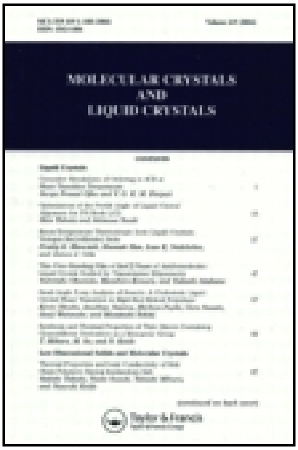

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Soliton Energetics in Extended Peierls-Hubbard Models: A Quantum Monte Carlo Study

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SOLITON ENERGETICS IN EXTENDED PEIERLS-HUBBARD MODELS: A QUANTUM MONTE CARLO STUDY

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Abstract Using quantum Monte Carlo techniques, we study the effects of on-site (U) and nearest-neighbor (V) Hubbard interactions on the energetics of solitons in coupled electron-phonon (Peierls) models of quasi-one-dimensional materials.

The importance of understanding the combined effects of electron-phonon (Peierls) and electron-electron (Hubbard) interactions in real quasi-one-dimensional materials has in past few years become increasingly clear. Several recent studies,[1-6] using exact diagonalization[2,6] or quantum Monte Carlo techniques,[1,3-5] have established the need to go beyond earlier approximate treatments, including Hartree-Fock,[7-9] perturbative,[8] and variational methods.[10] In this brief note, we present partial results of a continuation of our previous study[5] of soliton energetics in Peierls-Hubbard models; details will be published elsewhere.[11]

The model Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2M} + \frac{K}{2}\sum_i (u_i - u_{i+1})^2 + \frac{U}{2}\sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma} + V\sum_i n_i n_{i+1}$$

$$+ \sum_{i,\sigma} (t_o - \alpha(u_i - u_{i+1}))(c^+_{i,\sigma} c_{i+1,\sigma} + c^+_{i+1,\sigma} c_{i,\sigma}) \qquad (1)$$

where $n_{i,\sigma} \equiv c^{+}_{i,\sigma} c_{i,\sigma}$ and $n_i = \sum_{\sigma} n_{i,\sigma}$. In the physical context in which H describes trans-$(CH)_x$, the displacements (u_i) of the (CH) units along the chain are coupled (with strength α) to the hopping term which transfers π-electrons between adjacent sites, the Hubbard U(>0) models the Coulomb repulsion occurring when two π-electrons of opposite spin ($\sigma = \pm\frac{1}{2}$) occupy the same site (i.e., (CH) unit), and the Hubbard V -- $0 < V < U/2$ -- describes nearest neighbor repulsion.

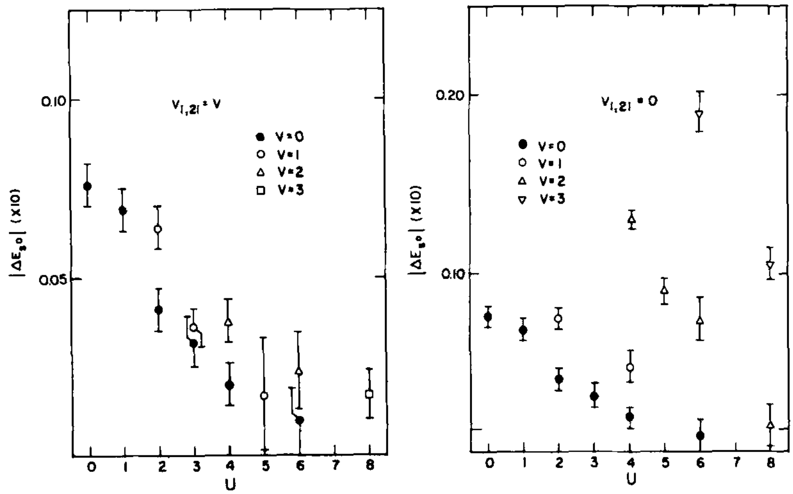

FIGURE 1 Magnitude of energy difference between neutral soliton and neutral dimer for N = 21: (a) $V_{1,21} = V$; (b) $V_{1,21} = 0$.

Using an "ensemble projector Monte Carlo" method[5,11] we have (for V = 0) previously[5] (1) established that dimerization presists even for large $U(\gtrsim 4t_0)$; (2) calculated neutral soliton creation energies; and (3) proved that "soliton doping" persists for $U \neq 0$. Here, in view of limitations of space, we focus exclusively on the energetics of charged and neutral solitons in the presence of both U and V. As previously,[5] we work with a fixed phonon configuration, which for the pure dimer is such that sequential transfer integrals alternate between $t_{\pm} \equiv t_o(1\pm2\delta)$, while for the "single site" soliton[5,11] is such that the bond alternation reverses about the central site. We choose an N = 4n+1 system (N = 21), which choice, together with the single site soliton, eliminates any elastic energy differences.

In Figs. 1 and 2 we plot $|\Delta E_S|$, the magnitude of the energy difference between the soliton (S) (which always has lower energy) and the dimer (D) versus U for the neutral (D^o,S^o) and positive (D^+,S^+) systems, respectively. The different symbols in each

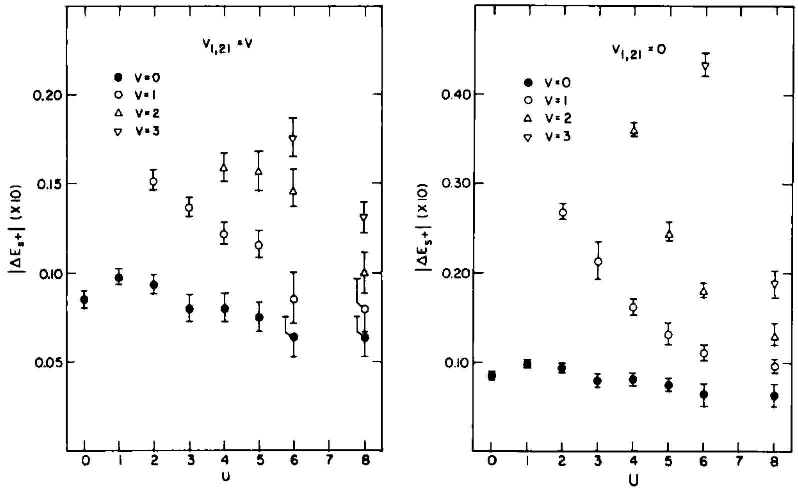

FIGURE 2 Magnitude of energy differences between charged soliton and charged dimer for N = 21: (a) $V_{1,21}$ = V (b) $V_{1,21}$ = 0.

figure refer to different values of V. Importantly, to obtain a result which can be extrapolated smoothly to the infinite chain, it is essential to assume that $V_{1,21} \neq 0$; that is, although there is no hopping between sites 1 and 21, one must include a "nearest neighbor" repulsion. A full explanation of this effect will be provided elsewhere.[11] Here we simply note that taking $V_{1,21} = 0$ artificially breaks the symmetry between S^+ and S^-. In the infinite chain, this symmetry should not be broken in our model; additional physical effects, such as a (σ-π) coupling, are required to break the symmetry. In Figs. 1 and 2, the parts labelled "a" have $V_{1,21} = V$ whereas those labelled "b" have $V_{1,21} = 0$; note the dramatic differences. Focusing only on the physically relevant "a" parts, we observe several important features. First, the ground state of an odd chain is a soliton for both charged and neutral systems even for nonzero U and V. Second, the degeneracy between S^o and S^+ is destroyed for nonzero U and V. Third, although it is not indicated on Fig. 2a, which shows only S^+, when $V_{1,21} = V$ our results show that $S^+ = S^-$, to within our Monte Carlo errors. Fourth, the neutral soliton stabilization energy decreases continuously with U (for V = 0) and with U-V (for $V \neq 0$). The charged soliton stabilization energy remains relatively flat as U is increased for V = 0, while for both U and V > 0 the charged soliton can be more stable than the pure Peierls (U = 0 = V) case. This very strong stabilization of the charged soliton may be responsible for its apparent ready formation in doping experiments.

REFERENCES

1. J. E. Hirsch and E. Fradkin, Phys. Rev. Lett. 49 402 (1982); Phys. Rev. B 27, 1680 and 4302 (1983).
2. S. Mazumdar and S. N. Dixit, Phys. Rev. Lett. 51, 292 (1983); Phys. Rev. B29, (1984).
3. J. E. Hirsch, Phys. Rev. Lett. 51 296 (1983).
4. J. E. Hirsch and M. Grabowski, Phys. Rev. Lett. 52, 1713 (1984).
5. D. K. Campbell, T. A. DeGrand and S. Mazumdar, Phys. Rev. Lett. 52, 1717 (1984).
6. Z. G. Soos and S. Ramasesha, Phys. Rev. Lett. 51, 2374 (1983); J. Chem. Phys., to be published.
7. K. R. Subbaswamy and M. Grabowski, Phys. Rev. B 24, 2168 (1981).
8. S. Kivelson and D. E. Heim, Phys. Rev. B 26, 4278 (1982).
9. H. Fukutome and M. Sasai, Prog. Theor. Phys. 69, 373 (1983).
10. P. Horsch, Phys. Rev. B 24, 7351 (1981).
11. D. K. Campbell, T. A. DeGrand and S. Mazumdar, in preparation.