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QUANTUM FLUCTUATION OF THE ORDER PARAMETER IN POLYACETYLENE

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Abstract The effects of the lattice quantum fluctuation upon the order parameter in the Peierls systems are studied using the Green's function technique. The order parameter is reduced compared with the adiabatic value but survives the quantum fluctuations in agreement with the Monte Carlo simulation results.

INTRODUCTION

In the standard model of the Peierls instability as well as the soliton excitation[2] the lattice distortion is treated as a c-number. However, the quantum fluctuations of the lattice are significant. The question whether the order parameter survives such fluctuation was discussed by Su[2] and Hirsch and Fradkin[3] using the Monte Carlo technique. The quantum corrections to the phonon frequencies and the soliton energy were considered by Nakahara and Maki.[4]

In this paper we briefly report the results of an analytical study on the effects of quantum fluctuations upon the dimerization. A coupled system of integral equations for the order parameter, the complex energy gap and the wave function renormalization is derived using the Green's function technique and is solved numerically for different sets of parameters. The order parameter is always reduced compared with the adiabatic value but the dimerization persists. In case of trans- $(CH)_x$ this reduction is of 8 % which is consistent with the Monte Carlo results. Details of this calculation will be published elsewhere.[5]

THE MODEL

We start from the discrete version of the SSH Hamiltonian.[1] After carrying out the Fourier transformation and shifting the momentum origin we end up with the following Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int} \tag{1}$$

$$\mathcal{H}_0 = \frac{\hbar\omega_0}{4}\frac{\eta^2(T)}{g^2(p,p)} + \sum_{q\neq 0}\hbar\omega_q b_q^+ b_q + \sum_p \xi_p C_p^+ \tau_3 C_p + \sum_p \eta(T) C_p^+ \tau_1 C_p \,, \tag{2}$$

$$\mathcal{H}_{int} = \sum_{\substack{p,p_1,q \\ q\neq 0}} \delta_{p_1,p+q}\, g(p_1,p)\, C_{p_1}^+ \tau_3 C_p (b_q + b_{-q}^+) \,, \tag{3}$$

where

$$g(p_1,p) = 2\alpha\sqrt{\frac{\hbar}{2NM\omega_b(q)}}\left(\cos(pa) + \cos(p_1 a)\right) \,, \tag{4}$$

$$\omega_b^2(q) = \omega_0^2 \cos(qa/2) \,, \tag{5}$$

$$\xi_p = 2t_0 \sin(pa) \,, \tag{6}$$

$$\omega_0^2 = 4K/M \,, \tag{7}$$

$$\eta(T) = g(p,p)\left(\langle b_0\rangle_T + \langle b_0^+\rangle_T\right) \tag{8}$$

and C_p^+, C_p the spinor fermion operators, τ_1, τ_3 the Pauli matrices, T the temperature. Unless specified otherwise, we will use the SSH set of parameters, namely, W = 4t = 10 eV, α =4.1 eV/Å, K= 21 eV/Å .

THE COUPLED SYSTEM OF EQUATIONS

In the continuum limit, the coupled system of equations for the order parameter and the renormalized Green's functions for electrons can be derived in the one-loop approximation either by use of the closed time-path Green's function formalism[6] or using the Matsubara technique.

The renormalized electron function can be written as

$$G^{-1} = Z(\omega)\omega - \tau_3 \xi_p - \phi(\omega)\tau_1 \tag{9}$$

The coupled system of equations for the order parameter $\eta(\omega)$, the complex gap function $\Delta(\omega) = \Phi / Z$ and the wave function renormalization $Z(\omega)$ is given by

$$(1 - Z(\omega))\,\omega = \int_0^\infty d\omega' R_e\left[\frac{\omega'}{(\omega'^2 - \Delta^2(\omega'))^{1/2}}\right] K_-(\omega,\omega') \quad , \tag{10}$$

$$\Delta(\omega) = \eta(0)/Z(\omega) - Z^{-1}(\omega)\int_0^\infty d\omega' R_e\left[\frac{\Delta(\omega')}{(\omega'^2 - \Delta^2(\omega'))^{1/2}}\right] K_+(\omega,\omega'), \tag{11}$$

$$\eta(0) = \lambda \int_0^\infty d\omega' R_e\left[\frac{\Delta(\omega)}{(\omega'^2 - \Delta^2(\omega'))^{1/2}}\right] \quad , \tag{12}$$

where

$$K_\pm(\omega) = \frac{1}{v_F}\int_0^\infty \frac{d\Omega}{2\pi} g^2(q_0) B(q_0,\Omega)\left[\frac{1}{\omega' + \Omega + \omega + i\delta} \pm \frac{1}{\omega' + \Omega - \omega - i\delta}\right] \tag{13}$$

$$\lambda = \frac{8\alpha^2 a}{\pi v_F K} \approx 0.408 \tag{14}$$

and $B(q,\Omega)$ is the phonon spectrum.

This system of equations is very similar to the Eliashberg equation in the strong coupling theory of superconductivity[7] although the physical content is different. The el-ph interaction is constructive there where as it is destructive here for the order parameter as seen from the negative sign in Eq. (11).

THE RESULTS

The system of equations (10) - (12) has been solved for the following phonon spectrum

$$B(q,\Omega) = \begin{cases} B_0\left[\frac{1}{(\Omega - \omega_q)^2 + \Gamma^2} - \frac{1}{(s^2+1)\Gamma^2}\right], & |\Omega - \omega_q| < s\Gamma \\ 0, \text{ otherwise.} \end{cases} \tag{15}$$

with $\omega_q = 0.1$ eV, $\Gamma = 0.03$ eV, $s = 3$ and B_0 determined from the normalization condition.

The results for the real and imaginary parts of $\Delta(\omega)$ and $Z(\omega)$ are shown in Figs. 1 and 2 correspondingly. As seen from the curve, the gap at the band edge $\Delta(\omega) = \omega$ is reduced

compared with the adiabatic value $\Delta_0 = 0.867$ eV. The order parameter defined by (8) which is also the asymptotic value of $\Delta(\omega)$ for large ω turns out to be $\eta(0) = 0.804$ eV. This value is 8 % reduced. Monte Carlo calculations give 15 %[3] or 20 %[2] reduction. In view of the approximation involved in the continuum limit such agreement should be considered satisfactory.

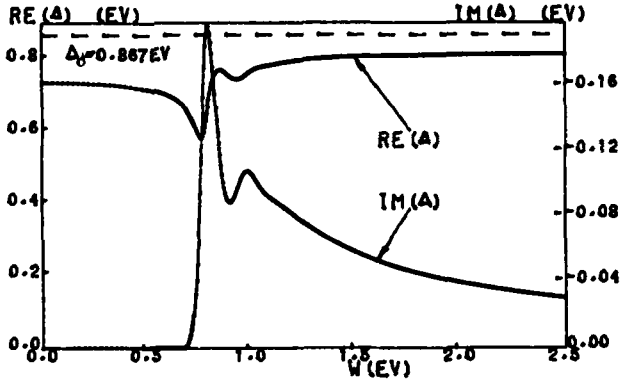

FIGURE 1 Real and imaginary parts of the gap parameter for α =4.1 eV/ Å.

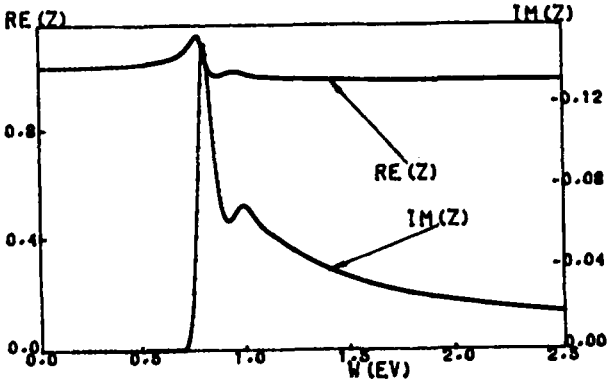

FIGURE 2 Real and imaginary parts for the wave function renormalization $Z(\omega)$ for α =4.1 eV/ Å.

We have examined the dependence of $\Delta(\omega)$ and $Z(\omega)$ upon various parameters. The results obtained are insensitive to the width of the phonon spectrum and its cut-off as well as the electron cut-

off which we take as 5 eV. However, the picture changes quite significantly if we modify the el-ph coupling constant α . The gap parameter for α = 3.2eV is plotted in Fig.3. Here we find more overtones which are suppressed by damping for stronger coupling.

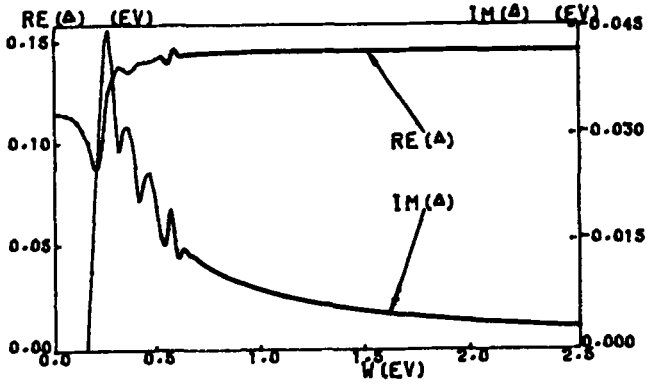

FIGURE 3 The gap parameter for α = 3.2 eV/ Å.

We have also calculated the density of states and the optical absorption with the lattice fluctuation being accounted for. These results will be reported elsewhere.[5] The work is in progress to consider the combined effects of the lattice fluctuation and the Coulomb correlation.

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