Continuum model of a Peierls system with a complex order parameter

B. Sriram Shastry
Tata Institute of Fundamental Research, Colaba, Bombay 400 005, India

W. P. Su
Department of Physics, University of Illinois at Urbana-Champaign, 1110 W. Green Street, Urbana, Illinois 61801

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We consider the continuum version of a one-dimensional model in which fermions are coupled with two phonon modes. Each mode is capable of producing dimerization, but together they are in competition, and the true ground state corresponds to only one of the two order parameters being nonzero in general. In the vicinity of a charged kink both order parameters are nonzero. We provide an analytical expression for the kink shape using the Fermi-level scheme which has been shown to be exact in another context. The gap-state energy and creation energy of the kink are also calculated. The model considered interpolates between the polyacetylene model and a model with continuous chiral symmetry in relativistic field theory.

I. INTRODUCTION

Stimulated by the success of the polyacetylene model[1] there have been many attempts to generalize it. One generalization consists of including one more phonon mode.[2,3] The internal modes of the ions in many molecular crystals which couple with the electronic density are examples. As a result of this extension the order parameter describing the lattice dimerization is a complex number. In general the ground states correspond either to a real or pure imaginary number. There are two kinds of kinks connecting the two degenerate ground states. The neutral kink has a real or pure imaginary order parameter and a midgap state as in the case of polyacetylene. The charged kinks have a complex order parameter. The position of the gap state and the creation energy are sensitive to the relative strength of the two electron-phonon couplings.[2,3]

In this paper we study the continuum model of such a system (Sec. II). Using the Fermi-level scheme[4] we solve the coupled equations to obtain the charged kink shape (Sec. III). We then examine the associated gap-state structure to estimate the creation energy (Sec. IV). Section V contains some discussions about the continuum electronic states and self-consistency of the solution.

II. CONTINUUM MODEL

In addition to the intersite displacement u_n of the nth ion we have an internal mode coordinate q_n which couples with the diagonal electronic charge density. Thus the discrete Hamiltonian is

$$H=-t_0\sum_n[1+\alpha(u_n-u_{n+1})](c_{n+1}^{\dagger}c_n+\text{H.c.})+\lambda\sum_n q_n c_n^{\dagger}c_n+\frac{K}{2}\sum_n(u_n-u_{n+1})^2+\frac{K'}{2}\sum_n q_n^2 . \tag{2.1}$$

We have neglected kinetic energy of the ions. The spin index is dropped for convenience. The c's are the usual fermionic field operator. The number of fermions is assumed to be $N/2$, where N is the number of ions. We define new variables by removing the rapidly varying phase factors from the fermion amplitudes ψ_n's and the classical fields u_n and q_n. Thus

$$a_n=(-1)^n\psi_{2n},\quad b_n=(-1)^n\psi_{2n-1},\qquad \chi_n=\frac{\lambda}{t_0}q_{2n},\quad \bar{\chi}_n=-\frac{\lambda}{t_0}q_{2n-1},\qquad \Phi_n=\frac{2\alpha}{t_0}(u_{2n+1}-u_{2n}),\quad \bar{\Phi}_n=-\frac{2\alpha}{t_0}(u_{2n}-u_{2n-1}) , \tag{2.2}$$

with $1<n<N/2$. A continuum theory is obtained by replacing the first differences by derivatives and equating χ and Φ with $\bar{\chi}$ and $\bar{\Phi}$, respectively. The resulting energy functional[2,3,5] is

$$E=\int_0^L dx\sum_{\alpha}{}'[\chi(|a_\alpha|^2-|b_\alpha|^2)-\Phi(a_\alpha^*b_\alpha+b_\alpha^*a_\alpha)+(b_\alpha'a_\alpha^*-a_\alpha'b_\alpha^*)]+\left[\frac{K't_0}{\lambda^2}\right]\int_0^L\chi^2dx+\left[\frac{Kt_0}{4\alpha^2}\right]\int_0^L\Phi^2dx , \tag{2.3}$$

where $L=N/2$, $b'=db/dx$, etc. $\delta E/\delta a^*=0$ and $\delta E/\delta b^*=0$ give the Dirac equations

$$(\epsilon_\alpha-\chi)a_\alpha=b_\alpha'-\Phi b_\alpha ,\qquad (\epsilon_\alpha+\chi)b_\alpha=-a_\alpha'-\Phi a_\alpha , \tag{2.4}$$

while $\delta E/\delta\lambda=0$ and $\delta E/\delta\Phi=0$ give the self-consistent equations

$$\Phi=\frac{2\alpha^2}{Kt_0}\sum_\alpha{}'(\alpha_\alpha^* b_\alpha+b_\alpha^* a_\alpha)\ ,$$
$$\chi=\frac{\lambda^2}{2K't_0}\sum_\alpha{}'(|b_\alpha|^2-|a_\alpha|^2)\ . \tag{2.5}$$

$a_\alpha(x)$ and $b_\alpha(x)$ are solutions of (2.4) with energy ϵ_α. In (2.3) and (2.5) α runs over all occupied states.

III. FERMI-LEVEL SCHEME

In the Fermi-level scheme[4] one replaces the sum (2.5) over all occupied states by the topmost extended state in the filled valence band with energy ϵ_0. ϵ_0 is determined by Eqs. (2.4) and (2.5) in the uniform ground state exactly as in the case of polyacetylene. With this replacement we have

$$\Phi=|\epsilon_0|(p_2+p_1)ab\ ,$$
$$\chi=|\epsilon_0|p_2(b^2-a^2)\ , \tag{3.1}$$

where

$$p_2=\frac{\lambda^2 N}{4K't_0}\Lambda_2,\quad p_1=\frac{2\alpha^2 N\Lambda_1}{Kt_0}-p_2\ .$$

Λ_1 and Λ_2 approach $1/|\epsilon_0|$ in the strong-coupling limit, but here we take them as parameters to be fixed from (2.5). Equation (3.1) together with Eqs. (2.4),

$$(\epsilon_0-\chi)a=b'-\Phi b\ ,$$
$$(\epsilon_0+\chi)b=-a'-\Phi a\ , \tag{3.2}$$

uniquely determine Φ, χ, a, and b. By rescaling the coordinate and the lattice fields appropriately

$$x\to x/(-\epsilon_0)\ ,$$
$$\Phi\to\Phi|\epsilon_0|\ , \tag{3.3}$$
$$\chi\to\chi|\epsilon_0|\ ,$$

one arrives at the Dirac equations

$$b'=-a(1-p_1b^2-p_2a^2)\ ,$$
$$a'=b(1-p_1a^2-p_2b^2) \tag{3.4}$$

and the self-consistency equations

$$\Phi=(p_1+p_2)ab\ ,$$
$$\chi=p_2(b^2-a^2)\ . \tag{3.5}$$

In the following we will mainly be concerned with a one kink solution such that

$$\chi\underset{x\to\pm\infty}{\to}0\ ,$$
$$\Phi\underset{x\to+\infty}{\to}-1,\quad \Phi\underset{x\to-\infty}{\to}1\ . \tag{3.6}$$

This corresponds to a positively charged kink in which the gap state is empty. The negatively charged kink solution can be obtained by using the charge conjugation transformation.[2]

An important conservation law which follows from (3.4) is

$$a^4+b^4-\frac{2}{p_2}(a^2+b^2)+\frac{2p_1}{p_2}a^2b^2=\text{const}\ . \tag{3.7}$$

This allows a^2 to be expressed in terms of b^2,

$$p_2a^2=(1-p_1b^2)-(p_+p_-)^{1/2}|b^2-1/p_+|\ , \tag{3.8}$$

where $p_+=p_1+p_2$ and $p_-=p_1-p_2$. Equations (3.4) can therefore be integrated to give

$$a(x)=\frac{\cosh(\theta x)}{(p_+)^{1/2}[\sinh^2(\theta x)+\frac{1}{2}(1+\theta)]^{1/2}}\ ,$$
$$b(x)=\frac{-\sinh(\theta x)}{(p_+)^{1/2}[\sinh^2(\theta x)+\frac{1}{2}(1+\theta)]^{1/2}} \tag{3.9}$$

and

$$\Phi(x)=\frac{-\sinh(2\theta x)}{\cosh(2\theta x)+\theta},\quad \chi(x)=\frac{-(1-\theta^2)}{\cosh(2\theta x)+\theta}\ . \tag{3.10}$$

$\theta=(p_-)^{1/2}/(p_+)^{1/2}$ depends only on the ratio of the two coupling constants. Polyacetylene corresponds to $p_2=0$ or $\theta=1$. Equation (3.10) reduces to $\chi=0$ and $\Phi(x)=-\tanh x$ as it should be. Notice in (3.10) the length scale is determined by θ^{-1}. Therefore the width of the charged kink or the coherence length is proportional to

$$l\sim 1/|\epsilon_0|\theta\ . \tag{3.11}$$

In the limit $p_1=p_2(\theta=0)$, $\Phi^2+\chi^2=\text{const}$. There is a continuous chiral symmetry[6] because the Hamiltonian is invariant under any rotation of the angle between Φ and χ. We have also obtained the many kink generalizations of solution (3.10). These are expressible in terms of Jacobian elliptic functions.[7]

IV. GAP STATE AND KINK CREATION ENERGY

By knowing the lattice field configurations (3.10) in principle, one can solve the Dirac equations for all the eigenstates. For lack of an exact solution we will try a power-series expansion for the bound state.

Through a change of variable

$$\zeta=\tanh(\theta x)\ , \tag{4.1}$$

one finds as $|\zeta|\to1$, both a and b behave as

$$a\to(1-\zeta^2)^\delta\ , \tag{4.2}$$

where

$$\delta=(1-\epsilon^2)^{1/2}/2\theta\ . \tag{4.3}$$

ϵ is the energy of the bound state to be determined. By substituting the following expressions:

$$a=f(1-\zeta^2)^\delta\ ,$$
$$b=g(1-\zeta^2)^\delta \tag{4.4}$$

in the Dirac equations, one has

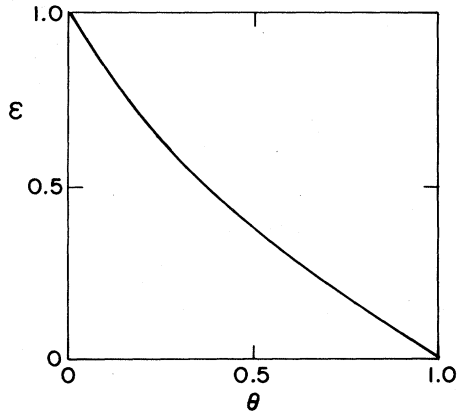

FIG. 1. Energy of the gap state ϵ as a function of the coupling ratio θ.

$$[\eta\epsilon+(1-\theta^2)(1-\zeta^2)]f = \left[\eta\theta(1-\zeta^2)\frac{\partial}{\partial\zeta}+2\zeta-2\eta\theta\delta\zeta\right]g \,,$$
$$[\eta\epsilon-(1-\theta^2)(1-\zeta^2)]g = \left[-\eta\theta(1-\zeta^2)\frac{\partial}{\partial\zeta}+2\zeta+2\eta\theta\delta\zeta\right]f \,, \tag{4.5}$$

where

$$\eta=(1+\theta)+\zeta^2(1-\theta) \,. \tag{4.6}$$

Since both f and g are analytic in $[-1,1]$ we can try power series with the right parity

$$f=c_1'\zeta+\cdots \,, \qquad g=c_0+c_2\zeta^2+\cdots \,, \tag{4.7}$$

in the zeroth-order approximation

$$\epsilon=1-\theta \,. \tag{4.8}$$

Thus the gap state is split off from the band edge by an energy θ. According to the uncertainty principle this is in agreement with (3.11). Since the kink creation energy is of the same order as the bound-state energy measured from the band edge, it is reasonable to assume that the kink creation energy is also proportional to $\theta\,|\,\epsilon_0\,|$.

A more accurate estimate of ϵ can be achieved by going to higher-order terms in ζ as in (4.7). By comparing the coefficients of the ζ terms in the first Dirac equation and the constant terms and the ζ^2 terms in the second Dirac equation, one has a set of homogeneous equations. The secular equation determines ϵ as a function of θ. The result is displayed in Fig. 1. It compares very well with a direct numerical solution of the Dirac equations.

V. CONTINUUM STATES AND SELF-CONSISTENCY

In the case of polyacetylene ($\theta=1$) the continuum states behave like a plane wave asymptotically, i.e., both $a(x)$ and $b(x)$ are proportional to e^{ikx} for both $x\to+\infty$ and $x\to-\infty$. In other words, the kink acts like a reflectionless potential for the electrons. Therefore $\Phi(x)$ in (2.5) is functionally proportional[4] to $a_\alpha^*(x)b_\alpha(x)+b_\alpha^*(x)a_\alpha(x)$ for every extended state α and the self-consistency is automatic. From some numerical studies of the Dirac equations it is found that this reflectionless property of the kink potential is lost for $\theta\neq1$. The determination of the continuum state is more complicated than the polyacetylene case and for the moment it is unknown if the solution (3.10) is exact or not.

To conclude, by using the Fermi-level scheme we have solved the coupled electron-phonon equations (2.4) and (2.5) for a complex Peierls system and have obtained the shape and creation energy of the charged kink. The solution has the desired property of interpolating between the pure amplitude kink (the polyacetylene case) and the phase kink in the chiral-symmetry limit.

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