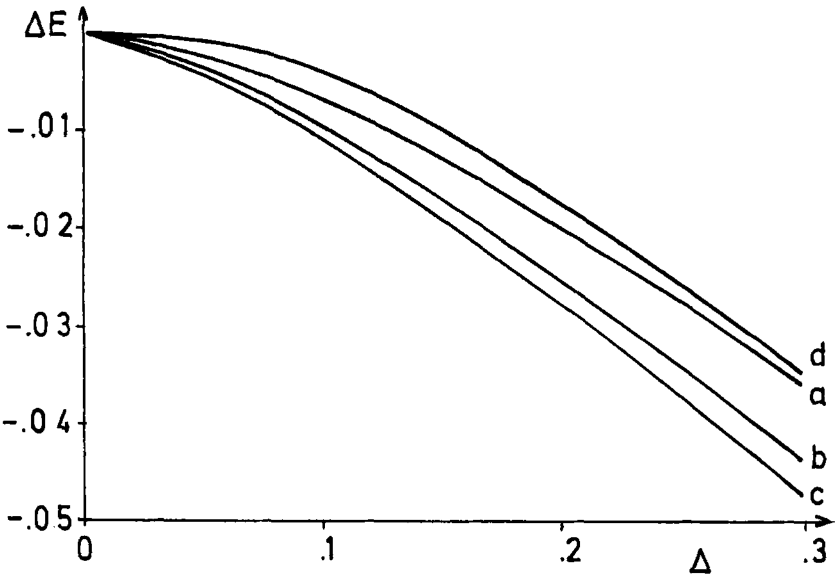

FIGURE 1 The ground state energy vs. Δ for $G^{\circ}/t_0 = 0$ (a), 1 (b), 2 (c), 3 (d).

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