Quantum corrections to solitons in polyacetylene

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(Received 16 June 1981)

The quantum corrections on the soliton in polyacetylene is studied within the continuum version of the Su, Schrieffer, and Heeger model. First, the optical-phonon spectrum in the presence of a soliton is determined. It is shown that the soliton generates two localized phonon modes; the one with $\omega=0$ corresponds to the translation of the soliton, while the other with $\omega\simeq 0.8\omega_0$ is Raman active where ω_0 is the optical-phonon frequency with $k=0$. The quantum correction to the soliton energy E_s is also calculated. We find the correction is rather important: $\delta E_s \simeq -\frac{1}{4}E_s$.

I. INTRODUCTION

The concept of solitons introduced by Su, Schrieffer, and Heeger[1] (SSH) and others[2–4] is central in interpreting the magnetic, optical, and electrical properties of pristine and lightly doped *trans*-polyacetylene. In the discrete model proposed by Su, Schrieffer, and Heeger,[1] two drastic assumptions are usually made: (a) The soliton is treated within the mean-field approximation, and (b) the Coulomb interaction between electrons is assumed to be small.

The object of the present paper is to clarify the nature of the first approximation. In the absence of topological disorder, Brazovskii and Dzyaloshinskii[5] have shown that the adiabatic approximation is justified when $\omega_0/(2\Delta) \ll 1$, where ω_0 is the zero-momentum optical-phonon frequency, and 2Δ is the Peierls energy gap. In the case of polyacetylene,[6] we can take $\omega_0 \sim 1400$ cm^{-1} and $2\Delta = 1.4$ eV which yields $\omega_0/(2\Delta) \sim 0.125$. Although in the presence of the soliton the same justification is assumed to hold,[1] it is worthwhile to study the validity of the mean-field approximation. For this purpose we make use of the semiclassical approach developed by Dashen, Hasslacher, and Neveu,[7] and others.[8] We shall first determine the (optical-) phonon spectrum in the presence of a soliton within the continuum version of the SSH model. We find that the phonon is drastically modified in the presence of soliton; there appear two phonon modes with frequencies below ω_0: The one with $\omega=0$ corresponds to the translational motion of the soliton, while the other with $\omega\simeq 0.82\omega_0$ should be Raman active. The second mode may correspond to the Raman-active mode observed experimentally in lightly doped polyacetylene,[6,9] although the predicted frequency appears somewhat higher than that observed experimentally. It is noteworthy that the phonon obtained here is very similar to that of the ϕ^4 model.[7] With the help of the phonon spectrum thus determined, the quantum correction (i.e., the second-order adiabatic correction) to the soliton energy is found to be $\delta E_s = -0.60\omega_0$, which reduces the soliton energy by roughly $\frac{1}{4}$. Therefore, the quantum correction to the soliton energy is rather important. On the other hand, it is shown that the quantum correction to the soliton mass is extremely small (a few percent of the mean-field soliton mass) and can be neglected.

Making use of the present results, together with the known quantum limit of the Gross-Neveu model,[10,11] we can establish within the perturbation calculation that (a) the dimerized configuration is the stable ground state of the SSH model even when the quantum fluctuations of lattice are included, (b) the soliton is a stable excitation in the system, and (c) the polaron state[10,12,13] in the SSH model is also stable. Indeed, (a) follows from (b) as in the case of the sine-Gordon system,[14] while (b) follows from the fact that $E_p < 2E_s$, where E_p and E_s are the polaron energy and the soliton energy which include quantum corrections.

II. PHONON SPECTRUM

Before going into analysis of the phonon spectrum in the presence of a soliton, we shall first briefly describe the phonon spectrum in a soliton-free polyacetylene within the mean-field approximation. In the discrete model of Su, Schrieffer, and Heeger, the bare photon spectra are given by

$$\omega_A^2(k)=\omega_Q^2\sin^2\left[\frac{a}{2}k\right],$$

and (1)

$$\omega_O^2(k)=\omega_Q^2\cos^2\left[\frac{a}{2}k\right],$$

where $\omega_A(k)$ and $\omega_O(k)$ are the acoustic- and optical-phonon frequencies, respectively, and a is the lattice constant. When the electron-loop corrections are included, the optical frequency is modified as

$$\omega_O^2(k)=\omega_Q^2[2\lambda F(\eta)]\cos^2\left[\frac{a}{2}k\right]$$
$$=\omega_0^2F(\eta)\cos^2\left[\frac{a}{2}k\right], \quad (2)$$

while the correction to the acoustic-phonon frequency is negligible.[15] Here,

$$F(\eta)=\eta^{-1}(1+\eta^2)^{1/2}\sinh^{-1}\eta, \quad (3)$$

and

$$\eta=\tfrac{1}{2}(\xi k),$$
$$\omega_0=(2\lambda)^{1/2}\omega_Q, \quad (4)$$
$$\xi=v_F/\Delta,$$

and λ is the dimensionless coupling constant.

The phonon spectra, Eqs. (1) and (2), are shown in Fig. 1. The spectra are essentially same as that calculated by Schulz[16] for the case $k_F=\pi/2a$. Furthermore, in the region of small k (i.e., $ak \ll 1$) the present results agree with those obtained by Mele and Rice[17] for the finite discrete system, although in the region $ak\simeq\pi/2$, our results differ from theirs. This may be due to the coupling with other modes, which is not considered in the present model. The derivation of Eq. (2) is given in Appendix A.

Here we note simply that the electronic polarization induces a large modification on the optical phonon but has little effect on the acoustic phonon. In the following we shall consider a system described by the Hamiltonian[3]:

$$H_c=\frac{1}{2g^2}\int dx[\dot{\Delta}^2(x)+\omega_Q^2\Delta^2(x)]$$
$$+\sum_s\int dx\,\psi_s^\dagger(x)[-iv_F\sigma_3\partial_x$$
$$+\sigma_1\Delta(x)]\psi_s(x), \quad (5)$$

where

$$\omega_Q^2=4K/M,$$
$$\Delta(x)=g(a/M)^{-1/2}\tilde{y}(x), \quad (6)$$

and $\tilde{y}_n=(-)^n y_n$ is the staggered lattice displacement. A dot on $\Delta(x)$ implies the time derivative. In most of previous analysis of the Hamiltonian (5), the first term has been neglected. To explore the role of this term on soliton is one of the principle objectives of the present paper.

In the following we shall first determine the phonon spectrum of a polyacetylene in the presence of a soliton. For this purpose we shall first calculate $\langle[\sigma_1,\sigma_1]\rangle(p,p')$, which gives rise to the mean-field correction to the phonon spectrum. Indeed, the phonon frequency in the presence of a soliton is given by solving

$$\omega^2\psi(p)=\omega_Q^2\cos^2\left[\frac{a}{2}p\right]$$
$$\times\left[\psi(p)-\frac{\lambda}{N_0}\int\frac{dp'}{2\pi}\chi(p,p')\psi(p')\right], \quad (7)$$

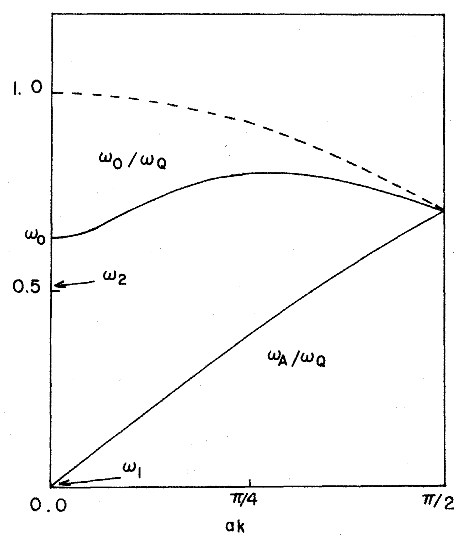

FIG. 1. Phonon frequencies in the SSH model are shown. The broken line represents the bare phonon frequencies, while the solid lines are the phonon frequencies where the electron-loop corrections are included. We have chosen $\lambda=0.2$ in the above calculation. ω_1 and ω_2 are two bound phonon states, which are generated in the presence of a soliton.

where

$$\chi(p,p')=\langle[\sigma_1,\sigma_1]\rangle(p,p') , \quad (8)$$

$N_0=(\pi v_F)^{-1}$ is the density of states for a one-spin state, and $\lambda=g^2N_0\omega_Q^{-2}$.

Making use of the method developed by Kivelson *et al.*[18] it is possible to separate $\chi(p,p')$ as

$$\chi(p,p')=4\pi N_0\left\{\left[\ln\left[\frac{W}{\Delta}\right]-F(\eta)\right]\delta(p-p')+\xi\,\mathrm{csch}[\pi(\eta-\eta')][\Phi(\eta)-\Phi(\eta')]+\xi\Phi(\eta,\eta')\right\} , \quad (9)$$

where

$$\Phi(\eta)=-\tfrac{1}{2}\int_{-\infty}^{\infty}dq\coth[\pi(q-\eta)]\times[q^{-1}(1+q^2)^{-1/2}\sinh^{-1}q+\tfrac{1}{2}\mathrm{Im}([q(q+i)]^{-1/2}\sin^{-1}\{2[q(q+i)]^{1/2}\})] , \quad (10)$$

$$\Phi(\eta,\eta')=\frac{\pi}{4}\int_{-\infty}^{\infty}dq(1+4q^2)^{-1/2}\mathrm{sech}[\pi(q-\eta)]\mathrm{sech}[\pi(q-\eta')] , \quad (11)$$

and $\eta=\frac{1}{2}(\xi p)$ and $\eta'=\frac{1}{2}(\xi p')$ and W is the full electronic bandwidth. Note that

$$\Delta=W\exp\left[-\frac{1}{2\lambda}\right] . \quad (12)$$

We shall give the derivation of Eq. (9) in Appendix B, since it is rather involved. Equation (7) is further simplified as

$$\omega^2\psi(p)=\omega_0^2\cos^2\left[\frac{a}{2}p\right]\left[F(\eta)\psi(p)-\int_{-\infty}^{\infty}K(\eta,\eta')d\eta'\psi(p')\right] , \quad (13)$$

with

$$K(\eta,\eta')=2\,\mathrm{csch}[\pi(\eta-\eta')][\Phi(\eta)-\Phi(\eta')]+2\Phi(\eta,\eta') , \quad (14)$$

and ω_0 and $F(\eta)$ have already been defined in Eqs. (3) and (4).

It appears a little difficult to make further progress with Eq. (13). However, if one imposes limits to the region of small p (i.e., $ap \ll 1$), Eq. (13) can be approximated by a Schrödinger-like equation,

$$\omega^2\tilde{\psi}(x)=\omega_0^2\left[\left[1-\frac{1}{12}\frac{d^2}{dx^2}-0.0206\,\mathrm{sech}^2x\right]\tilde{\psi}(x)-\tfrac{1}{2}\mathrm{sech}x\int dy\,K_0(|x-y|)\mathrm{sech}y\,\tilde{\psi}(y)\right] , \quad (15)$$

where $K_0(z)$ is the modified Bessel function, and $\tilde{\psi}(x)$ is the Fourier transform of $\psi(p)$. Here we take ξ as the unit of length. In deriving Eq. (15), we have neglected higher-order terms in d^2/dx^2. Then, Eq. (15) is solved variationally as

$$\left[\frac{\omega}{\omega_0}\right]^2=1+\left[\frac{1}{12}\int_{-\infty}^{\infty}dx\left[\frac{df}{dx}\right]^2-0.0206\int_{-\infty}^{\infty}dx\,\mathrm{sech}^2xf^2-\tfrac{1}{2}\int\int_{-\infty}^{\infty}dx\,dy\,\mathrm{sech}xf(x)\mathrm{sech}yf(y)K_0(|x-y|)\right]\left[\int_{-\infty}^{\infty}f^2dx\right]^{-1} . \quad (16)$$

By carefully choosing forms of variational functions $f_1(x)=\mathrm{sech}^{\nu}x$ and $f_2(x)=\tanh x\,\mathrm{sech}^{\mu}x$ where ν and μ are variational parameters, we find two bound states with

$$\omega_1^2=0.104\omega_0^2 \text{ with } \nu=1.95 , \quad (17)$$

and

$$\omega_2^2=0.737\omega_0^2 \text{ with } \mu=1.25 , \quad (18)$$

which curiously resemble the bound-state spectrum of the ϕ^4 theory.[7]

We note that the present results are also qualitatively very similar to those obtained earlier by Mele and Rice[17] within a phenomenological model. We should stress, however, that quantitatively those frequencies in the phenomenological model are somewhat different from ours. The above results may be somewhat improved by including the next-order terms,

$$\delta\omega^2 = -\omega_0^2 \left\{ \frac{1}{120} \int_{-\infty}^{\infty} \left[\frac{d^2 f}{dx^2} \right]^2 dx + 0.0169 \int_{-\infty}^{\infty} \mathrm{sech}^2 x \left[-2f\frac{d^2 f}{dx^2} + \left[\frac{df}{dx} \right]^2 \right] dx \right\} \left[\int_{-\infty}^{\infty} dx\, f^2 \right]^{-1} . \tag{19}$$

With these corrections, ω_1^2 and ω_2^2 are now given by $\omega_1^2 = 0.067\omega_0^2$ and $\omega_2^2 = 0.66\omega_0^2$, respectively.

From the translation invariance of the system the lowest eigenvalue should be $\omega_1^2 = 0$ with $f_1(x) = \mathrm{sech}^2 x$. Indeed, the result (17) is consistent with this because of the approximation introduced in going from Eq. (13) to Eq. (15). On the other hand, we believe that the value of ω_2 thus determined should be quite accurate; at least the first digit is reliable. This second mode is Raman active but does not appear in the infrared absorption.

Because of a close similarity between the continuum version of the SSH model and the ϕ^4 theory, it may be useful to compare these two cases. In Table I we present ω_1/ω_0, ω_2/ω_0, and the phase shift $\delta(k)$ for two models. In the case of the ϕ^4 theory, momentum k is normalized by ω_0/c, where ω_0 is the boson mass.

III. QUANTUM CORRECTION

In order to calculate the quantum correction to the soliton energy E_s, we need the phase shift suffered by phonons due to the presence of a soliton as well. Again, we shall determine the phase shift $\delta(k)$, by making use of the Bethe formula,[19] which should be accurate in the small k region. For this purpose we have to first find a solution $u_O(x)$, which satisfies

$$\mathscr{L}(u_O(x)) = 0 , \tag{20}$$

where

$$\mathscr{L}(u(x)) = -\frac{1}{12}\frac{\partial^2}{\partial x^2} u(x) - 0.0206\, \mathrm{sech}^2 x\, u(x) - \tfrac{1}{2}\, \mathrm{sech} x \int dy\, K_0(|x-y|) \times \mathrm{sech} y\, u(y) , \tag{21}$$

and

$$u_O(0) = 0 . \tag{22}$$

Furthermore, u_0 depends linearly on x for $x \gg 1$. In analogy to the u_0 solution in the case of the ϕ^4 theory we choose

$$u_O(x) = \tanh x + \alpha x + \beta x \tanh^2 x , \tag{23}$$

with α and β as variational parameters, which are determined so as to minimize the norm $||\mathscr{L}(u_0)||$. We find $\alpha = 0.21$ and $\beta = -1.04$, with $||\mathscr{L}(u_0)||^2 \sim 10^{-3}$. In terms of α and β, the scattering length b and the effective range r are given by

$$b = -(\alpha+\beta)^{-1} \cong 1.20 ,$$

and (24)

$$r = 2\int_0^{\infty} (v_0^2 - u_0^2)\, dx = 0.936 ,$$

where

$$v_0 = 1 + (\alpha+\beta)x .$$

Finally, the phase shift $\delta(k)$ is given by

$$\delta(k) = -2\tan^{-1}\left[\frac{bk}{1 - \frac{1}{2} brk^2} \right] , \tag{25}$$

where k is in the unit of ξ^{-1}. A factor of 2 in front of the right-hand side (rhs) of Eq. (25) arises from the definition of the phase shift in the one-dimensional system. The phase shift decreases monotonically from $\delta(0) = 2\pi$ to $\delta(\infty) = 0$ as k in-

TABLE I. The phonon spectra in the presence of a soliton in the TLM model and the ϕ^4 theory are shown. Here ω_1 and ω_2 are the frequencies of the localized modes and $\delta(k)$ is the phase shift of the phonon with momentum k.

Model	ω_1/ω_0	ω_2/ω_0	$-\tan[\frac{1}{2}\delta(k)]$
SSH	0	0.82	$1.2k/(1-0.56k^2)$
ϕ^4	0	$\sqrt{3}/2$	$1.5k/(1-0.5k^2)$

creases consistent with Levinson's theorem. With these results we can calculate the quantum correction to the soliton energy,

$$E_s=\frac{2}{\pi}\Delta+\delta E_s\ , \tag{26}$$

where

$$\delta E_s=\tfrac{1}{2}\sum_n(\omega_{sn}-\omega_{on})\ , \tag{27}$$

and ω_{sn} is the phonon frequency in the presence of a soliton, while ω_{on} is the phonon frequency in the perfectly dimerized state. Equation (27) is transformed as

$$\delta E_s=\tfrac{1}{2}\omega_2+\frac{1}{2\pi}\omega_0\int_0^{k_F}dk[F(\eta)]^{1/2}\cos\left[\frac{ak}{2}\right]\frac{d\delta(k)}{dk}\simeq-0.60\omega_0\ . \tag{28}$$

Comparing this mass correction to the one for the ϕ^4 theory where

$$\delta E_s=\left[\frac{1}{4\sqrt{3}}-\frac{3}{2\pi}\right]\omega_0\simeq-0.33\omega_0\ ,$$

the present mass renormalization appears rather large. We believe that this is due to the particular circumstance that in the SSH model the integral in Eq. (28) is cut off at the Fermi momentum, while in the ϕ^4 theory, the integral actually diverges logarithmically with the cutoff, which should be canceled by the other term[7] in E_s. Since $\omega_0/2\Delta\simeq10^{-1}$, the quantum correction is negative and roughly $\frac{1}{4}$ of E_s. Therefore, as far as the soliton energy is concerned, the quantum correction is sizable.

By making use of the method developed by Maki and Takayama,[20] we can also calculate the quantum correction to the soliton mass. However, it is easily seen the correction is of the order of $m(\omega_0/W)$, where m is the electron mass. Since the soliton mass is of the order of m, the present correction is less than the order of $10^{-2}m$, which is completely negligible.

IV. CONCLUDING REMARKS

Making use of the continuum version of the Su, Schrieffer, and Heeger (SSH) model, we have examined the quantum corrections to the soliton in polyacetylene. We have shown that the soliton produces a drastic modification in the optical-phonon spectrum; the soliton induces two bound states of phonon; one with $\omega=0$ corresponding to the translational motion of soliton, and the other with $\omega\simeq0.8\omega_0$ which should be Raman active. Furthermore, the effect of the modified phonon spectrum on the soliton energy is found rather important. Therefore, the examination of the quantum corrections to other properties of soliton are certainly desirable.

We note also that by eliminating $\Delta(x,t)$ our Hamiltonian (5) is transformed into

$$H=\sum_s\int dx\,\overline{\psi}_s(x,t)(-v_F\sigma_2\partial_x)\psi_s(x,t)-\tfrac{1}{2}\tilde{g}^2\sum_{ss'}\int dx\int dt'\overline{\psi}_s(x,t)\psi_s(x,t)\overline{\psi}_{s'}(x,t')\psi_{s'}(x,t')D(t-t')\ , \tag{29}$$

where

$$\overline{\psi}_s=\psi_s^+\sigma_1\ ,$$

$$D(t-t')=2i\omega_Q e^{-i\omega_Q|t-t'|}\ ,$$

and

$$\tilde{g}=g\omega_Q^{-1}=(\lambda/N_0)^{1/2}\ , \tag{30}$$

which reduces to the Gross-Neveu Hamiltonian in the limit $\omega_Q\to\infty$ (or M the ionic mass tends to 0), keeping $\tilde{g}$ finite. In the limit ω_Q tends to 0 (or $M\to\infty$), on the other hand, the mean-field theory becomes exact. Therefore, the Takayama–Lin-Liu–Maki (TLM) theory,[3] alias the SSH model, lies in between the mean-field theory and the full quantum theory of Gross-Neveu model. In this context our analysis of E_s demonstrates within perturbation calculation that the dimerized state in the SSH model is stable even in the presence of quantum corrections, which follows from the fact $E_s>0$ [see Eqs. (26) and (28)]. Furthermore, we can prove the stability of the polaron state[10,12,13] in the SSH model as follows. The polaron state is stable when

$$E_p\le2E_s\ , \tag{31}$$

where

$$E_p = \frac{2\sqrt{2}}{\pi}\Delta + \delta E_p \ ,$$

and δE_p (<0) is the quantum correction to E_p. If the accepted value of ω_0 in polyacetylene is inserted, the rhs of Eq. (31) becomes

$$2E_s \simeq \frac{3}{\pi}\Delta \ . \tag{32}$$

Therefore, it is easy to see that Eq. (31) is satisfied for polyacetylene even when δE_p is neglected. It will be of great interest, therefore, to explore the consequence of the polaron state in polyacetylene.

ACKNOWLEDGMENT

We are grateful to Lu Yu for providing us with his notes for the calculation of optical absorption due to soliton in polyacetylene, which were extremely helpful to us. One of us (K.M.) would like to thank E. Fradkin and J. Hirsch at the Institute for Theoretical Physics at the University of California at Santa Barbara for illuminating conversations on the relation between the SSH model and the Gross-Neveu model. The present work was supported by the National Science Foundation under Grant No. DMR 79-16903.

APPENDIX A: THE OPTICAL-PHONON—SELF-ENERGY CORRECTION IN THE PERFECTLY DIMERIZED STATE

The self-energy correction due to the single electron loop is given by

$$\prod_{O}(k,\omega) = g^2\omega_Q^{-2}\cos^2\left[\frac{a}{2}k\right]\langle[\sigma_1,\sigma_1]\rangle(k,\omega) \ . \tag{A1}$$

Making use of the electron Green's function in the perfectly dimerized state,

$$G^0(k,\omega_n) = (i\omega_n - v_F k\sigma_3 - \Delta\sigma_1)^{-1} \ , \tag{A2}$$

we obtain

$$\langle[\sigma_1,\sigma_1]\rangle(k) = 2T\sum_n \int \frac{dp}{2\pi}\mathrm{Tr}[\,\sigma_1 G^0(\omega_n,p)\sigma_1 \times G^0(\omega_n,p+k)] \ . \tag{A3}$$

In the above expressions we have neglected the phonon frequencies, as they are much smaller than 2Δ. At $T=0$ K the sum over the Matsubara frequency ω_n is replaced by an integral and we obtain

$$\langle[\sigma_1,\sigma_1]\rangle = 2N_0\left[\ln\left[\frac{W}{\Delta}\right] - F(\eta)\right] \ , \tag{A4}$$

where

$$F(\eta) = \eta^{-1}(1+\eta^2)^{1/2}\sinh^{-1}\eta \ , \tag{A5}$$

and $N_0 = (\pi v_F)^{-1}$, and $\eta = \frac{1}{2}\xi k$.

Substituting (A4) into (A1), we obtain Eq. (2) in the text, where

$$\lambda = g^2 N_0 \omega_Q^{-2} \ ,$$

and we have made use of the relation (12).

APPENDIX B: THE OPTICAL-PHONON— SELF-ENERGY CORRECTION IN THE PRESENCE OF SOLITON

We shall limit ourselves to the optical phonon only for simplicity, since the effect on the acoustic-phonon spectrum due to a soliton is rather small. We shall calculate $\langle[\sigma_1,\sigma_1]\rangle(p,p') \equiv \chi(p,p')$ in the presence of a soliton. As in the calculation of the optical absorption,[18] $\chi(p,p')$ splits in two terms $\chi(p,p') = \chi^{(1)}(p,p') + \chi^{(2)}(p,p')$, where $\chi^{(1)}(p,p')$ involves the midgap state, while $\chi^{(2)}(p,p')$ is given in terms of the scattering states only. Furthermore, $\chi^{(1)}(p,p')$ and $\chi^{(2)}(p,p')$ are given by

$$\chi^{(1)}(p,p') = 4\frac{L}{2\pi}\int_{-\infty}^{\infty} dk\, E_k^{-1} M_k(p) M_k^*(p') \tag{B1}$$

and

$$\chi^{(2)}(p,p') = 4\left[\frac{L}{2\pi}\right]^2 \int\int_{-\infty}^{\infty} dk\, dk' (E_k + E_k')^{-1} M_{k,k'}(p) M_{k,k'}^*(p') \ , \tag{B2}$$

where

$$M_k(p) = \frac{i}{2\sqrt{L\xi}}\int dx\, e^{i(k-p)x}\mathrm{sech}\left[\frac{x}{\xi}\right] = -\frac{\pi}{2}i\left[\frac{\xi}{L}\right]^{1/2}\mathrm{sech}\left[\frac{\pi}{2}\xi(k-p)\right] \ , \tag{B3}$$

$$M_{k,k'}(p)=-\frac{i}{2L}\int dx\, e^{i(k-k'-p)x}\left[\frac{k'}{E'_k}+\frac{k}{E_k}+i\Delta(x)\left[\frac{1}{E_k}-\frac{1}{E'_k}\right]\right]$$
$$=-\frac{i}{L}\left\{(\cos\phi+\cos\phi')\frac{\sin[(L/2)(k-k'-p)]}{k-k'-p}\right.$$
$$\left.-(\sin\phi-\sin\phi')\left[\frac{\pi}{2}\xi\,\mathrm{csch}\left[\frac{\pi}{2}\xi(k-k'-p)\right]-\frac{\cos[(L/2)(k-k'-p)]}{k-k'-p}\right]\right\}, \quad \text{(B4)}$$

$\phi=\tan^{-1}(\Delta/k)$, $\phi'=\tan^{-1}(\Delta/k')$, and $E_k=(k^2+\Delta^2)^{1/2}$. Hereafter we shall put $v_F=1$ for simplicity. Equations (B3) and (B4) follow from the exact electron solutions in the presence of a soliton:

$$\psi_B=\begin{bmatrix}1\\-i\end{bmatrix}\frac{1}{2\sqrt{\xi}}\mathrm{sech}\left[\frac{x}{\xi}\right], \quad \text{(B5)}$$

$$\psi_k^{\pm}=\frac{e^{ikx}}{2\sqrt{L}}\begin{bmatrix}1\pm[k+i\Delta(x)]/E_k\\ i(1\mp[k+i\Delta(x)]/E_k)\end{bmatrix}, \quad \text{(B6)}$$

Furthermore, a small correction in the normalization of ψ_k cancels out exactly the correction terms due to the change in the electron density of states. Substituting (B3) into (B1), we easily find $\chi^{(1)}(p,p')$:

$$\chi^{(1)}(p,p')=\pi^2\xi^{-1}\int_{-\infty}^{\infty}dk\,E_k^{-1}\mathrm{sech}\left[\frac{\pi}{2}\xi(k-p)\right]\mathrm{sech}\left[\frac{\pi}{2}\xi(k-p')\right]. \quad \text{(B7)}$$

On the other hand, in order to calculate $\chi^{(2)}(p,p')$, we shall first reduce $M_{k,k'}(p)$ to

$$M_{k,k'}(p)=-\frac{2i\cos[\frac{1}{2}(\phi'+\phi)]}{L}\left[(-1)^{\nu-\nu'}\frac{\cos[(L/2)p]}{k-k'-p}\right.$$
$$\left.+\sin[\tfrac{1}{2}(\phi'-\phi)]\frac{\pi}{2}\xi\,\mathrm{csch}\left[\frac{\pi}{2}\xi(k-k'-p)\right]\right], \quad \text{(B8)}$$

where use is made of the boundary conditions[18] on k and k':

$$Lk+\phi=2\pi\nu\,,$$
$$Lk'+\phi'=2\pi(\nu'+\tfrac{1}{2})\,. \quad \text{(B9)}$$

(Note here k is associated with electron, while k' is associated with hole.) Substituting this into (B2), $\chi^{(2)}(p,p')$ is broken down to two terms:

$$\chi^{(2)}(p,p')=\chi_1^{(2)}(p,p')+\chi_2^{(2)}(p,p')\,. \quad \text{(B10)}$$

The first term is calculated as follows:

$$\chi_1^{(2)}(p,p')=\left[\frac{2}{\pi}\right]^2\int\int_{-\infty}^{\infty}dk\,dk'(E_k+E_{k'})^{-1}\cos^2[\tfrac{1}{2}(\phi'+\phi)]\frac{\cos[(L/2)p]}{(k-k'-p)}\frac{[(L/2)p']}{(k-k'-p')}$$
$$=\left[\frac{2}{\pi}\right]^2\int_{-\infty}^{\infty}dq\left[\ln\frac{W}{\Delta}-F(\tfrac{1}{2}\xi q)\right]\frac{\cos[(L/2)p]\cos[(L/2)p']}{p-p'}\left[\frac{1}{q-p}-\frac{1}{q-p'}\right]$$
$$\simeq\frac{4}{\pi}\left[\ln\frac{W}{\Delta}-F(\tfrac{1}{2}\xi p)\right]\frac{\sin[(L/2)(p-p')]}{p-p'}=4\left[\ln\frac{W}{\Delta}-F(\eta)\right]\delta(p-p')\,, \quad \text{(B11)}$$

where use is made of the relation

$$\int_{-\infty}^{\infty}dq\frac{1}{q-p}=\sum_{n=-\infty}^{\infty}\left[n+\frac{1}{2}-\frac{Lp}{2\pi}\right]^{-1}=\psi\left[\frac{1}{2}-\left\{\frac{Lp}{2\pi}\right\}\right]-\psi\left[\frac{1}{2}+\left\{\frac{Lp}{2\pi}\right\}\right]=\pi\tan[(L/2)p]\,, \quad \text{(B12)}$$

where

$$\{z\}=z \bmod 1\ , \tag{B13}$$

and $\psi(z)$ is the diagamma function. Therefore, $\chi_1^{(2)}(p,p')$ recovers the term in the perfectly dimerized state. On the other hand, $\chi_2^{(2)}(p,p')$ is given by

$$\begin{aligned}\chi_2^{(2)}(p,p')&=\pi^{-2}\int\int_{-\infty}^{\infty} dk\, dk'(E_k+E_{k'})^{-1}(\sin\phi-\sin\phi')^2\\ &\qquad\times\left[\frac{\pi}{2}\xi\right]^2 \operatorname{csch}\left[\frac{\pi}{2}\xi(k-k'-p)\right]\operatorname{csch}\left[\frac{\pi}{2}\xi(k-k'-p)\right]\\ &=4\operatorname{csch}\left[\frac{\pi}{2}\xi(p-p')\right][\Phi(p)-\Phi(p')]\ ,\end{aligned} \tag{B14}$$

where

$$\begin{aligned}\Phi(p)&=\tfrac{1}{16}\xi^2\int\int_{-\infty}^{\infty} dk\, dk'(E_k+E_{k'})^{-1}(\sin\phi-\sin\phi')^2\coth\left[\frac{\pi}{2}\xi(k-k'-p)\right]\\ &=\xi\int_{-\infty}^{\infty} dq\, F_1(q)\coth\left[\frac{\pi}{2}\xi(q-p)\right]\ ,\end{aligned} \tag{B15}$$

and

$$\begin{aligned}F_1(q)&=\xi\int_{-\infty}^{\infty} dk\frac{1}{E_k^2E_{k-q}^2}\frac{(E_k-E_{k-q})^2}{(E_k+E_{k-q})}\\ &=-\frac{1}{4}\left[\eta^{-1}(1+\eta^2)^{-1/2}\sinh^{-1}\eta-\tfrac{1}{2}\operatorname{Re}\left[\frac{1}{\sqrt{\eta(\eta+i)}}\sin^{-1}[2\sqrt{\eta(\eta+i)}]\right]\right]\ ,\end{aligned} \tag{B16}$$

where $\eta=\frac{1}{2}(\xi q)$. From (B7), (B11), and (B14) we obtain Eq. (13) in the text. It is difficult to make further progress analytically However, for small η, (B16) can be calculated as

$$F_1(q)\cong\tfrac{1}{2}\left(\tfrac{1}{15}\eta^2-\tfrac{4}{63}\eta^4+\tfrac{872}{1365}\eta^6+\cdots\right)\ , \tag{B17}$$

which yields

$$\Phi(p)\cong 0.0103p+0.008\,425p^3-0.0026p^5\ , \tag{B18}$$

where we write ξp as p.

Then, for small p and p', $\chi^{(2)}(p,p')$ becomes

$$\chi_2^{(2)}(p,p')=4\operatorname{csch}\left[\frac{\pi}{2}(p-p')\right][0.0103(p-p')+0.008\,425(p^3-p'^3)]\ , \tag{B19}$$

of which the Fourier transform is given by

$$\tilde{\chi}_2^{(2)}(p,p')=8\operatorname{sech}^2 x\,\delta(x-x')[0.0103+0.008\,425(\partial_x^2+\partial_x\partial_{x'}+\partial_{x'}^2)]\ . \tag{B20}$$

Similarly, $\chi_1^{(2)}(p,p')$ can be expanded as

$$\chi_1^{(2)}(p,p')=4\left[\ln\frac{W}{\Delta}-\left[1+\frac{1}{12}p^2-\frac{1}{120}p^4\cdots\right]\right]\delta(p-p')\ , \tag{B21}$$

whose Fourier transform is given by

$$\tilde{\chi}_1^{(2)}(x,x')=4\left[\ln\frac{W}{\Delta}-\left[1-\frac{1}{12}\frac{d^2}{dx^2}-\frac{1}{120}\frac{d^4}{dx^4}\cdots\right]\right]\delta(x-x')\ . \tag{B22}$$

Combining these expressions, we easily find Eq. (15) of the text.

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