Variational approach to the quantum lattice fluctuations in the Su-Schrieffer-Heeger model: The ground state

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We have studied the effect of quantum lattice fluctuations on the dimerized ground state of the half-filled Su-Schrieffer-Heeger (SSH) model. Our results show that, at least in the weak-coupling limit, quantum lattice fluctuations change the functional dependence of the gap $\Delta(0)$ on the coupling constant even if the ratio $\omega_\pi/4t$ is small (but finite). In the spin-$\frac{1}{2}$ case our result is the same as that predicted by Fradkin and Hirsch. But in the spinless case we still predict a long-range dimerization order even if the coupling is weak and $\omega_\pi/4t$ is finite. We have shown by numerical calculations that our variational approach gives a good description of the continuous variation of the gap $\Delta(0)$ in the fermionic spectrum as a function of the coupling constant v or the phonon frequency ω_π. By using the same input parameters as those of SSH we get a 12% reduction of the gap $\Delta(0)$ compared with the adiabatic value. The calculated electron density of states does not have the inverse-square-root singularity but does have a peak around $\Delta(0)$. There is a significant tail below the peak. These are consistent with the observed optical absorption coefficient in undoped *trans*-polyacetylene.

I. INTRODUCTION

In the last decade or so the physics of one-dimensional electron-phonon systems has attracted the considerable attention of both theoretists and experimentalists.[1] In the studies of properties of a quasi-one-dimensional system such as polyacetylene, Su, Schrieffer, and Heeger[2] (SSH) proposed a model Hamiltonian in which the phonons interact with the electrons by modifying the electron hopping matrix elements,

$$H=-\sum_{n,\sigma} t(c^{\dagger}_{n,\sigma}c_{n+1,\sigma}+c^{\dagger}_{n+1,\sigma}c_{n,\sigma}) -\sum_{n,\sigma}\alpha(u_n-u_{n+1})(c^{\dagger}_{n,\sigma}c_{n+1,\sigma}+c^{\dagger}_{n+1,\sigma}c_{n,\sigma}) +\sum_n\left[\frac{1}{2M}p_n^2+\frac{K}{2}(u_n-u_{n+1})^2\right]. \quad (1)$$

The notations in it are as usual.[1,2] Within the adiabatic approximation, that is, treating the phonon degrees of freedom classically, SSH have used this Hamiltonian to uncover a wealth of interesting physics.[2] In the half-filled-band case, the system undergoes a Peierls instability and the ground state is dimerized with an energy gap $2\Delta(0)$. The optical absorption coefficient of the perfectly dimerized lattice has an inverse-square-root edge singularity at $\omega=2\Delta(0)$ and there is no absorption inside the gap. However, the observed optical absorption is quite different. The singularity is absent, and there is a significant tail below the maximum.[3-5] This indicates that there exist tails of electron density of states (DOS) extending into the gap.

Attempts have been made to explain the discrepancy between theory and experiment in terms of three-dimensional interactions[6] (they cannot account for the large tail), disorder[7] (this is not consistent with the fact that the tail structure is observed clearly in very good samples), direct photoproduction of soliton-antisoliton pairs,[8-13] and the quantum lattice fluctuations (as a source of disorder) described by a random potential with Gaussian correlations.[14] In this work we show that an electron DOS consistent with the observed optical absorption coefficient can be obtained for the original SSH model by taking into account the effect of quantum lattice fluctuations, without assuming the virtual soliton-antisoliton pairs production or the phenomenological random potential connected with the fluctuations.

The theoretical analysis becomes much more difficult when the quantum lattice fluctuations are taken into account. Scalapino and Sugar[15] raised the question whether the dimerization could survive the quantum lattice fluctuations if the ionic mass is lower than some critical value. Su,[16] Fradkin and Hirsch,[17] and Takahashi[13] have calculated the electronic and lattice structure of the half-filled SSH model by the adiabatic or the nonadiabatic Monte Carlo simulations, and concluded that the Peierls dimerization can survive the quantum lattice fluctuations but with a reduction [20% in Ref. 16, 15% in Ref. 17, and 7% in Ref. 13 by using the same input parameters as those of SSH (Ref. 2)] of the order parameter compared with the adiabatic value. In the work of Fradkin and Hirsch,[17] they found that the low-energy behavior of the system of finite ionic mass is governed by the zero-mass limit of the theory, an n-component Gross-Neveu model[18] where n is the number of spin states. They pointed out that for weak coupling the gap in the fermionic spectrum behaves like

$$\Delta(0)\sim\exp\left[-\frac{\pi}{2(n-1)v}\right], \quad (2)$$

where $v=\alpha^2/Kt$ is the coupling constant. This should be compared with the adiabatic result

$$\Delta_c(0)\sim\exp\left[-\frac{\pi}{2nv}\right] . \tag{3}$$

So Fradkin and Hirsch[17] concluded that for spinless electrons quantum lattice fluctuations destroy the Peierls dimerization for small coupling constant if the ionic mass is finite. Su, Wang and Yu[19] studied the same problem by using the Green's-function technique and found a 8% reduction of the gap function compared with the adiabatic value. Caron and Bourbonnais[20] calculated the $T=0$ K phase diagram of the continuous version of SSH model by using the renormalization procedure but their method is limited to the weak-coupling limit. McKenzie and Wilkins[14] proposed to mimic the effect of quantum lattice fluctuations by means of a random potential with Gaussian correlations; but this approach is mainly phenomenological and also limited to the continuous version of SSH model.

In this work, besides getting an electron DOS consistent with the observed optical absorption coefficient, we shall discuss the functional dependence of gap $\Delta(0)$ on the coupling constant v and phonon frequency $\omega_\pi=2\sqrt{K/M}$. In particular, for the input parameters of SSH (Ref. 2) a 12% reduction of $\Delta(0)$ will be derived compared with the adiabatic value. Furthermore, for a weak-coupling case an analytical formula for $\Delta(0)$ will be obtained,

$$\Delta(0)\sim\exp\left[-\frac{\pi}{2v}\right] , \tag{4}$$

for spin-$\frac{1}{2}$ electrons and finite ionic mass. This is the same as that [Eq. (2)] predicted by Fradkin and Hirsch.[17] However, for spinless electrons our result is

$$\Delta(0)\sim\exp\left[-\frac{\pi}{v}\right] , \tag{5}$$

being different from Eq. (2) and predicting that even for the spinless electrons the Peierls dimerization persists for an arbitrary coupling constant.

Throughout this paper we put $\hbar=1$ and $k_B=1$.

II. THEORY

We start by using the original SSH Hamiltonian Eq. (1), in which the operators for the lattice modes, u_n and p_n, can be expanded by using the phonon creation and annihilation operators,

$$u_n=\sum_q\sqrt{1/2MN\omega_q}(b^\dagger_{-q}+b_q)\exp(iqn) , \tag{6}$$

$$p_n=i\sum_q\sqrt{M\omega_q/2N}\,(b^\dagger_{-q}-b_q)\exp(iqn) . \tag{7}$$

N is the total number of cells. Here $\omega_q^2=(4K/M)\sin^2(q/2)$. Thus, H becomes

$$\begin{aligned}H=&-\sum_{n,\sigma}t(c^\dagger_{n,\sigma}c_{n+1,\sigma}+c^\dagger_{n+1,\sigma}c_{n,\sigma})\\&+\sum_q\omega_q(b^\dagger_q b_q+\tfrac{1}{2})\\&+\frac{1}{\sqrt{N}}\sum_{k,q,\sigma}g(k+q,k)(b^\dagger_{-q}+b_q)c^\dagger_{k+q,\sigma}c_{k,\sigma} .\end{aligned} \tag{8}$$

The coupling function $g(k+q,k)$ is defined as

$$g(k+q,k)=-2i\alpha\sqrt{1/2M\omega_q}[\sin k-\sin(k+q)] . \tag{9}$$

In order to determine the thermodynamical properties of the coupling system we derive the free energy as follows. Following the Bogoliubov's thermodynamical variational principle,[21] an upper bound of the free energy $F(T)$ can be written as

$$\begin{aligned}F(T)<&F_0(T)\\&=-\frac{1}{\beta}\ln\mathrm{Tr}[\exp(-\beta H_0)]\\&\quad+\mathrm{Tr}[\exp(-\beta H_0)(H-H_0)]/Z+\mu N_e ,\end{aligned} \tag{10}$$

$Z=\mathrm{Tr}[\exp(-\beta H_0)]$ and $\beta=1/T$. Here H is given by Eq. (1) and H_0 is a trial Hamiltonian. We introduce an unitary operator $\exp[-S(T)]$ to write the trial Hamiltonian H_0 as

$$H_0=\exp[-S(T)]H_0'\exp[S(T)] , \tag{11}$$

with the definition of $S(T)$,

$$S(T)=\frac{1}{\sqrt{N}}\sum_{k,q,\sigma}\frac{g(k+q,k)}{\omega_q}(b^\dagger_{-q}-b_q)\delta(k+q,k)c^\dagger_{k+q,\sigma}c_{k,\sigma} . \tag{12}$$

Here we introduce for H_0 the variational function $\delta(k',k)$, which is a function of the energies of the incoming and outgoing electrons in the electron-phonon scattering process. The form of $\delta(k',k)$ will be defined later. As the operators under the trace operation can commute with each other, one can rewrite $F_0(T)$ as

$$\begin{aligned}F_0(T)=&-\frac{1}{\beta}\ln\mathrm{Tr}\{\exp[S(T)]\exp(-\beta H_0)\exp[-S(T)]\}\\&+\mathrm{Tr}\{\exp[S(T)]\exp(-\beta H_0)\exp[-S(T)]\exp[S(T)](H-H_0)\exp[-S(T)]\}/Z+\mu N_e\\=&-\frac{1}{\beta}\ln\mathrm{Tr}[\exp(-\beta H_0')]+\mathrm{Tr}[\exp(-\beta H_0')(H'-H_0')]/Z+\mu N_e ,\end{aligned} \tag{13}$$

where

$$H'=\exp[S(T)]H\exp[-S(T)] . \tag{14}$$

The thermodynamical variational principle means that the variational function introduced by the unitary operator $\exp[-S(T)]$ should be adjusted so that $F_0(T)$ reaches a stable minimum. Note that the variational function $\delta(k',k)$ is only used for H_0, all parameters in H, Eq. (1), remain fixed.

The unitary transformation in Eq. (14) can be done as follows. We divide the Hamiltonian H [Eq. (8)] as $H=H^0+H^1$, where H^0 contains the first two terms and H^1 the last term. Then the transformation can be done order by order,

$$H'=H^0+H^1+[S,H^0]+[S,H^1]+\tfrac{1}{2}[[H^0,S],S]+O(\alpha^3) .$$

The first-order terms in the transformed Hamiltonian H' are

$$\begin{aligned} H^1+[S,H^0]=&\frac{1}{\sqrt{N}}\sum_{k,q,\sigma} g(k+q,k)(b^\dagger_{-q}+b_q)c^\dagger_{k+q,\sigma}c_{k,\sigma} \\ &-\frac{1}{\sqrt{N}}\sum_{k,q,\sigma} g(k+q,k)\delta(k+q,k)(b^\dagger_{-q}+b_q)c^\dagger_{k+q,\sigma}c_{k,\sigma} \\ &+\frac{1}{\sqrt{N}}\sum_{k,q,\sigma}\frac{g(k+q,k)}{\omega_q}(\epsilon_k-\epsilon_{k+q})\delta(k+q,k)(b^\dagger_{-q}-b_q)c^\dagger_{k+q,\sigma}c_{k,\sigma} , \end{aligned} \tag{15}$$

where ϵ_k is the bare band function for electrons: $\epsilon_k=-2t\cos k$. Now we can choose the functional form of $\delta(k+q,k)$ to make the contribution of these first-order terms as small as possible. It is easy to see that one can choose

$$\delta(k+q,k)=1/(1+|\epsilon_{k+q}-\epsilon_k|/\omega_q) , \tag{16}$$

thus the sum of first-order terms proportional to $b^\dagger_{-q}c^\dagger_{k+q,\sigma}c_{k,\sigma}$ is zero when $\epsilon_k<\epsilon_{k+q}$ and that proportional to $b_q c^\dagger_{k+q,\sigma}c_{k,\sigma}$ is zero when $\epsilon_k>\epsilon_{k+q}$. We note that the ground state $|G\rangle$ of H^0, the noninteracting system, is a direct product of a Fermi sea $|FS\rangle$ and a phonon vacuum state $|\mathrm{ph},0\rangle$:

$$|G\rangle=|FS\rangle|\mathrm{ph},0\rangle . \tag{17}$$

If we choose $\delta(k+q,k)$ as above, the first-order matrix element of $H^1+[S,H^0]$ between this ground state and the lower-lying excited states is zero. In this work we will introduce a variational parameter γ in $\delta(k+q,k)$,

$$\delta(k+q,k)=1/(1+\gamma|\epsilon_{k+q}-\epsilon_k|/\omega_q) . \tag{18}$$

When $\gamma=1$ this definition is the same as that in Eq. (16). We believe that for $\gamma>1$ the effect of higher-order terms has been taken into account partly. Here we would note the following two points: (1) γ is the only variational parameter we introduced in this work; (2) if γ is fixed to be 1 [as that in Eq. (16)], all the following results do not change qualitatively. The second-order terms are listed in the Appendix.

We choose the trial Hamiltonian H'_0 as

$$\begin{aligned} H'_0=\exp(-R)\Bigg[&\sum_q \omega_q(b^\dagger_q b_q+\tfrac{1}{2})+\sum_{k,\sigma}E_k c^\dagger_{k,\sigma}c_{k,\sigma} \\ &+\sum_{k>0,\sigma} i\Delta_k(c^\dagger_{k,\sigma}c_{k-\pi,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k,\sigma})\Bigg]\exp(R) . \end{aligned} \tag{19}$$

Here

$$R=-\sum_n(-1)^n u_0\sqrt{M\omega_\pi/2}(b^\dagger_n-b_n) \tag{20}$$

and $\exp(-R)$ is a displacement operator:

$$\exp(R)u_n\exp(-R)=(-1)^n u_0+\sum_q\sqrt{1/2MN\omega_q}(b^\dagger_{-q}+b_q)\exp(iqn) . \tag{21}$$

We note that Δ_k and E_k in H'_0 are not variational functions. They are determined by the transformed Hamiltonian H'.

We substitute H' and H'_0 into Eq. (13) and get the free energy $F_0(T)$,

$$\begin{aligned} F_0(T)=&2Ku_0^2N[1+2c(c-1)]+\frac{1}{\beta}\sum_q\ln\left[2\sinh\frac{\beta\omega_q}{2}\right]-\frac{1}{\beta}\sum_{k>0,\sigma}\ln[2+2\cosh(\beta W_k)] \\ &-\frac{1}{2N}\sum_{k'>0,k>0,\sigma}\frac{|g(k'-\pi,k)|^2}{\omega_{k'-\pi-k}}\delta(k'-\pi,k)[2-\delta(k'-\pi,k)] \\ &\times[1-\langle c^\dagger_{k,\sigma}c_{k,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k-\pi,\sigma}\rangle\langle c^\dagger_{k',\sigma}c_{k'\sigma}-c^\dagger_{k'-\pi,\sigma}c_{k'-\pi,\sigma}\rangle] . \end{aligned} \tag{22}$$

Details of the derivation are shown in the Appendix. Here the fermionic spectrum in the dimerized state is

$$W_k=\sqrt{E_k^2+\Delta_k^2}\ . \tag{23}$$

The renormalized band function is

$$E_k=\epsilon_k-\frac{1}{N}\sum_{k'>0}(\epsilon_k+\epsilon_{k'})\frac{|g(k'-\pi,k)|^2}{\omega_{k'-\pi-k}^2}\coth\left[\frac{\beta\omega_{k'-\pi-k}}{2}\right]\delta^2(k'-\pi,k)$$
$$-\frac{1}{N}\sum_{k'>0}\frac{|g(k'-\pi,k)|^2}{\omega_{k'-\pi-k}}\delta(k'-\pi,k)[2-\delta(k'-\pi,k)]\langle c_{k',\sigma}^{\dagger}c_{k',\sigma}-c_{k'-\pi,\sigma}^{\dagger}c_{k'-\pi,\sigma}\rangle\ . \tag{24}$$

The gap function is

$$\Delta_k=4\alpha u_0\sin(k)][c-\tfrac{1}{2}\delta(k,k-\pi)]\ , \tag{25}$$

where

$$c=1+\frac{1}{N}\sum_{k>0,\sigma}\frac{2\alpha^2}{K}\sin(k)\delta(k-\pi,k)\frac{\Delta_k}{4\alpha u_0 W_k}\tanh\frac{\beta W_k}{2}\ . \tag{26}$$

The equation to determine u_0 is

$$1=\frac{2}{N}\sum_{k>0,\sigma}\frac{2\alpha^2}{K}\sin(k)[1-\delta(k-\pi,k)]\frac{\Delta_k}{4\alpha u_0 W_k}\tanh\frac{\beta W_k}{2}\ . \tag{27}$$

In this paper we deal with the $T=0$ ground state, thus $\tanh(\beta W_k/2)=1$ and $\coth[\beta\omega_{k'-\pi-k}/2]=1$ in all above equations. Equations (26) and (27) are basic equations in our theory. If $\delta(k',k)=0$ we have $c=1$ from (26) and (27) becomes the same as that in the adiabatic theory.[2,17,19] In our theory $\delta(k-\pi,k)$ has the form [see Eq. (18)]

$$\delta(k-\pi,k)=\frac{1}{1+(4t\gamma/\omega_\pi)|\cos(k)|}\ . \tag{28}$$

This function is shown in Fig. 1 where we use numerical value $\omega_\pi/2t=0.0327$. As will be obtained in Sec. IV, for this value of ω_π and $v=0.32$ we have $\gamma=1.469$. $\delta(k-\pi,k)$ has a sharp peak at $k=\pm\pi/2$, the Fermi points in the one-dimensional case. The height of the peak is 1 and the width of it is $2k_0$, where k_0 is determined by

$$\delta(\pi/2-k_0-\pi,\pi/2-k_0)=\tfrac{1}{2}\ .$$

Thus

$$\cos(\pi/2-k_0)=\omega_\pi/4t\gamma$$

or

$$k_0=\sin^{-1}\left[\frac{\omega_\pi}{4t\gamma}\right]\approx\frac{\omega_\pi}{4t\gamma}\ . \tag{29}$$

In the case of Fig. 1, $2k_0=0.022$, so the peak is very narrow. This is to say that only those electrons near the Fermi point $\pi/2$ $(-\pi/2)$ can be scattered by those near $-\pi/2$ $(\pi/2)$ through the electron-phonon interaction and contribute to the reduction of the gap $\Delta(0)$ compared with the adiabatic value. This fact is similar to that in the Bardeen-Cooper-Schrieffer theory[22] for superconductivity, only those electrons near the Fermi surface form Cooper pairs via a phonon-induced effective attraction.

We note that, since

$$1-\delta(k-\pi,k)=\frac{(4t\gamma/\omega_\pi)|\cos(k)|}{1+(4t\gamma/\omega_\pi)|\cos(k)|}\ , \tag{30}$$

the logarithmic singularity in the integration of Eq. (27) in the weak-coupling limit and adiabatic case,[2] $\int_0^{\pi/2}dk/\cos(k)$, is removed by the factor $1-\delta(k-\pi,k)$ as long as the ratio $\omega_\pi/4t\gamma$ is finite. However, now the logarithmic singularity appears in the integration of Eq. (26). The change of the singularity in these integrations may result in a change of the analytical form of the gap $\Delta(0)$. We shall show this in next section.

Comparing Eq. (25) with that in the adiabatic case,[2] $\Delta_k=4\alpha u_0\sin(k)$ [the gap $\Delta_c(0)=4\alpha u_0$], we have the gap in the nonadiabatic case,

$$\Delta(0)=4\alpha u_0 c\ , \tag{31}$$

if the ratio $\omega_\pi/4t\gamma$ is small and thus the second term in the square bracket of Eq. (25) can be omitted.

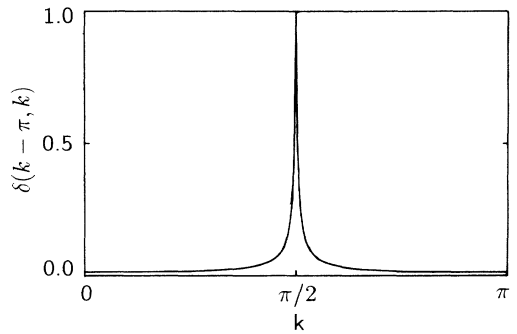

FIG. 1. The variational function $\delta(k-\pi,k)$ [Eq. (28)] vs k relation. $v=0.32$, $\omega_\pi/2t=0.0327$, and $\gamma=1.469$.

III. WEAK-COUPLING LIMIT

First, let us discuss the weak-coupling limit $v=\alpha^2/Kt\to 0$. In this limit we can put the variational parameter $\gamma=1$ [because that, as was mentioned after Eq. (18), $\gamma>1$ is used to take into account partly the effect of higher-order terms of v] and the renormalization band function E_k to be the same as the bare one: $E_k=\epsilon_k$. Thus, Eqs. (26) and (27) become

$$c=1+\frac{2vr}{\pi}\int_0^{\pi/2}dk\,\sin^2(k)\frac{c-0.5r/[r+\cos(k)]}{r+\cos(k)}\left[\cos^2k+4vx^2\sin^2k\left[c-\frac{0.5r}{r+\cos(k)}\right]^2\right]^{-1/2}, \tag{32}$$

$$1=\frac{4v}{\pi}\int_0^{\pi/2}dk\,\sin^2(k)\cos(k)\frac{c-0.5r/[r+\cos(k)]}{r+\cos(k)}\left[\cos^2k+4vx^2\sin^2k\left[c-\frac{0.5r}{r+\cos(k)}\right]^2\right]^{-1/2}, \tag{33}$$

where $r=\omega_\pi/4t$ is a parameter related to the nonadiabaticity and x is a dimensionless parameter proportional to u_0, $x=u_0\sqrt{K/t}$. It is easy to see that the logarithmic singularity appears in the integration of Eq. (32) and does not in that of Eq. (33). As r is a small quantity ($r<0.05$ throughout this paper), in the following calculations we shall omit all terms of order r^1 and higher. Thus, the gap is

$$\Delta(0)/2t=2d=2\sqrt{v}xc\ . \tag{34}$$

The integrations in Eqs. (32) and (33) can be done as follows:

$$\begin{aligned}c&=1+\frac{2vr}{\pi}\int_d^1 dx\frac{\sqrt{1-x^2}}{x}\frac{c-0.5r/(r+x)}{r+x}\\&\approx 1+\frac{v}{\pi}(2c-1)\ln\frac{2}{d}-\frac{v}{\pi}(2c-1)\ln\frac{2}{r+d}\ ,\end{aligned} \tag{35}$$

$$\begin{aligned}1&=\frac{4v}{\pi}\int_d^1 dx\sqrt{1-x^2}\frac{c-0.5r/(r+x)}{r+x}\\&\approx\frac{4vc}{\pi}\ln\frac{2/e}{r+d}\ .\end{aligned} \tag{36}$$

For $r=0$ (adiabatic limit), the solution of Eq. (35) is $c=1$ and from Eq. (36) we get

$$\Delta_c(0)=\frac{8t}{e}\exp\left[-\frac{\pi}{4v}\right], \tag{37}$$

which is the same as that of the adiabatic solution.[2,17,19] When $r>0$ is a finite quantity, the solution of these two equations is

$$\Delta(0)=\frac{8t}{e}\exp\left[-\frac{\pi}{2v}\right]. \tag{38}$$

Comparing (38) with (37) one can see that the formula for gap when $r>0$ is very different from that when $r=0$. The ratio

$$\Delta(0)/\Delta_c(0)=\exp\left[-\frac{\pi}{4v}\right] \tag{39}$$

goes to zero when $v\to 0$. This indicates that the quantum lattice fluctuations have changed the low-energy behaviors of the coupling system even if the nonadiabatic parameter r is small.

The form of the gap when r is finite, Eq. (38), is the same as that predicted by Fradkin and Hirsch[17] for spin-$\frac{1}{2}$ electrons. Their conclusion is that when r is finite the low-energy behavior of the coupling system is governed by the zero-mass limit of the theory, an n-component (n is the number of spin states) Gross-Neveu model,[18] and the gap in the fermionic spectrum behaves like

$$\Delta(0)\sim\exp\left[-\frac{\pi}{2(n-1)v}\right]. \tag{40}$$

Thus they also predicted that for spinless electrons quantum lattice fluctuations destroy the long-range dimerization order for the small coupling constant if the ionic mass is finite. However, if the number of spin states n is written explicitly in our formulas our result will be

$$\Delta(0)\sim\exp\left[-\frac{\pi}{nv}\right] \tag{41}$$

for a weak-coupling limit and finite r. When $n=2$ these two equations are the same. But when $n=1$, the spinless case, Eq. (41) still predicts that a long-range dimerization order persists even in the weak-coupling limit. This conclusion is the same as that of Ref. 19.

IV. GENERAL CASE

In the general case we have to do the numerical calculations for determining the variational parameter γ and cannot get the analytical formulas as those in Sec. III. We list some of our numerical results in Figs. 2–4.

Figure 2 shows the gap $\Delta(0)$ and the optimum value of variational parameter γ as functions of the coupling constant v in the case of $\omega_\pi/2t=0.0327$. For comparison, the short-dashed line is the result of adiabatic approximation. It is obvious that quantum lattice fluctuations reduce the gap $\Delta(0)$ compared with the adiabatic value $\Delta_c(0)$, and the ratio $\Delta(0)/\Delta_c(0)$ is a monotonically increasing function of v. Equation (39) shows that this ratio is 0 at the $v\to 0$ limit. It goes to 0.98 at $v=0.5$. For the input parameters used by SSH:[2] $K=21$ eV/Å^2, $t=2.5$ eV, $\alpha=4.1$ eV/Å, $M=3145$ eV^{-1}/Å^2, we have $v=0.32$ and $\omega_\pi/2t=0.0327$. Figure 2 shows that the reduction for this case is 12% [$\Delta(0)/\Delta_c(0)=0.88$]. Here we list some results of previous authors for this redution:

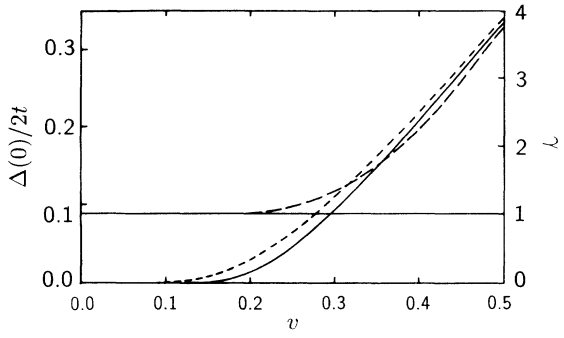

FIG. 2. The gap $\Delta(0)$ (solid line) and the optimum value of variational parameter γ (long-dashed line) as functions of the coupling constant v. $\omega_\pi/2t=0.0327$. The short-dashed line is the result of the adiabatic approximation.

20% of Ref. 16, 15% of Ref. 15, 7% of Ref. 13, 8% of Ref. 19.

The optimum value of variational parameter γ is a monotonically increasing function of v. It goes up from $\gamma=1$ at the $v\to 0$ limit to $\gamma=3.763$ at $v=0.5$. This may be an indication that the effect of the higher-order terms (of order α^3 and higher) has been taken into account partly, as was mentioned after Eq. (18). On the other hand, since the effect of quantum lattice fluctuations is the strongest at the $v\to 0$ limit (the reduction is nearly 100%), we can say that the weaker the effect of quantum lattice fluctuations, the larger is γ.

Figure 3 shows the gap $\Delta(0)$ and the optimum value of variational parameter γ as functions of the phonon frequency ω_π in the case of $v=0.32$. The horizontal short-dashed line is the result of adiabatic approximation: $\Delta_c(0)/2t=0.13$. We can see clearly that the quantum lattice fluctuations gradually reduce the gap $\Delta(0)$ when the phonon frequency ω_π increases. The ratio $\Delta(0)/\Delta_c(0)=0.65$ for $\omega_\pi/2t=0.1$. The optimum value of variational parameter γ is a monotonically decreasing function of ω_π. This means that the stronger the effect of quantum lattice fluctuations, the smaller is γ.

For calculating the electron DOS $\rho(E)$ we use the input parameters of SSH,[2] $v=0.32$ and $\omega_\pi/2t=0.0327$. $\rho(E)$ is defined as[2]

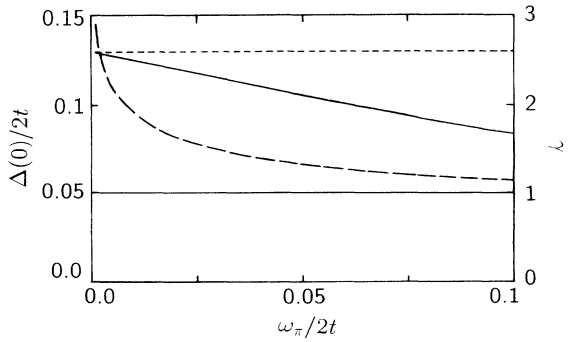

FIG. 3. The gap $\Delta(0)$ (solid line) and the optimum value of variational parameter γ (long-dashed line) as functions of the phonon frequency $\omega_\pi/2t$. $v=0.32$. The horizontal short-dashed line is the result of the adiabatic approximation.

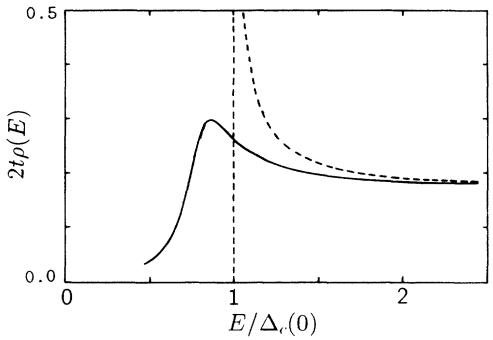

FIG. 4. The electron DOS. $\omega_\pi/2t=0.0327$ and $v=0.32$. The dashed line is the result of the adiabatic approximation.

$$\rho(E)=\frac{1}{2\pi}\frac{1}{|dW_k/dk|}\bigg|_{W_k=E}. \tag{42}$$

Here $W_k=\sqrt{E_k^2+\Delta_k^2}$ and E_k and Δ_k are shown in Eqs. (24) and (25), respectively. In Fig. 4, we show our result for the electron DOS $\rho(E)$ compared with that of the adiabatic approximation (dashed line in the figure) using the same input parameters. The inverse-square-root singularity disappears but there is a peak around $E=\Delta(0)$, which has a displacement from the adiabatic value $\Delta_c(0)$ (the vertical dashed line in the figure): $\Delta(0)/\Delta_c(0)=0.88$. Besides, there is a significant tail below the peak. As the optical absorption coefficient $\alpha(\omega)$ of the band-to-band direct transition is proportional to the joint density of states,[23]

$$\alpha(\omega)\sim\rho(E=\omega/2)\ , \tag{43}$$

we conclude that our calculated DOS is in consistent with the observed optical absorption coefficient in undoped *trans*-polyacetylene.[3–5]

Comparing our gap function [see Eqs. (25) and (28)]

$$\Delta_k=4\alpha u_0\sin(k)\left[c-\frac{1}{2}\frac{1}{1+(4t\gamma/\omega_\pi)|\cos(k)|}\right] \tag{44}$$

with that in the adiabatic approximation: $\Delta_k=4\alpha u_0\sin(k)$, one can see that the subgap states come from the quantum lattice fluctuations, i.e., the second term in the square bracket of Eq. (44).

V. CONCLUSIONS

We have studied the effect of quantum lattice fluctuations on the dimerized ground state of the half-filled SSH model. Our results show that, at least in the weak-coupling limit, quantum lattice fluctuations change the functional dependence of the gap $\Delta(0)$ on the coupling constant v even if the ratio $\omega_\pi/4t$ is small (but finite). In the spin-$\frac{1}{2}$ case our result is the same as that predicted by Fradkin and Hirsch.[17] But in the spinless case we still predict a long-range dimerization order even if the coupling is weak and $\omega_\pi/4t$ is finite. We have shown by numerical calculations that our variational approach gives a good description of the continuous variation of the gap $\Delta(0)$ in the fermionic spectrum as a function of the cou-

pling constant v or the phonon frequency ω_π. By using the same input parameters as those of SSH (Ref. 2) we get a 12% reduction of the gap $\Delta(0)$ compared with the adiabatic value. The calculated electron DOS $\rho(E)$ does not have the inverse-square-root singularity but have a peak around $E=\Delta(0)$. There is a significant tail below the peak. These are in consistent with the observed optical absorption coefficient in undoped *trans*-polyacetylene.

From our work we can say that the main effect of quantum lattice fluctuations is twofold. One is to lower the effective dimerization potential seen by electrons, as is represented by the factor $1-\delta(k-\pi,k)$ in Eq. (27) or in the fifth term of Eq. (A3) for $F_0(T)$. The other is to induce an interaction term of electrons, the last one in Eq. (A2). The Hartree-Fock approximation is used to decouple the interaction term and leads to $c>1$, as shown in Eq. (26). As was mentioned before, Eqs. (26) and (27) are two basic equations in our theory.

In our model system, quantum lattice fluctuations compete with the long-range dimerization order and the physical properties of the system should be determined by this competition. Figure 1 shows that this competition influences mainly those electrons near the Fermi points $\pm\pi/2$. Figures 2 and 3 show the effect of this competition with varying v and ω_π: When v is small but ω_π large, the quantum lattice fluctuations dominate; when v is large but ω_π small, the long-range dimerization order dominates.

In this work, our main interest is concentrated on the small ω_π case ($\omega_\pi/2t<0.1$ throughout this paper) because this is the case of practical interest. If the ratio $\omega_\pi/2t$ is large it might be necessary to reconsider the functional form of the variational function $\delta(k',k)$. We leave this problem for further investigation.

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APPENDIX

In this appendix we show mathematical details of the analysis in Sec. II. Equation (13) gives the upper bound of the free energy,

$$F_0(T)=-\frac{1}{\beta}\ln \mathrm{Tr}[\exp(-\beta H_0')]+\mathrm{Tr}[\exp(-\beta H_0')(H'-H_0')]/Z+\mu N_e \ , \tag{A1}$$

where H_0' is given by Eq. (19) and H' is the transformed Hamiltonian Eq. (14). The second order terms in H' can be collected as follows:

$$\begin{aligned}[S,H^1]+\tfrac{1}{2}[[H^0,S],S]=&\frac{1}{2N}\sum_{q,q'}\sum_{k,k',\sigma}\frac{g(k+q,k)g(k'+q',k')}{\omega_q\omega_{q'}}(b^\dagger_{-q}-b_q)(b^\dagger_{-q'}-b_{q'})(\epsilon_{k+q}-\epsilon_k)\\
&\times\delta(k+q,k)\delta(k'+q',k')[c^\dagger_{k+q,\sigma}c_{k',\sigma}\delta_{k'+q',k}-c^\dagger_{k'+q',\sigma}c_{k,\sigma}\delta_{k+q,k'}]\\
&+\frac{1}{2N}\sum_{q,q'}\sum_{k,k',\sigma}\frac{g(k+q,k)g(k'+q',k')}{\omega_q}(b^\dagger_{-q}-b_q)(b^\dagger_{-q'}+b_{q'})[2\delta(k+q,k)\\
&-\delta(k+q,k)\delta(k'+q',k')][c^\dagger_{k+q,\sigma}c_{k',\sigma}\delta_{k'+q',k}-c^\dagger_{k'+q',\sigma}c_{k,\sigma}\delta_{k+q,k'}]\\
&-\frac{1}{N}\sum_{q}\sum_{k,\sigma}\sum_{k',\sigma'}\frac{g(k+q,k)g(k'-q,k')}{\omega_q}\\
&\times[2\delta(k+q,k)-\delta(k+q,k)\delta(k'-q,k')]c^\dagger_{k+q,\sigma}c_{k,\sigma}c^\dagger_{k'-q,\sigma'}c_{k',\sigma'} \ .\end{aligned} \tag{A2}$$

Here $\delta_{k'+q',k}$ is the Kronecker δ symbol. All terms of higher order than α^2 in H' will be omitted in the following treatment. Substituting H_0' and H' into Eq. (A1) we can get an upper bound of the free energy

$$
\begin{aligned}
F_0(T)=&2Ku_0^2N+\frac{1}{\beta}\sum_q \ln\left[2\sinh\frac{\beta\omega_q}{2}\right]-\frac{1}{\beta}\sum_{k>0,\sigma}\ln[2+2\cosh(\beta W_k)]\\
&+\sum_{k>0,\sigma}\epsilon_k\langle c^\dagger_{k,\sigma}c_{k,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k-\pi,\sigma}\rangle\\
&+\sum_{k>0,\sigma}4i\alpha u_0\sin(k)[1-\delta(k,k-\pi)]\langle c^\dagger_{k,\sigma}c_{k-\pi,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k,\sigma}\rangle\\
&+\frac{1}{N}\sum_{k'}\sum_{k>0,\sigma}\frac{|g(k',k)|^2}{\omega^2_{k'-k}}\coth\left[\frac{\beta\omega_{k'-k}}{2}\right](\epsilon_{k'}-\epsilon_k)\delta^2(k',k)\langle c^\dagger_{k,\sigma}c_{k,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k-\pi,\sigma}\rangle\\
&-\frac{1}{2N}\sum_{k'>0,k>0,\sigma}\frac{|g(k'-\pi,k)|^2}{\omega_{k'-\pi-k}}\delta(k'-\pi,k)[2-\delta(k'-\pi,k)]\\
&\qquad\times[1+\langle c^\dagger_{k,\sigma}c_{k,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k-\pi,\sigma}\rangle\langle c^\dagger_{k',\sigma}c_{k',\sigma}-c^\dagger_{k'-\pi,\sigma}c_{k'-\pi,\sigma}\rangle]\\
&\qquad+\frac{1}{2N}\sum_{k>0,\sigma}\sum_{k'>0,\sigma'}\frac{2\alpha^2}{K}\sin(k)\sin(k')\delta(k-\pi,k)[2-\delta(k',k'-\pi)]\\
&\qquad\qquad\times\langle c^\dagger_{k,\sigma}c_{k-\pi,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k,\sigma}\rangle\langle c^\dagger_{k',\sigma'}c_{k'-\pi,\sigma'}-c^\dagger_{k'-\pi,\sigma'}c_{k',\sigma'}\rangle\\
&\qquad\qquad-\sum_{k>0,\sigma}E_k\langle c^\dagger_{k,\sigma}c_{k,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k-\pi,\sigma}\rangle\\
&\qquad\qquad-\sum_{k>0,\sigma}i\Delta_k\langle c^\dagger_{k,\sigma}c_{k-\pi,\sigma}-c^\dagger_{k-\pi,\sigma}c_{k,\sigma}\rangle\ ,
\end{aligned}
\tag{A3}
$$

where the spectrum for the elementary excitations in the dimerized state is

$$W_k=\sqrt{E_k^2+\Delta_k^2}\ . \tag{A4}$$

The gap function Δ_k and the renormalized band function E_k will be determined later. The thermodynamical averaging $\langle\cdots\rangle$ is defined as

$$\langle\cdots\rangle=\mathrm{Tr}[\exp(-\beta H_0')\cdots]/\mathrm{Tr}[\exp(-\beta H_0')]\ . \tag{A5}$$

Because of the quadratic form of the trial Hamiltonian H_0', in deriving $F_0(T)$ [Eq. (A3)] we have decoupled the correlation term by means of the Wick's theorem:

$$
\begin{aligned}
\langle c^\dagger_{k+q,\sigma}c_{k,\sigma}c^\dagger_{k'-q,\sigma'}c_{k',\sigma'}\rangle=&\delta_{q,-\pi}\langle c^\dagger_{k-\pi,\sigma}c_{k,\sigma}\rangle\langle c^\dagger_{k'+\pi,\sigma'}c_{k',\sigma'}\rangle+\delta_{q,\pi}\langle c^\dagger_{k+\pi,\sigma}c_{k,\sigma}\rangle\langle c^\dagger_{k'-\pi,\sigma'}c_{k',\sigma'}\rangle\\
&+\delta_{k+q,k'}\delta_{\sigma,\sigma'}\langle c^\dagger_{k+q,\sigma}c_{k+q,\sigma}\rangle\langle c_{k,\sigma}c^\dagger_{k,\sigma}\rangle\ .
\end{aligned}
\tag{A6}
$$

E_k and Δ_k in $F_0(T)$ should be determined by minimizing $F_0(T)$,

$$\frac{\delta F_0(T)}{\delta E_k}=0\quad\text{and}\quad\frac{\delta F_0(T)}{\delta\Delta_k}=0\ .$$

By differentiating it is easy to get

$$
\begin{aligned}
E_k=&\epsilon_k-\frac{1}{N}\sum_{k'>0}(\epsilon_k+\epsilon_{k'})\frac{|g(k'-\pi,k)|^2}{\omega^2_{k'-\pi-k}}\coth\left[\frac{\beta\omega_{k'-\pi-k}}{2}\right]\delta^2(k'-\pi,k)\\
&-\frac{1}{N}\sum_{k'>0}\frac{|g(k'-\pi,k)|^2}{\omega_{k'-\pi-k}}\delta(k'-\pi,k)[2-\delta(k'-\pi,k)]\langle c^\dagger_{k',\sigma}c_{k',\sigma}-c^\dagger_{k'-\pi,\sigma}c_{k'-\pi,\sigma}\rangle\ ,
\end{aligned}
\tag{A7}
$$

$$\Delta_k=4au_0\sin(k)[c-\tfrac{1}{2}\delta(k,k-\pi)]\ , \tag{A8}$$

where

$$c=1+\frac{1}{N}\sum_{k>0,\sigma}\frac{2\alpha^2}{K}\sin(k)\delta(k-\pi,k)\frac{\Delta_k}{4\alpha u_0W_k}\tanh\frac{\beta W_k}{2}\ . \tag{A9}$$

The equation to determine u_0 is

$$\frac{\partial F_0(T)}{\partial u_0}=0\ ,$$

which results in

$$1=\frac{2}{N}\sum_{k>0,\sigma}\frac{2\alpha^2}{K}\sin(k)[1-\delta(k-\pi,k)]\frac{\Delta_k}{4\alpha u_0 W_k}\tanh\frac{\beta W_k}{2} . \tag{A10}$$

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