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SOLITON EXCITATIONS IN POLYACETYLENE AND RELATIVISTIC FIELD THEORY MODELS*

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A continuum model of a Peierls-dimerized chain, as described generally by Brazovskii and discussed for the case of polyacetylene by Takayama, Lin-Liu and Maki (TLM), is considered. The continuum (Bogliubov-de Gennes) equations arising in this model of interacting electrons and phonons are shown to be equivalent to the static, semiclassical equations for a solvable model field theory of self-coupled fermions – the $N = 2$ Gross-Neveu model. Based on this equivalence we note the existence of soliton defect states in polyacetylene that are additional to, and qualitatively different from, the amplitude "kinks" commonly discussed. The new solutions do not have the topological stability of kinks but are essentially conventional strong-coupling polarons in the dimerized chain. They carry spin ($\frac{1}{2}$) and charge ($\pm e$). In addition, we discuss further areas in which known field theory results may apply to a Peierls-dimerized chain, including relations between phenomenological ϕ^4 and continuum electron-phonon models, and the structure of the fully quantum versus mean field theories.

1. Introduction

The subject of intrinsic defect (or inhomogeneous) states in conjugated polymers has received close renewed attention in the last two years, both experimentally and theoretically [1]. The simplest case is that of dimerized polyacetylene ($(CH)_x$) and this has been studied in especial detail [2], including possible soliton (defect)-based doping and transport characteristics, which are of great technological potential [2].

Previous discussions [1–10] have focused almost exclusively on the *kink*-like soliton states. These appear as extended *structural* inhomogeneities in the C-C backbone of $(CH)_x$ interpolating between the two degenerate dimerized phases of trans-$(CH)_x$. Again, most treatments have viewed $(CH)_x$ as a prototype Peierls-dimerized system, neglecting electron-electron interactions. Within the Peierls electron-phonon interaction models, band-gap *electronic* defect levels, necessarily accompanying the structural distortions, are readily determined. With further analysis, spin characteristics can also be identified. In their theoretical analysis, Su, Schrieffer and Heeger [3] (SSH) worked directly with a discrete lattice, adiabatic mean-field hamiltonian and imposed a hyperbolic tangent (tanh) kink form on the

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staggered atomic displacement coordinate (the Peierls amplitude order parameter). Using standard 1-electron Green function theory, they identified the associated electronic defect level and numerically optimized the tanh profile. This suggested a defect ~ 15 C-C units wide so that for most properties discrete lattice effects are not expected to be important. It is, therefore, not surprising that Brazovskii [5] and Takayama, Lin-Liu and Maki [6] (TLM) have obtained many of the SSH results working in a continuum limit of the SSH model. Brazovskii and TLM show that the tanh order-parameter profile is an *exact* solution (in the continuum limit) of the self-consistent equations of motion for phonon and electron operators determined in a variational scheme. Although lacking realistic discreteness, this approach has the important advantage of being analytic and therefore is a very useful guide to studies with more complete hamiltonians. The approach has, for instance, been used to study widely separated kink-antikink pairs [11] as well as soliton "lattices," [7] which may play a role in understanding the insulator-metal transition observed [2, 7, 9] under doping in $(CH)_x$.

A less immediate but potentially valuable feature of the continuum model is the connections that exist between it and certain model field theories. It is these connections that we wish to explore and exploit in this paper. Some important aspects of these connections have been noted elsewhere [7, 12] and suggest that a useful dialogue can be established in this area between field theory and condensed matter physics. In particular, we expand here on the previous observation [13]* that a formal equivalence between the equation of a relativistic model field theory and the continuum model of a Peierls-dimerized chain allows one to predict the existence of new inhomogeneous states in materials such as $(CH)_x$. These states (which are essentially strong polarons**) have, in fact, been seen very recently in discrete lattice simulations [15]*** and are in good agreement with the continuum theory [13]. In addition, based on recent model field theory studies, we comment on the usefulness of phenomenological ϕ-four (ϕ^4) field theory descriptions of polyacetylene which have been advocated by some authors [8–10] and questioned by others [3, 6].

* Although the emphasis in these two articles is quite different, the major new results in each is the existence of the polaron excitation within the standard continuum model of $(CH)_x$; the results of the two calculations of this excitation are in complete agreement.

** It is straightforward to construct a conventional 2-band polaron theory for the Peierls-dimerized chain. This will be reported separately (see also ref. [14a]). Here we only note that, as is common in one-dimensional polaron theories (e.g., ref. [14b]), certain approximations reduce the polarons to solutions of a non-linear Schrödinger (NLS) equation. Recall that NLS is a valid description of extended, *small* amplitude breathers of both sine-Gordon and ϕ^4-like models. We emphasize that the strong-coupling polaron solution (3.8) solving the TLM equations is distinctly non-perturbative. The static polaron solution found in sect. 3 is, of course, the lowest member of a polaron *band*. This band corresponds to the dynamic NLS solitons or to the $(CH)_x$ analogs of the Gross-Neveu breathers discussed in sect. 4. Finally, we note that polarons do not require degenerate ground states as do kinks. Thus they can be anticipated as stable excitations in a much more general class of conjugated polymers than trans-$(CH)_x$, including cis-$(CH)_x$ (c.f. Brazovskii and Kirova, ref. [13]).

*** We are especially grateful to these authors for detailed discussion of their results.

More specifically, we note an exact formal equivalence between the Brazovskii/TLM continuum equations [5, 6] for $(CH)_x$ and the *static*, *semiclassical* equations for a recently studied solvable model field theory: the $N = 2$ Gross-Neveu model [16, 17]. Using this equivalence, we establish the existence of localized solutions additional to, and qualitatively different from, the amplitude kinks on which previous discussions have focussed. These new localized solutions imply the existence of further soliton-like excitations (polarons) in polyacetylene. From a solid-state perspective the polaron state is entirely expected qualitatively. However, the field theory connection offers the clearest derivation and allows us to unify kinks and polarons within the same model. In the present article we shall concentrate on presenting the polaron solutions and clarifying the equivalence that has led to their discovery. In sect. 2 we introduce the continuum model for polyacetylene and show that, in the mean field approximation, it leads to a set of coupled equations – also called [6] the Bogliubov-de Gennes equations – relating the electron and phonon fields. We then show that these same equations have recently arisen in the study of the static solutions to the semiclassical equations of the $N = 2$ Gross-Neveu field theory model. In sect. 3, we discuss the static solutions to the continuum equations for $(CH)_x$ and, using the formal connection to the field theory model and known properties of its solutions, derive the explicit form of the polaron solution in polyacetylene. For completeness, in the appendix we present the necessary details of the construction of the polaron solution directly from the continuum, self-consistent electron phonon equations for $(CH)_x$. In sect. 4 we pursue this field theory connection further by stressing that, beyond this explicit but limited quantitative equivalence of the static equations, there are a number of known or potential qualitative similarities among the Gross-Neveu, self-consistent, continuum electron-phonon, and ϕ^4 (coupled to fermion) models, including time-dependent properties and solutions. Finally, we speculate on the possible implications of field theory models for the fully quantum mechanical treatment of the properties of polyacetylene. In sect. 5 we conclude with a discussion of questions and problems for further research.

Since one of our aims will be to bridge the gap between the condensed matter/many-body and field theory languages, we attempt in the following sections to give more detail than might be necessary in an article for specialists in either discipline separately. Nonetheless, since we must begin somewhere, we assume that serious readers will at least peruse the articles describing the SSH lattice model of polyacetylene [3], its continuum limit [5–7] and the semiclassical analysis of the Gross-Neveu model [16] before studying our results in detail.

2. The continuum electron-phonon and Gross-Neveu models

In this section we introduce both the continuum electron-phonon model of a Peierls-dimerized chain and the Gross-Neveu field theory and establish an exact

formal equivalence for the static, semiclassical (mean field) equations of these theories. Since polyacetylene is the prototype Peierls-dimerized material, we shall use these nomenclatures interchangeably.

Beginning from the lattice hamiltonian of SSH, a sequence of approximations described (for example) by TLM leads in the continuum limit to an effective adiabatic mean-field hamiltonian in terms of the (real) gap parameter Δ and electron field Ψ of the form

$$H = \int \mathrm{d}y \left\{ \frac{\omega_Q^2}{g^2} \Delta^2(y) + \Psi^\dagger(y) \left[-iv_F \sigma_3 \frac{\partial}{\partial y} + \Delta(y)\sigma_1 \right] \Psi(y) \right\} \tag{2.1a}$$

$$= \int \mathrm{d}y \left\{ \frac{\omega_Q^2}{g^2} \Delta^2(y) - iv_F u(y) \frac{\partial u}{\partial y}(y) + iv_F v(y) \frac{\partial v}{\partial y}(y) \right.$$

$$\left. + \Delta(y)[u^*(y)v(y) + v^*(y)u(y)] \right\}, \tag{2.1b}$$

where ω_Q^2/g^2 is the net effective electron-phonon coupling constant [3, 6], σ_i; is the ith Pauli matrix and $\Psi(y) = \begin{pmatrix} u(y) \\ v(y) \end{pmatrix}$. For consistency with the notion of TLM we have suppressed the electron spin index, s. Variation of H with respect to the electron field yields the equation of motion for the single-particle electron wave functions,

$$E_n u_n(y) = -iv_F \frac{\partial}{\partial y} u_n(y) + \Delta(y) v_n(y), \tag{2.2a}$$

$$E_n v_n(y) = +iv_F \frac{\partial}{\partial y} v_n(y) + \Delta(y) u_n(y), \tag{2.2b}$$

whereas variation of H with respect to Δ leads to the self-consistent gap equation

$$\Delta(y) = \frac{-g^2}{2\omega_Q^2} \sum_{n,s}{}' (v_n^*(y)u_n(y) + u_n^*(y)v_n(y)). \tag{2.2c}$$

Here, for undoped $(CH)_x$, the summation is over the two spin states (labeled by s) for every energy level (labeled by n) in the valence band; thus the sum is up to the Fermi energy, which is chosen to be zero. In eq. (2.2c) the wave functions are assumed to be normalized to unity:

$$\int_{-\infty}^{\infty} \mathrm{d}y \{ |u_n(y)|^2 + |v_n(y)|^2 \} = 1. \tag{2.3}$$

Eqs. (2.2), which form the basis of the continuum model of polyacetylene, are referred to by TLM as the Bogliubov-de Gennes equations. This terminology stems from their earlier appearance in the theory of inhomogeneous superconductors [18]. To make the present application to polyacetylene clear, we shall henceforth refer to them as the self-consistent, continuum electron-phonon equations.

Perhaps the most striking change in going from the lattice to the continuum theory is in the single electron spectrum. The naive lattice model – that is, the lattice model before Peierls distortion effects are included – has the typical band structure spectrum of a periodic system; in $(CH)_x$, the band is exactly half-filled, as shown in fig. 1a, and, naively, polyacetylene appears to be a metal. When the ground state of the lattice theory is actually calculated [3], the Peierls distortion effects produce a gap in the spectrum at the Fermi surface, as shown in fig. 1b. Since the lower (valence) band is full, $(CH)_x$ is, in fact, an insulator.

To obtain the continuum model, one linearizes the electron spectrum around the Fermi surface. This leads to the (apparently) linear, gapless (Luttinger-like) spectrum shown in fig. 1c and (apparently) reflected in eqs. (2.2a) and (2.2b), in which, assuming $\Delta(y) = 0$ in the ground state, the electron spectrum appears to be simply $E(k) = \pm k v_F$. However, if one actually solves for the ground state in the continuum model, one finds explicitly that the Peierls distortion leads to a (uniform dimerized) ground state with $\Delta = \Delta_0 \neq 0$, so that a gap of $2\Delta_0$ emerges between the (filled) valence band and the (empty) conduction band; this is illustrated in fig. 1d.

Although we shall reserve for sect. 3 most of our discussion of the solutions to (2.2), for purposes of establishing clearly the equivalences with the field theory model we need to exhibit here the explicit form of the ground-state solution to (2.2). One finds [5, 6] that $\Delta(y) = \Delta_0$, where Δ_0 is related to the other parameters of the theory according to

$$\Delta_0 = W \exp\left(-\pi v_F \omega_Q^2 / g^2\right). \tag{2.4}$$

Here W, the full band width, is related, as indicated by figs. 1c, 1d, to the wave vector cut-off K by

$$W = 2\sqrt{K^2 v_F^2 + \Delta_0^2} \simeq 2 K v_F. \tag{2.5}$$

The approximate equality in (2.5) assumes $K v_F \gg \Delta_0$, a weak coupling limit reasonably satisfied in $(CH)_x$ where [3, 6] $W \simeq 10$ eV, $\Delta_0 \simeq 0.75$ eV. The normalized electron wave functions in the valence band – that is, with $E_n < 0$ – are labeled by a continuous wave vector, k, and have the form

$$u_n(x) \equiv u(k; x) = N_k' e^{ikx} \left(\frac{-v_F k + \omega + \Delta_0}{v_F k} \right), \tag{2.6a}$$

$$v_n(x) \equiv v(k; x) = N_k' e^{ikx} \left(\frac{-v_F k - \omega - \Delta_0}{v_F k} \right), \tag{2.6b}$$

with

$$\omega = +\sqrt{k^2 v_F^2 + \Delta_0^2}\,, \qquad E_n \equiv E(k) = -\omega, \tag{2.6c}$$

$$N_k' = \frac{1}{2}\frac{1}{\sqrt{2\pi}}\left(\frac{\omega - \Delta_0}{\omega}\right)^{1/2}. \tag{2.6d}$$

By direct evaluation of the right-hand side of eq. (2.2c) using the electron wave functions in eq. (2.6), one can show that this self-consistent gap equation is satisfied for $\Delta = \Delta_0$ given by equation (2.4) [6].

Actually, eqs. (2.2), thinly disguised, have recently arisen in yet another context: namely, they are exactly equivalent to the *static* versions of the *semiclassical* equations [16] of the $N = 2$ Gross-Neveu model field theory [17]. To see this equivalence, we recall that the Gross-Neveu model is a one-space, one-time dimensional theory of self-coupled fermions, described by the relativistic lagrangian density

$$\mathcal{L}(x) = \sum_{\alpha=1}^{N}\left\{\overline{\Psi}^{\alpha}(x)\left(i\gamma_\mu \frac{\partial}{\partial x_\mu}\right)\Psi^{\alpha}(x)\right\} + \tfrac{1}{2}g_{GN}^2\left(\sum_{\alpha=1}^{N}\overline{\Psi}^{\alpha}(x)\Psi^{\alpha}(x)\right)^2. \tag{2.7}$$

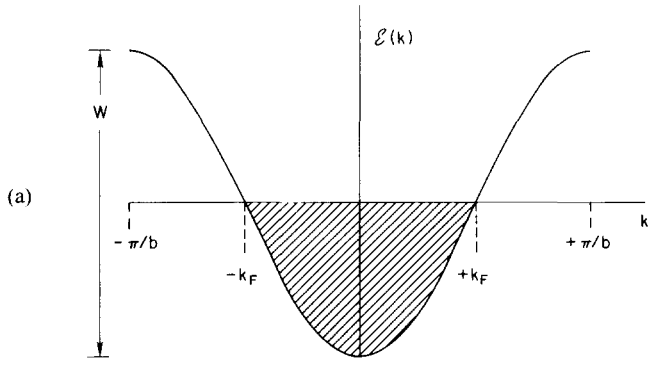

Fig. 1. Successive approximations to the single electron energy levels in $(CH)_x$. (a) The apparent single electron spectrum of a half-filled band material, such as $(CH)_x$, before the Peierls distortion effects are included. W is the full band width. Recall that in $(CH)_x$, $\pi/b = 2k_F$. (b) A schematic illustration of the actual single electron spectrum in $(CH)_x$ after Peierls distortion effects are included. Note the gap, $2\Delta_0$, between the filled valence and empty conduction bands. (c) The approximate Luttinger-like (linear, gapless) electronic spectrum obtained by expanding the spectrum of (a) around $k = k_F$ and shifting the energy scale so that the Fermi energy is zero. The linear dispersion relation is $E(k) = \pm v_F k$. (d) The electronic spectrum produced from (b) when the Peierls distortion and, for $(CH)_x$, consequent dimerization are included. The non-zero gap parameter, Δ_0, is determined self-consistently as described in the text. Note the relation among the full band width, W, the "cut-off" momentum, k_F, and Δ_0, which relation is used in the discussion of renormalization in the text.

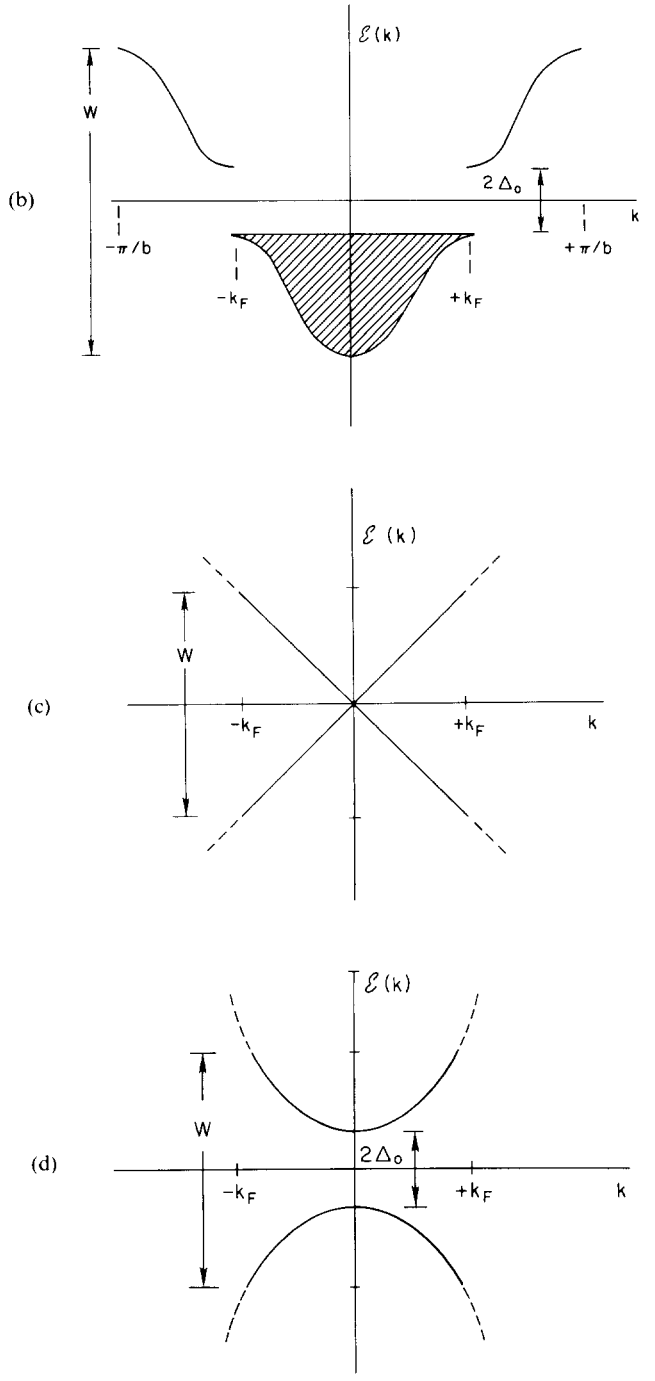

Fig. 1 (continued).

Here γ_μ ($\mu = 0, 1$) are the Dirac γ matrices in two dimensions; we shall use the convention $\gamma_0 = \sigma_3$ and $\gamma_1 = i\sigma_1$. Recall that $\overline{\Psi} = \Psi^\dagger \gamma_0$. For each α, Ψ is a two-component Dirac spinor $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$; the internal SU($N$) symmetry index $\alpha = \{1, \ldots, N\}$ labels the "particle type." Apart from this internal symmetry, the lagrangian possesses a "chiral symmetry", in that it is invariant under $\psi \to \psi' = \gamma_5 \psi$, with $\gamma_5 \equiv \gamma_0 \gamma_1$. This model was originally proposed [17] as an example of an asymptotically free* field theory exhibiting dynamical spontaneous symmetry breaking of the chiral symmetry** [20]. It has also been studied in the semiclassical approximation, and the complete particle spectrum has been calculated [16]. Recently, some exact properties of the full quantum field theory [21, 22], including the exact S-matrix, have been found [21]. For comparison to the continuum model of $(CH)_x$, however, we need to concentrate only on the semiclassical results obtained by Dashen, Hasslacher, and Neveu [16] (henceforth DHN). In their calculation, the Gross-Neveu model was studied in terms of the (equivalent) lagrangian density

$$\mathcal{L}(x) = \sum_{\alpha=1}^{N} \overline{\Psi}^\alpha(x) \left(i\gamma_\mu \frac{\partial}{\partial x_\mu} \right) \Psi^\alpha(x) - g_{\mathrm{GN}} \sigma(x) \sum_{\alpha=1}^{N} \overline{\Psi}^\alpha(x) \Psi^\alpha(x) - \tfrac{1}{2}\sigma^2(x). \tag{2.8}$$

The *formal* field equations resulting from this lagrangian are a Dirac equation

$$\left(i\gamma_\mu \frac{\partial}{\partial x_\mu} - g_{\mathrm{GN}} \sigma(x) \right) \Psi^\alpha(x) = 0, \qquad \alpha = 1, \ldots, N, \tag{2.9a}$$

and a "self-consistency" equation for $\sigma(x)$, which is schematically of the form

$$\sigma(x) = -g_{\mathrm{GN}} \text{“}\overline{\Psi}(x)\Psi(x)\text{”}. \tag{2.9b}$$

Here the quotation marks indicate that the formal expression $\overline{\Psi}(x)\Psi(x)$ must be correctly interpreted (see below). Already these equations, when written in terms of components $\Psi_1(x)$ and $\Psi_2(x)$, are qualitatively strikingly similar to the electron-

* The adjective "asymptotically free" applied to a field theory means that the renormalization group effective momentum-dependent coupling constant, $g_{\mathrm{eff}}(q^2)$, decreases to zero as the momentum squared, q^2, approaches infinity. The interest in "asymptotic freedom" arises primarily because it has been shown that the non-abelian gauge theory currently thought to describe strong interactions – quantum chromodynamics (QCD) – is asymptotically free. Hence simpler theories exhibiting asymptotic freedom are useful theoretical tools. See, for example, ref. [19].

** "Dynamical spontaneous symmetry breaking" occurs when quantum corrections of some sort – 1-loop fermion corrections, in the Gross-Neveu model – lead to a ground state which "breaks" – that is, does not have – a symmetry possessed by the original classical lagrangian. See refs. [17, 20]. We stress that in the semiclassical analysis of the GN only these 1-loop fermion corrections are incorporated. In the fully quantum GN theory (see sect. 4), *all* quantum fluctuations are included.

phonon equations (2.2). To establish that this correspondence can indeed be made exact, we begin by noting that although the fermions in the lagrangians (2.7) and (2.8) appear formally massless, dynamical symmetry breaking [20] implies that the "free" solutions, to eqs. (2.9) have $\sigma(x) = \sigma_0 \neq 0$; this produces a mass gap and leads to the spectrum shown in fig. 2. A comparison of figs. 1 and 2 (correctly) suggests that this dynamical symmetry breaking is the analog of the (uniform) dimerization $\Delta(x) = \Delta_0$ in $(CH)_x$.

To pursue the equivalence further, we note that for a time-independent $\sigma(x)$ the Dirac equation can be studied [16] in terms of the stationary solutions defined by $\Psi^\alpha(x,t) \equiv e^{-i\omega_n t}\Psi^\alpha(n;x)$ for which eq. (2.9a) becomes

$$\left\{\omega_n\gamma_0 + i\gamma_1\frac{\partial}{\partial x} - g_{GN}\sigma(x)\right\}\Psi^\alpha(n;x) = 0, \tag{2.10a}$$

or, in terms of components,

$$\omega_n\Psi_1^\alpha(n;x) = \frac{\partial}{\partial x}\Psi_2^\alpha(n;x) + g_{GN}\sigma(x)\Psi_1^\alpha(n;x), \tag{2.10b}$$

$$\omega_n\Psi_2^\alpha(n;x) = -\frac{\partial}{\partial x}\Psi_1^\alpha(n;x) - g_{GN}\sigma(x)\Psi_2^\alpha(n;x). \tag{2.10c}$$

Here as usual α is the particle-type index. Eq. (2.10) is immediately seen to be precisely equivalent to the electron part of the continuum electron-phonon equa-

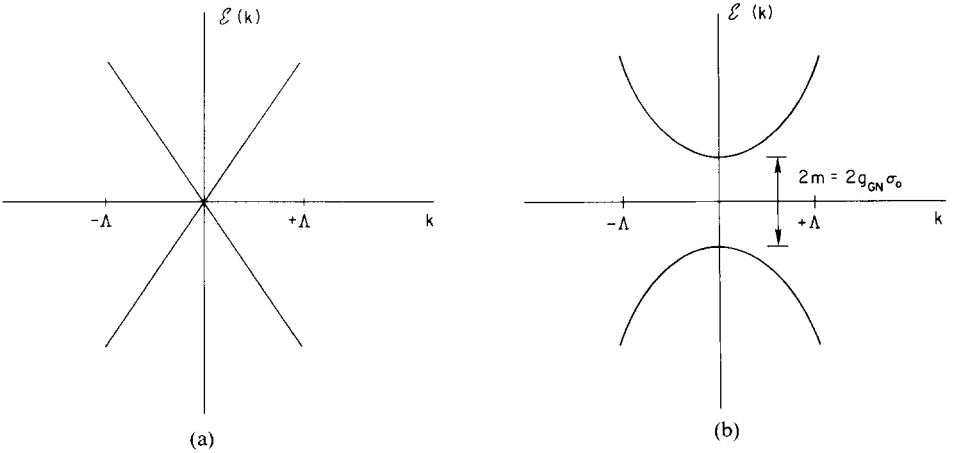

Fig. 2. Successive approximations to the energy spectrum in the Gross-Neveu model. (a) The apparent Luttinger-like (linear, gapless) spectrum for the single particle states of the Dirac equation in the Gross-Neveu model. Here Λ represents the ultraviolet cut-off required to define the theory precisely. (b) The actual "free" fermion spectrum of the Dirac equation in the Gross-Neveu model showing the presence of the mass gap induced by the dynamical symmetry breaking. Again Λ represents the required ultraviolet cut-off.

tions, (2.2a) and (2.2b), by making the transformations $\Psi_1 \to \frac{1}{2}(u+v)$, $\Psi_2 \to -\frac{1}{2}i(u-v)$, $g_{GN}\sigma \to \Delta$, and $y \to v_F x$ and performing some straightforward algebra.

To establish the equivalence of the Gross-Neveu self-consistency equation, (2.9b), and the self-consistent gap equation, (2.2c), requires a little more care. For clarity, we make the argument for constant $\sigma(x) = \sigma_0$. In this case, as shown by DHN, the correct interpretation of the formal equation (2.9b) is

$$Z(\Lambda)\sigma_0 = -g_{GN} \sum_{\substack{\alpha, n \\ \omega_n < 0}} \bar{\Psi}^\alpha(n; x)\Psi^\alpha(n; x). \tag{2.10d}$$

In eq. (2.10d), $Z(\Lambda)$ represents the ultraviolet renormalization – Λ is the ultraviolet momentum cut-off – necessary to cancel the divergence of the infinite (as $\Lambda \to \infty$) sum over $\bar{\Psi}\Psi$. As indicated in eq. (2.10d), this sum is over all states – i.e., all $\Psi^\alpha(n; x)$ satisfying eq. (2.10a) – with energy less than zero. Intuitively, it is clear that this "Dirac negative energy sea" must be filled completely, for otherwise the supposed ground state with $\sigma(x) = \sigma_0$ would not be the lowest energy state. Clearly, the sum over the negative energy sea is analogous to the sum over the valence band in $(CH)_x$. Further, note that the sum over α in eq. (2.10d) just introduces an overall factor of N, since the α dependence of eq. (2.10a) is trivial; this is just like the spin sum in the continuum electron-phonon equation. The explicit form of $Z(\Lambda)$ is, as shown by DHN,

$$Z(\Lambda) = \frac{g_{GN}^2}{\pi} \int_0^\Lambda \frac{dk}{(k^2 + m^2)^{1/2}} \tag{2.11a}$$

$$= \frac{g_{GN}^2}{\pi} N \ln \frac{\Lambda + \sqrt{\Lambda^2 + m^2}}{m}, \tag{2.11b}$$

where $m \equiv g_{GN}\sigma_0$. The consistency of the Gross-Neveu equations (2.10) is easily demonstrated. The normalized *negative energy* solutions to (2.10a) are, for each α,

$$\Psi(n; x) \equiv \Psi(k; x) = N_k \begin{pmatrix} 1 \\ \dfrac{ik}{\omega - m} \end{pmatrix} e^{ikx}, \tag{2.12}$$

where

$$\omega = +\sqrt{k^2 + m^2}, \qquad N_k = \frac{1}{\sqrt{2\pi}} \left(\frac{\omega - m}{2\omega} \right)^{1/2},$$

with $m = g_{GN}\sigma_0$. Thus

$$\bar{\Psi}(k;x)\Psi(k;x) = |\Psi_1(k;x)|^2 - |\Psi_2(k;x)|^2 = -\frac{m}{2\pi\omega}, \quad (2.13a)$$

$$\sum_{\substack{\alpha,n;\\ \omega_n<0}} \bar{\Psi}^\alpha(n;x)\Psi^\alpha(n;x) = -\frac{N}{2\pi}\int_{-\Lambda}^{\Lambda} \frac{dk\, m}{\sqrt{k^2+m^2}}. \quad (2.13b)$$

Since $m = g_{GN}\sigma_0$, the consistency of eq. (2.10d) follows immediately from eqs. (2.13b) and (2.11).

Although this consistency is obviously directly analogous to that of the gap equation in $(CH)_x$, establishing an exact equivalence between (2.10d) and (2.2c) at first appears to present a problem, for the renormalization factor $Z(\Lambda)$ in the field theory seems to have no counterpart in the condensed matter case. A bit more thought establishes that this is not a difficulty. In the solid state context if the limit, K, of the sum over wave vectors were allowed to approach infinity, a similar "divergence" would occur because the *linearization* of the dispersion relation about the half-filled band removes the true lower energy cut-off of the band. But as suggested by fig. 1, in the case of a dimerized chain, the consistency of the linearization approximation with the true spectrum requires the identification of the actual full band width, W, with the energy at the wave vector cut-off, K, as already indicated in eq. (2.5). Indeed, the relation between Δ_0 and W [eq. (2.4)] is just the requirement that the self-consistency equation for Δ be solved with a "renormalization constant" equal to 1. We can achieve a comparable situation in the field theory context by choosing σ_0 such that

$$m = g_{GN}\sigma_0 = 2\Lambda \exp\left(-\pi/Ng_{GN}^2\right). \quad (2.14)$$

Using this result, from eq. (2.11b) it follows that $Z(\Lambda) = 1$. Although this choice might at first appear unconventional in a field theory analysis, it is, in fact, completely equivalent* to the standard prescription that renormalizes the theory by requiring the second derivative of the effective potential to be unity at an arbitrary subtraction point, σ_S [17].

Clearly eq. (2.14) is the field theory counterpart of the relation between the band gap and full band width, eq. (2.4), in the condensed matter problem. There is an important difference in interpretation, however, since both Δ_0 *and* W are measurable in $(CH)_x$ whereas in the field theory, only m is measurable; Λ is an unphysical cut-off introduced to make the theory finite. Actually, eq. (2.14) illustrates rather

* Although this prescription is indeed equivalent to that used by Gross and Neveu in ref. [17], it is not identical. Their Λ is a cut-off on the modulus of the euclidean two-vector ($k_0^2 + k_1^2 \leq \Lambda^2$) whereas we, following DHN in ref. [16], use Λ as a cut-off on the spatial part only ($|k_1| < \Lambda$). This leads eventually to a trivial numerical difference between our eq. (2.14) and the corresponding eq. (4.19) in ref. [17].

transparently three crucial concepts developed in recent field theory studies and embodied in the Gross-Neveu model. Let us digress briefly to clarify these points.

First, as noted above, the original Gross-Neveu lagrangian [eq. (2.7)] possesses a discrete "chiral symmetry" (γ_5 invariance) and appears to describe massless fermions. Nonetheless, the actual ground state – that is, the vacuum – contains a filled Dirac sea of *massive* fermions and is *not* invariant under $\Psi \to \gamma_5 \Psi$. This is "dynamical spontaneous symmetry breaking." Second, for fixed N, the original lagrangian contains only one parameter: the *dimensionless* coupling constant, g_{GN}. In the final, renormalized theory, the one physical parameter, as suggested by (2.14), is the *dimensional* quantity the fermion mass [17]. This is the phenomenon of "dimensional transmutation" [20]. Third, eq. (2.14) correctly reflects the "asymptotic freedom" [19] of the Gross-Neveu model, for if one insists on a fixed m – to define the same theory – as $\Lambda \to \infty$, then the coupling constant, g_{GN}^2 must go to the zero like one over the logarithm of Λ.

With the above choice of σ_0, making the formal identification $g_{\mathrm{GN}}^2 = g^2/2\omega_{\mathrm{Q}}^2$, and noting that because of the change of independent variable, a relative factor of v_{F} comes in the normalization of wave functions between (2.10d) and (2.2c), we see that these equations can be exactly transformed into each other, provided we choose $N = 2$ to correspond to the correct spin degeneracy in the continuum $(\mathrm{CH})_x$ equations. Thus the continuum, self-consistent electron-phonon equations for $(\mathrm{CH})_x$ are precisely equivalent to the static, semiclassical equations for the $N = 2$ Gross Neveu model, and we can immediately translate solutions from one model to the other.

3. Static solutions: ground state, kinks and polarons

The static solutions to the semiclassical equations have been analyzed, and systematically constructed, by DHN [16]. Since we have shown that the adiabatic mean field equations for $(\mathrm{CH})_x$ are equivalent, the same techniques can be immediately applied to them. Alternatively, one can simply translate, according to (2.11), known solutions from the Gross-Neveu model to $(\mathrm{CH})_x$. To stress the field theory connection while explicitly exhibiting the constructive method, we follow a dual course. In the appendix the method for constructing solutions is briefly summarized and the form of the solutions are derived in Gross-Neveu language. In the present section, we translate these solutions into the explicit forms appropriate to $(\mathrm{CH})_x$.

As first shown by DHN and as illustrated in the appendix, there are three classes of solutions to eqs. (2.10) for static $\sigma(x)$. The first class, with $\sigma(x) = \sigma_0$ given by (2.14), corresponds to the vacuum – with, of course, the filled Dirac negative energy sea – in the Gross-Neveu model. In sect. 2 we have already shown that this translates into the ground state – with the filled valence band – in $(\mathrm{CH})_x$. The explicit forms for the wave functions in both models are given in sect. 2.

The second class of solutions to the Gross-Neveu model are the "kinks," with, as shown in the appendix,

$$\sigma(x) = \sigma_0 \tanh mx. \tag{3.1}$$

These exist for any N and always have a zero energy, $\omega_0 = 0$, bound state which can, by the Pauli principle, be occupied by up to $n_0 = N$ fermions. Obviously, these translate to the familiar "kink" solitons in $(CH)_x$, which have been extensively discussed elsewhere [5, 6]. For completeness, we quote the explicit form of the solutions in $(CH)_x$. For $\Delta(y)$ one has

$$\Delta(y) = \Delta_0 \tanh(\Delta_0 y / v_F) \tag{3.2a}$$

and for the "midgap" state ($\varepsilon_n \equiv \varepsilon_0 = 0$)

$$u_0(y) = N_0 \operatorname{sech}(\Delta_0 y / v_F), \tag{3.2b}$$

$$v_0(y) = -iN_0 \operatorname{sech}(\Delta_0 y / v_F), \tag{3.2c}$$

with

$$N_0 = \sqrt{\frac{\Delta_0}{4v_F}}\,.$$

The *negative* energy scattering solutions corresponding to the valence band electronic states are

$$u_n(y) \equiv u_-(k; y) = N_k e^{iky}\left[\tanh\frac{\Delta_0}{v_F} y + i\left(\frac{\omega - kv_F}{\Delta_0}\right)\right], \tag{3.2d}$$

$$v_n(y) \equiv v_-(k; y) = -iN_k e^{iky}\left[\tanh\frac{\Delta_0}{v_F} y - i\left(\frac{\omega + kv_F}{\Delta_0}\right)\right], \tag{3.2e}$$

with

$$\omega = +\left(\Delta_0^2 + k^2 v_F^2\right)^{1/2}, \qquad N_k = \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{\Delta_0}{\omega}\,.$$

It is straightforward to verify that these functions satisfy the continuum electron-phonon equations (2.2). The form of the kink solution and the electron density, $|u_0|^2 + |v_0|^2$, in the midgap state are shown in fig. 3a.

The third class of solutions [16] to the static, semiclassical equations of the Gross-Neveu model can be called "bags." As the corresponding solutions in $(CH)_x$ have only recently been found, first numerically [15] and then analytically [13], let us first describe the qualitative features of the solutions in some detail. The bag

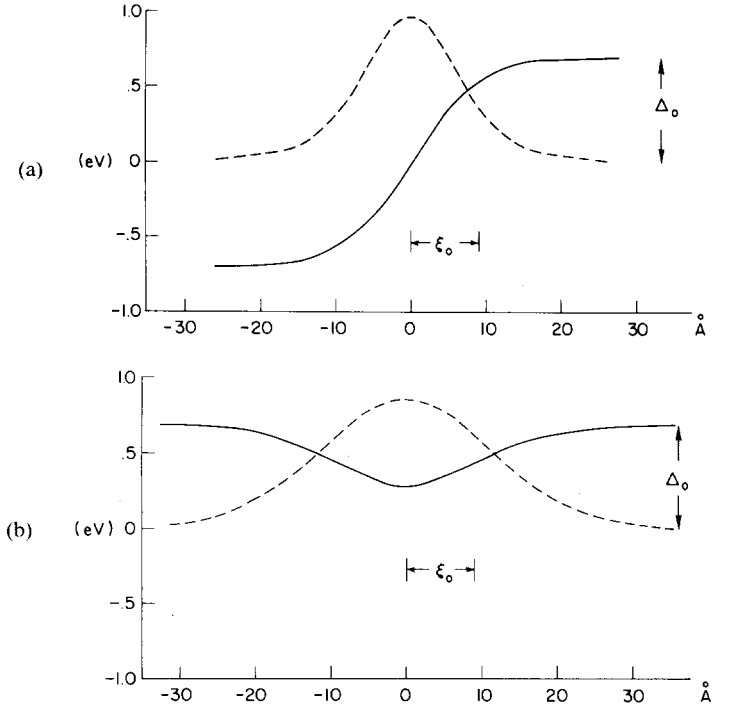

Fig. 3. A comparison (continuum electron-phonon model) of the gap parameter $\Delta(x)$, solid line, for (a) the "kink" excitation, and (b) the static "polaron" excitation. The vertical scale is in eV, the horizontal one in Å (for parameter values relevant to $(CH)_x$ [3]). The dashed lines indicate (in arbitrary units) the electron density $\Psi_0^+(x)\Psi_0(x)$ in (a) the "midgap" state ($\omega_0 = 0$), and (b) the "bound state" ($\omega_0 < \Delta_0$) (see text for nomenclature).

topology differs importantly from that of the kink; rather than interpolating between the two degenerate ground states, $\pm\sigma_0$, the σ field for the bag has a localized "dimple," as shown in fig. 3b. This "dimple" acts as a potential in the Dirac equation, producing a *single* positive energy bound state* at $E = \omega_0 < m$ and modifying the continuum, as illustrated in fig. 4. As shown by DHN and reviewed in the appendix, for general N there exist bag-like, self-consistent solutions – that is, solutions satisfying *both* eqs. (2.10a) and (2.10d) – in which all negative energy states (including the bound state with $E = -\omega_0$) are occupied by N fermions and the positive energy bound state is occupied by $1 \leqslant n_0 \leqslant N-1$ fermions. Further, by the charge conjugation symmetry* of the equations, there exist "antiparticle" – in the

* With only a σ field present, the energy levels of the Dirac equation are "charge conjugation symmetric": that is, for every positive energy level, $\varepsilon_+ = \omega_n$, there is a negative energy level with $\varepsilon_- = -\omega_n$. In fact, the components of the Dirac wave function, Ψ_1 and Ψ_2, are simply interchanged in going from the state with ε_+ to that with ε_-. In terms of u and v this implies, using (2.11), that $u \to iv$ and $v \to -iu$. Note that the special state $\varepsilon = 0$ – the "midgap" electronic state induced by the kink "potential" – is its own charge conjugate.

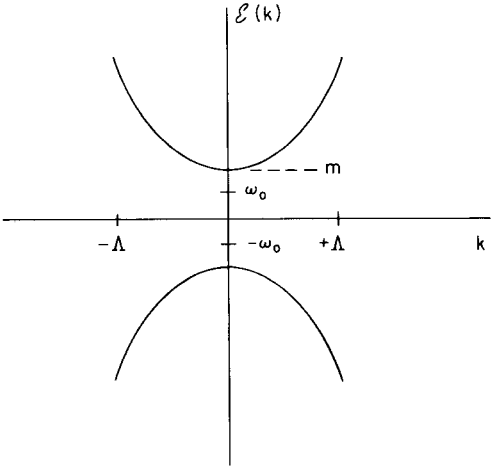

Fig. 4. The energy spectrum of the Dirac equation in the presence of the "bag" $\sigma(x)$. Note the occurrence of a single positive energy bound state at $E(0)=\omega_0<m$. The symmetry between positive and negative energy states follows directly from eqs. (2.10b) and (2.10c).

solid state application, "hole" – solutions in which the negative energy bound state is occupied by only $m_0<N$ fermions. For those excitations in which n_0 fermions occur in a positive energy bound state, the value of ω_0 for which the self-consistency equations is satisfied is given by $\omega_0(n_0)=m\cos\theta(n_0)$ [16] where, as sketched in the appendix,

$$\theta(n_0)=\frac{n_0}{N}\left(\frac{\pi}{2}\right). \tag{3.3}$$

The energy of the corresponding bag-like excitation is

$$E(n_0)=\frac{2}{\pi}Nm\sin\theta(n_0). \tag{3.4}$$

The expression for the bag energy provides an insightful interpretation of this excitation. For $n_0/N\ll 1$, expanding (3.4) gives

$$E(n_0)\simeq n_0 m-\frac{n_0^3 m\pi^2}{24N^2}+\cdots, \tag{3.5}$$

which shows that in this limit the excitation can be viewed as a weakly bound state of n_0 elementary fermions of mass m. Conversely, for $n_0\simeq \mathrm{O}(N), \theta\simeq \mathrm{O}(\frac{1}{2}\pi)$, so

$$E(n_0)\lesssim\frac{2}{\pi}Nm. \tag{3.6}$$

Recalling that the energy of a kink in the Gross-Neveu model is

$$E_K = \frac{N}{\pi} m, \tag{3.7}$$

we see that in this limit, the bag energy approaches that of two kinks. We shall return to these results later.

Intuitively, the existence of the bag excitations can be understood as a balance between the "pressure" of the fermions – pushing "out" and preventing the σ field from "collapsing" to $\sigma(x) = \sigma_0$ – and that of the σ field – pushing "in" and trapping the fermions in the localized well*. This implies that, in contrast to the kink-like excitations, in which the single Dirac bound state having $\omega_0 = 0$ can be occupied or not, for the bags the presence of fermions in the positive energy bound state – or, equivalently, their absence from the negative energy bound state, in the case of antiparticle or hole excitation – is essential to the existence of the excitation.

To translate these bag-like solutions from the Gross-Neveu model to polyacetylene, we note that since $(CH)_x$ corresponds to the $N = 2$ semiclassical equations, one expects a *single* bag-like excitation with $n_0 = 1$; the state with $n_0 = 2$ is, as a comparison of eqs. (3.4) and (3.7) suggests, in fact identical to a kink and antikink pair infinitely far apart. As noted above, the $n_0 = 1$ excitation corresponds to the presence of a single additional, unpaired electron in the $(CH)_x$ chain and consequently has the standard relation of charge $(-e)$ and spin $(\frac{1}{2})$. Since the electron is trapped in a field driven by its coupling to phonons*, this excitation is clearly a "polaron" [14]. The fact that the continuum electron-phonon model of $(CH)_x$ admits (in an approximate form) both conventional strong-coupling polarons and amplitude kinks will be a useful starting point for studying these particle-like excitations (and their interactions) in a *unified* theory.

In the appendix, we show how to construct explicitly these "polaron" or "bag" solutions, using techniques related to the inverse scattering method [16, 23–25]. Translating the forms of σ in (A.20) and of Ψ in (A.21) and (A.22) via the transformation in eq. (2.11), we find for $\Delta(y)$,

$$\begin{aligned}\Delta(y) &= \Delta_0 - K_0 v_F \{\tanh[K_0(y+y_0)] - \tanh[K_0(y-y_0)]\} \\ &= \Delta_0 - (K_0 v_F)^2 \omega_0^{-1} \operatorname{sech}[K_0(y+y_0)] \operatorname{sech}[K_0(y-y_0)], \end{aligned} \tag{3.8a}$$

* Note that in the Gross-Neveu model the fermions are self-interacting and the σ field is essentially introduced as an "auxiliary" field. Actually, one can show (see ref. [16]) that the σ field does correspond to a true bound state and acquires non-trivial dynamics in the time-dependent semiclassical formalism. In the context of $(CH)_x$, the phonon field is *ab initio* dynamical and it is the electron coupling via phonons that leads to the polaron state. Nonetheless, for static σ (or Δ) fields, the equations are identical.

and for the positive energy bound state, $E = +\omega_0$, the wave functions

$$u_0(y) = N_0\{(1-i)\mathrm{sech}[K_0(y+y_0)] + (1+i)\mathrm{sech}[K_0(y-y_0)]\}, \quad (3.8b)$$

$$v_0(y) = N_0\{(1+i)\mathrm{sech}[K_0(y+y_0)] + (1-i)\mathrm{sech}[K_0(y-y_0)]\}. \quad (3.8c)$$

Here

$$K_0 v_F = \sqrt{\Delta_0^2 - \omega_0^2}, \qquad N_0 = \tfrac{1}{4}\sqrt{K_0},$$

$$\tanh K_0 y_0 = \frac{\Delta_0 - \omega_0}{K_0 v_F}.$$

The negative energy bound state follows simply from eqs. (3.8b) and (3.8c) by the transformation $u_{-0} \equiv u|_{E=-\omega_0} = iv_0$ and $v_{-0} \equiv v|_{E=-\omega_0} = -iu_0$, while the *negative* energy scattering states have the forms

$$u_-(k;x) = N_k'' e^{ikx}[(\omega + \Delta_0 - kv_F) - \gamma(1+i)t_+ + \delta(1-i)t_-], \quad (3.8d)$$

$$v_-(k;x) = -N_k'' e^{ikx}[(\omega + \Delta_0 + kv_F) - \gamma(1-i)t_+ + \delta(1+i)t_-], \quad (3.8e)$$

where

$$t_\pm \equiv \tanh[K_0(y \pm y_0)], \qquad \omega = \sqrt{k^2 v_F^2 + \Delta_0^2},$$

$$\gamma \equiv \tfrac{1}{2}K_0 v_F\left[1 - \frac{ikv_F}{\omega - \Delta_0}\right], \qquad \delta \equiv \tfrac{1}{2}K_0 v_F\left[1 + \frac{ikv_F}{\omega - \Delta_0}\right],$$

$$N_k'' = \frac{1}{2\sqrt{2\pi}}\sqrt{\frac{\omega - \Delta_0}{\omega(k^2 v_F^2 + K_0^2 v_F^2)}}.$$

By direct calculation, one can verify that these forms for u and v satisfy the electron part of the continuum $(CH)_x$ equations – our eqs. (2.2a) and (2.2b) – for *any* value of ω_0 in the range $0 \leq \omega_0 \leq \Delta_0$. However, as the results for the Gross-Neveu model imply [16], only for

$$\omega_0 = K_0 v_F = \sqrt{\tfrac{1}{2}}\,\Delta_0 \quad (3.9)$$

is the $(CH)_x$ "gap" equation – our (2.2c) – *also* satisfied*. To verify this in detail,

* One could also imagine taking the form of $\Delta(y)$ given by (3.8a) as an ansatz and then varying y_0 to satisfy (2.2c); this would, of course, reproduce (3.9) and would be conceptually similar to the method used to find the self-consistent kink solution in ref. [6]. However, because of the constraints among all the parameters in (3.8a), it is hard to imagine "guessing" such an ansatz *a priori*.

recall that the polaron solution corresponds to the presence of an additional, unpaired electron beyond those in the valence band. We see that the precise form of eq. (2.2c) for these solutions is

$$\Delta(y)=\frac{-g^2}{2\omega_Q^2}\Big\{1\cdot(u_0^*v_0+v_0^*u_0)+2(u^*_{-0}v_{-0}+v^*_{-0}u_{-0})$$

$$+2\int_{-K}^{K}\mathrm{d}k\,u^*_-(k;x)v_-(k;x)+v^*_-(k;x)u_-(k;x)\Big\}. \quad (3.10)$$

Using the explicit forms of the electron wave functions from eqs. (3.8), one can verify the consistency of eq. (3.10) as follows:

$$\Delta(y)=\frac{-g^2}{2\omega_Q^2}\Bigg\{1\cdot\frac{\omega_0}{2v_F}(t_+-t_-)-2\cdot\frac{\omega_0}{2v_F}(t_+-t_-)$$

$$-\frac{2}{2\pi}\int_{-K}^{K}\frac{\mathrm{d}k}{\sqrt{k^2v_F^2+\Delta_0^2}}\left[\Delta(y)-\frac{\omega_0^2K_0v_F}{k^2v_F^2+K_0^2v_F^2}(t_+-t_-)\right]\Bigg\} \quad (3.11a)$$

$$=\left\{\frac{g^2}{\pi\omega_Q^2}\int_0^K\frac{\mathrm{d}k}{\sqrt{k_0^2v_F^2+\Delta_0^2}}\right\}\Delta(y)$$

$$-\frac{g^2}{2\omega_Q^2}(t_+-t_-)\left\{\frac{2}{\pi}\int_0^K\frac{\mathrm{d}k\,\omega_0^2K_0v_F}{\left[k^2v_F^2+\Delta_0^2\right]^{1/2}\left[k^2v_F^2+K_0^2v_F^2\right]}-\frac{\omega_0}{2v_F}\right\}. \quad (3.11b)$$

Now the first term in brackets in eq. (3.11b) is just 1, by the definition of Δ_0. Hence, for eq. (3.10) to be consistent, the second term in brackets must vanish. We note that

$$\frac{2}{\pi}\int_0^K\frac{\mathrm{d}k\,\omega_0^2K_0v_F}{\left[k^2v_F^2+\Delta_0^2\right]^{1/2}\left[k^2v_F^2+K_0^2v_F^2\right]}=\frac{2}{\pi}\omega_0^2K_0v_F\left[\frac{1}{v_F}\frac{1}{K_0v_F}\frac{1}{\omega_0}\tan^{-1}\left(\frac{\omega_0}{K_0v_F}\right)\right], \quad (3.12)$$

where, consistent with the previous approximations and the rapid fall-off of the integrand, we have taken the $K \to \infty$ limit of the integral. Using result (3.12) to evaluate the second term in brackets in eq. (3.11b) we see that setting it to 0 requires

$$\frac{2}{\pi}\frac{\omega_0}{v_F}\tan^{-1}\left(\frac{\omega_0}{K_0 v_F}\right) - \frac{\omega_0}{2v_F} = 0, \tag{3.13a}$$

or

$$\tan^{-1}\left(\frac{\omega_0}{K_0 v_F}\right) = \tfrac{1}{4}\pi, \tag{3.13b}$$

so that indeed $\omega_0 = K_0 v_F = \sqrt{\tfrac{1}{2}}\,\Delta_0$, as asserted above. From eq. (3.4) we observe that the energy of this excitation is

$$E(n_0 = 1) = \frac{2}{\pi} \cdot 2 \cdot \Delta_0 \sin\tfrac{1}{4}\pi \tag{3.14a}$$

$$= \frac{2\sqrt{2}}{\pi}\Delta_0 \tag{3.14b}$$

$$\simeq 0.90\Delta_0. \tag{3.14c}$$

The energy of the single additional electron in the localized bag (polaron) excitation is thus *less* than that (Δ_0) in the lowest conduction band state. Further, it is also less than the energy required to create, and place a *single* electron into, a kink/antikink pair, since [5, 6] $E_{\bar{K}} + E_K = 2(2/\pi)\Delta_0$. Since topological constraints require kinks to be produced in $K\bar{K}$ pairs, the polaron is the lowest energy state available to a *single* electron. The form of the polaron solutions and its comparison with the amplitude kink are shown in fig. 3.

Although the polaron is a true solution to the coupled equations (2.2) only for $K_0 v_F = \sqrt{\tfrac{1}{2}}\,\Delta_0$, considering its form for arbitrary K_0 in the range $0 < K_0 v_F < \Delta_0$ provides useful insight. For $K_0 \to \Delta_0/v_F$, $\tanh K_0 y_0 \to 1$ and, from (3.8a), we see that $\Delta(y)$ looks like a widely separated kink and antikink. Note that since this limit corresponds to $\theta(n_0) \to \tfrac{1}{2}\pi$, this result corroborates the previous comments based on the energy of the polaron. For $K_0 y \ll \Delta_0/v_F$, one has $\omega_0 \to \Delta_0$ and that $\Delta(y) - \Delta_0$ approaches a shallow ($-\mathrm{sech}^2 K_0 y$) structure; both these results are characteristic of the conventional weakly bound polaron described, in certain circumstances [14] by a non-linear Schrödinger equation. With $K_0 = \sqrt{\tfrac{1}{2}}\,\Delta_0$, our polaron is ambivalent about its parentage.

From (3.8a) it follows that the characteristic polaron width is

$$\begin{aligned} 2y_0 &= (2/K_0)\tanh^{-1}\left[K_0 v_F/(\Delta_0+\omega_0)\right] \\ &= \left(Wa/\Delta\sqrt{2}\right)\ln\left(1+\sqrt{2}\right) \\ &\simeq 1.24\zeta_0 \\ &\simeq 10.8\text{Å (for } (CH)_x \text{ [3, 6])}. \end{aligned} \tag{3.15}$$

Here ζ_0 is the kink width parameter. The value of Δ at the polaron center is

$$\Delta_{\min} \equiv \Delta(0) = \Delta_0\left(\sqrt{2}-1\right). \tag{3.16}$$

From (3.14) the polaron binding energy is

$$\begin{aligned} \text{BE}_p &\simeq 0.10\Delta_0 \\ &\simeq 0.07 \text{ eV (for } (CH)_x \text{ [3, 6])}. \end{aligned} \tag{3.17}$$

Apart from the recent discovery of this analytic form in the continuum model [13], the polaron has been independently observed in a numerical simulation [15] of single electron injection in a *lattice* model of $(CH)_x$ which makes the same adiabatic mean-field approximations as (2.1). All of the continuum polaron results above are in good agreement with these discrete simulations, in the same way that the continuum kink features compare favorably with lattice results. Furthermore, the numerical simulations [15] revealed a polaron "instability" – that is, the absence of a polaron state – for the (hypothetical) *spinless* electron case. This result is immediately understood from our discussion of the semiclassical spectrum of the Gross-Neveu model; *spinless* electrons in $(CH)_x$ correspond to the $N = 1$ Gross-Neveu equations, and, as eqs. (3.3) and (3.4) suggest, these are no bag-like or "polaron" states – only kinks – in this case.

4. Further model field theory implications for polyacetylene

In a separate article we shall pursue the physical implications of polarons (and the possible time-dependent extensions mentioned below), in $(CH)_x$ including their potential effects in specific types of doping, their possible role as "doorway" states to $K\overline{K}$ pair production or annihilation, their implications for tunnel injection experiments*, and the possibility of polaron transport mechanisms**. However,

* We thank S. Etemad and J.R. Schrieffer for discussions on this point.

** We thank D. Emin for discussions on this point.

here we turn to a number of additional field theory connections that may provide further insight into solitons in $(CH)_x$. To avoid any possible confusion, let us state our perspective in this section quite precisely. In the previous sections we have established that an exact formal equivalence holds between two sets of equations, and hence that the previously known solutions of one set can be translated into solutions of the other. Although this has provided an important quantitative insight into polarons in continuum models of polyacetylene, it is in a sense an "accident" that the bag-like solutions were first discovered in the context of the semiclassical Gross-Neveu equations; one could have found the polaron solutions directly by applying inverse scattering techniques to the continuum model of $(CH)_x$ with no mention of a field theory connection. In addition, as we have indicated and will discuss further below, the full dynamics of $(CH)_x$ differ from those of the Gross-Neveu fermions even at the semiclassical – let alone fully quantum mechanical – level. Thus, if one goes beyond the static solutions treated above, no precise quantitative connections can be made. Nonetheless, as we shall see, if one looks for possible qualitative similarities, a number of interesting suggestions follow from pursuing this field theory connection.

Perhaps the most striking qualitative suggestion comes from known results on the full quantum Gross-Neveu model [21, 22] and may have bearing on the existence of polaron-like excitations in the full quantum – as opposed to adiabatic mean field – theory of $(CH)_x$. Although our results here have established that the polarons are genuine solutions to the adiabatic mean field equations, one can question whether in a fuller description of the dynamics of $(CH)_x$ – as provided, for example, by the SSH lattice hamiltonian with non-trivial quantum corrections – the polaron solutions persist. Technically, this question can be phrased in terms of the stability of polaron-like states under perturbations to the adiabatic mean field equations. This stability question is both difficult and important, for unlike the individual kinks, the bags are *not* guaranteed to be stable by general topological considerations. Further, in this regard, a cursory glance at the Gross-Neveu analogy proves worrying [5], for in the *full, quantum* theory [21, 22] of the Gross-Neveu model, it has been shown that, for the case $N=2$, *only* kink-like excitations exist★; the bag-like states disappear in the full quantum theory with exact Gross-Neveu dynamics. However, as we have constantly stressed, the equivalence of the adiabatic mean field equations in $(CH)_x$ is to the *static, semiclassical* equations of the Gross-Neveu model. Indeed, it is clear that the full dynamics of even the continuum model of $(CH)_x$ – let alone the underlying SSH lattice model – *differ* from those of the Gross-Neveu model, for in deriving the adiabatic mean field hamiltonian, an explicit term involving $\dot{\Delta}^2(y)$ was dropped. As an inspection of equation (2.8) shows, there is *no* $\dot{\sigma}^2(x)$ term in the full

★ Interestingly, in ref. [23], Witten obtains the "absence of bags" result by mapping the $N=2$ quantum Gross-Neveu model into two decoupled quantum sine-Gordon systems. Note the relation to Horovitz' results in ref. [7] and the question of charge/spin degrees of freedom. We thank V.J. Emery for discussions of this point.

Gross-Neveu model. Thus the detailed results for the full quantum Gross-Neveu model can *not* be translated directly to $(CH)_x$, and one can not conclude from studies of the $N=2$ quantum Gross-Neveu theory that polaron excitations should not exist in polyacetylene. Nonetheless, this aspect of the Gross-Neveu model underscores the importance of studying polaron stability in $(CH)_x$. Although one could certainly study this question – probably by numerical (e.g., quantum Monte Carlo) techniques only – in the full, quantum, time-dependent continuum model, we believe that since the underlying lattice theory is closer to the true physics, it is most sensible to study the question of polaron stability numerically in that context.

Apart from this – possibly negative – implication, the field theory connection provides a number of additional insights into, and suggests further possible studies of, solitons in polyacetylene. As a first example, let us return to semiclassical or mean field approaches and consider the relation between the continuum coupled electron-phonon description of kink-like solitons in $(CH)_x$ and recent attempts [8–10] to apply a ϕ^4 theory to these same excitations. The use of ϕ^4 theory (which is motivated by a Landau-Ginzburg expansion) in this context is subject to (and has received [3, 6, 7]) the *a priori* criticism that since the $(CH)_x$ ground-state energy varies as $E_0(\Delta_0) \sim \Delta_0^2 \ln \Delta_0^2$ [26] and is strongly non-local, the conventional Landau-Ginzburg gradient expansion must fail in small amplitude regimes. And yet, comparison of the results with those of the coupled electron phonon theory indicates that the ϕ^4 theory, at least qualitatively, *can* describe the kink-like solutions. A perhaps illuminating perspective on this apparently puzzling circumstance can be gained by referring to known results on a similar circumstance in field theory: namely, the qualitative similarities between the Gross-Neveu model [16, 17] and the one-space, one-time dimensional scalar ϕ^4 field theory described by the lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\left(\partial_\mu \phi \partial^\mu \phi\right) - \tfrac{1}{4}\lambda\left(\phi^2 - f^2\right)^2, \tag{4.1}$$

where f is a constant [27–29]. In this ϕ^4 theory, the lowest-order "effective potential" which determines the ground state has the simple polynomial form

$$V(\phi) = \tfrac{1}{4}\lambda\left(\phi^2 - f^2\right)^2 \tag{4.2}$$

from which one sees immediately the two degenerate ground states with non-zero values of $\phi - \phi_0 = \pm f$; this is explicit (rather than dynamical) spontaneous symmetry breaking. For the Gross-Neveu model, the effective potential for the σ field must be calculated *dynamically* [20] and the result contains a term of the form [17]

$$V(\sigma) \propto \sigma^2 \ln \sigma^2 \tag{4.3}$$

in direct analogy to the full $(CH)_x$ result [26]. This form of $V(\sigma)$ leads to the *dynamical* spontaneous symmetry breaking result $\sigma = \pm\sigma_0$, for the ground state. In

both theories, as a further consequence of the two-fold degeneracy leading to this spontaneous symmetry breaking, there exist topological kink-solitons [12, 27, 28]. Thus, despite the fact that the effective potential for the (composite) scalar field σ in the Gross-Neveu model can *not* be expanded around $\sigma = 0$, both the structure of the symmetry breaking and the existence of kink-like solutions are correctly modeled by a polynomial – namely ϕ^4 – effective potential with the appropriate minima. The structural similarity between the Gross-Neveu model and ϕ^4 theory goes further. If fermions are coupled to the ϕ field in the ϕ^4 model via the standard Yukawa interaction, the full lagrangian becomes [27–29]

$$\mathcal{L} = \sum_{\alpha=1}^{N} \bar{\Psi}^{\alpha}(i\gamma\partial - g\phi)\Psi^{\alpha} + \tfrac{1}{2}(\partial^{\mu}\phi)(\partial_{\mu}\phi) - \tfrac{1}{4}\lambda(\phi^2 - f^2)^2. \tag{4.4}$$

One can study this lagrangian semiclassically [25] in two related but separate cases that have interest for comparisons to $(CH)_x$. First, one can treat only the "bound-state" fermions in the Dirac potential, ignoring the negative energy sea. Alternatively, the full effects of the negative continuum can also be included. In both cases one finds that not only zero energy fermion states coupled to the ϕ^4 kinks, with unusual spin/charge assignments [12] but also that bag-like (polaron) excitations, qualitatively similar to those in the semiclassical Gross-Neveu equations, exist [25]. Indeed, for a particular ratio ($\lambda = 2g^2$) of ϕ^4 coupling constants in (4.4), the functional forms for Δ and the u_i and v_i for the ϕ^4 plus fermion "polaron" are *identical* to those given in (3.8) [25]. Only the relation determining K_0 – the analog of (3.3) – is different. For other ratios of λ/g^2, analytic forms of the polaron solution are not available, but numerical results confirm their existence [30]. Thus the ϕ^4 model of $(CH)_x$, even without explicitly including valence electron effects, *does* contain essentially the same polaron found in the continuum electron-phonon model: in solid state language, the ϕ^4 potential is, in a sense, imitating the effects of valence band electrons. Notice, however, the important role in ϕ^4 models of spatial gradient terms which determine the kink and polaron characteristic sizes. Such terms are absent in the *continuum* electron-phonon model and their role is played instead by nonlocalities coming from the valence band electrons (or "negative energy fermion sea" in the Gross-Neveu language).

Other previous field theory studies, which have noted the relation between ϕ^4 plus fermions and the Gross-Neveu model [29], may also prove useful in studies of polyacetylene. For instance, in the limit that N (the number of different fermion fields) approaches infinity, the ϕ^4 (with fermions) and Gross-Neveu models become formally equivalent [29]. Despite its apparently formal nature, this large-N result may be relevant to $(CH)_x$ because it is known that semiclassically (although not, as noted earlier, in the fully quantum theory) the $N = 2$ theory does exhibit the generic large N behavior.

Despite the striking qualitative successes of the ϕ^4 modeling outlined above, it is necessarily phenomenological. It would seem most likely to encounter difficulties over *details* of *dynamics*. This brings us to a final aspect of the field theory connection that deserves mention: namely, known field theory results on non-static solutions. In the semiclassical Gross-Neveu equations, time-periodic "breather"-like solutions have been found analytically [16]. Further, recent numerical studies [31] establishing the existence – and apparent stability – of similar time-periodic breather-like solutions to ϕ^4 suggest that such solutions are "robust" under changes in the theory that preserve fundamental symmetry properties. It is thus natural to speculate that breather-like – that is, localized, time-dependent – solutions may exist in $(CH)_x$. Unfortunately, in view of the absence in the Gross-Neveu model of a term comparable to the explicit $\dot{\Delta}^2(y)$ term in the full $(CH)_x$ continuum hamiltonian, one can not simply translate the known analytic or numerical results from field theory to polyacetylene, although the field theory forms may provide a convenient basis for perturbative approaches. In view of their strong potential interest, we feel such solutions should be sought in numerical studies of realistic models of $(CH)_x$; indeed, there may actually be preliminary evidence in existing simulations [15]. A second crucial aspect of time-dependent solutions is the important role such excitations may play as kink decay channels. Kink(K)/antikink($\overline{\text{K}}$) scattering in ϕ^4 is known [32] to have a very interesting structure. In particular, although the K and $\overline{\text{K}}$ reflect from each other at high relative velocity, at low relative velocity they form a trapped, quasi-periodic decaying state [32]. Further, for intermediate velocities, there is an interesting resonance phenomenon. In the Gross-Neveu model, on the other hand, an analytic formula exists which describes semiclassical $\text{K}\overline{\text{K}}$ scattering: from the form of the (time-dependent) σ field which describes such a collision, [32]

$$\sigma(x,t) = \frac{v\cosh 2\gamma x - \cosh 2v\gamma t}{v\cosh 2\gamma x + \cosh 2v\gamma t}, \tag{4.5}$$

with $\gamma = (1-v^2)^{-1/2}$, one sees that for all velocities the kink and antikink reflect; this "preservation of form" is a consequence of the infinite number of conservation laws underlying the complete integrability of the Gross-Neveu model [16, 21, 33]. One possible approach to understanding the differences is in studying the fluctuation spectra around kink profiles in the two models [34].

The existence of breathers and the persistence and details of resonances in $\text{K}\overline{\text{K}}$ scattering for more fundamental models of $(CH)_x$ is again something which is probably best addressed in very careful numerical simulations. Breather-kink collision processes in polyacetylene will also be interesting, as they are in the field theories themselves, and all of these details will presumably bear on questions of soliton transport and lifetime.

It may be helpful to note that the static Gross-Neveu bag solution can, for given n_0, be shown to be the lowest energy (static) member of a family of Gross-Neveu breather solutions [16]. This suggests that one should think of the putative breathers

in $(CH)_x$ as the *band* of polaron states anticipated from general solid state experience [14]. That they should not, in $(CH)_x$, have infinite lifetimes and "ideal" collisions (as in Gross-Neveu) is also expected in terms of "shake-off phonon" effects.

5. Concluding comments

Our aim in this paper has been to continue the emerging dialogue [7, 12] in the area of polyacetylene and related materials, between field theory and solid state physics. We used lessons from model relativistic field theories (the $N = 2$ Gross-Neveu and ϕ^4 with coupled fermions) to illuminate relations (and differences) among various theoretical models of Peierls-dimerized chains – discrete lattice hamiltonians [3, 26] continuum interacting electron-phonon models [4–7] and phenomenologically motivated ϕ^4 Landau-Ginzburg-like descriptions [8–10]. In particular, we identified polaron-soliton solutions [13] in good agreement with those observed in recent numerical simulations [15].

A number of topics remain for future discussion and further work. Apart from the crucial questions of interpreting observed experimental phenomena in $(CH)_x$ in terms of any of the existing soliton based models [2, 35], it is clearly important to understand the full richness of the predictions of those models. Time-dependent properties are being studied further using time-dependent terms appropriate to $(CH)_x$ but with Gross-Neveu dynamics as an indicator for numerical and perturbational studies of breathers, $K\bar{K}$ and K-breather scattering. Similarly, the full quantum theories must be analyzed. The possibly discouraging indications [5, 21, 22] of full $N = 2$ Gross-Neveu quantum dynamics (that breathers, including the bag limit, are destabilized by quantum fluctuations) may well be invalidated by the differing dynamics in $(CH)_x$. Further, one might question the utility of literal one-dimensional field theories in real materials like $(CH)_x$ – a mean field description may actually be *more* appropriate than an exactly one-dimensional quantum theory, or at least correlation lengths may be large on a characteristic chain length scale. It is also essential to include Coulomb interactions, both to examine the relative effects on kinks [36] *and* polarons, and also to admit elementary exciton modes into the models, as well as possible bi-polaron or polaron-exciton states. Finally, we note that *lattice* Gross-Neveu models have been analyzed [37] which preserve complete integrability and support discrete generalizations of kinks, polarons and breathers. The possible implications of these results for $(CH)_x$ will be described separately. They may be important in the $(CH)_x$ context because of small numerical differences [6] between soliton descriptions in discrete [15] and continuum models [13].

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Appendix

EXPLICIT CONSTRUCTION OF THE STATIC SOLUTIONS

In this appendix we present in brief form a systematic method for constructing the solutions to the continuum electron-phonon model for polyacetylene. To tie in more directly with the previous field theory literature, we shall construct the solutions in the σ and Ψ form; the translation into Δ, u, and v is then immediate, using eqs. (2.11).

Summarized very succinctly, the method starts from the observation that for static σ fields the Dirac part of the semiclassical equations is simply a standard potential scattering problem having in general both a discrete (bound states) and continuous (scattering states) spectrum. For any given σ, one can solve directly for all the scattering data. Conversely, using the "trace identities" [16, 24, 25] appropriate to the Dirac equation [25, 38], one can rewrite certain expressions involving integrals over the fields entirely in terms of the scattering data. In fact, for the Gross-Neveu model, one can replace the expression for the action [16]

$$S(T) = \int_0^T \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}x \, \mathcal{L}(\sigma, \Psi) \tag{A.1}$$

in terms of the fields by an equivalent expression in terms of the (as yet undetermined) scattering data – bound-state energies and normalizations and the reflection coefficient – associated with the "potential" (a known expression in terms of σ) in the Dirac equation. Then, instead of varying S functionally with respect to the fields σ and Ψ to obtain the field equations (2.9), one determines the scattering data directly by varying S with respect to them. Knowing the scattering data, one has only to solve the inverse problem for the Dirac equation [23] to reconstruct σ and the Ψ_i.

The utility of the method really follows from the simplicity of the expression for S in terms of the scattering data. In particular, extremizing S with respect to the reflection coefficient leads to the result that the Dirac potential is reflectionless [16, 25]. Using this result and (without loss of generality for the present problem [16]) assuming that there is only one positive energy bound state, one finds after renormalization that the semiclassical action can be expressed as

$$S/T = -n_0\omega_0 - \frac{2N}{\pi}K_0 + \frac{2N}{\pi}\omega_0 \tan^{-1}\frac{K_0}{\omega_0}, \tag{A.2}$$

where ω_0 and $K_0 \equiv \sqrt{m^2 - \omega_0^2}$ are the positive energy, bound-state energy and momentum defined in the text. Introducing $\omega_0 = m\cos\theta$ and $K_0 = m\sin\theta$ and varying (A.2) with respect to θ yields

$$N\sin\theta\left(\frac{2\theta}{\pi} - \frac{n_0}{N}\right) = 0, \tag{A.3}$$

which determines the non-trivial solutions $\theta \equiv \theta(n_0)$ precisely as indicated in eq. (3.3). Similarly, since for static solutions $E = -S/T$, substituting the solution to (A.3) into (A.2) yields

$$E(n_0) = \frac{2N}{\pi} m \sin\theta(n_0), \tag{A.4}$$

which is just eq. (3.4).

To reconstruct σ and the Ψ_i, we can use the techniques developed by Frolov [23] who established that a matrix generalization of the Gelfand-Levitan [39] -Marchenko [40] formalism is applicable to the one-dimensional Dirac equation. The procedure can be simply summarized. From the scattering data one forms a matrix kernel $F(x, y) = F_S(x, y) + F_{BS}(x, y)$; for reflectionless potentials, which is the case in which we are interested, the scattering contribution, F_S, vanishes and only the bound state contribution remains. In our representation of the Dirac matrices and for the case of a single positive energy bound state, ω_0, and its "charge symmetric" negative counterpart at $-\omega_0$, one finds [25]

$$F_{BS}(x, y) = e^{-K_0(x+y)}(c_+ M_+ + c_- M_-) \tag{A.5}$$

where the matrices $M_\pm$ are given by

$$M_+ = \begin{bmatrix} \dfrac{m+\omega_0}{m-\omega_0} & \dfrac{m+\omega_0}{K_0} \\ \dfrac{m+\omega_0}{K_0} & 1 \end{bmatrix}, \tag{A.6a}$$

$$M_- = \begin{bmatrix} 1 & \dfrac{m+\omega_0}{K_0} \\ \dfrac{m+\omega_0}{K_0} & \dfrac{m+\omega_0}{m-\omega_0} \end{bmatrix} \tag{A.6b}$$

and for the charge symmetric case $c_+ = c_- = c_0$. In (A.6), as usual $\omega_0 \equiv +(m^2 - K_0^2)^{1/2}$.

From the kernel F one constructs the transformation operator $K(x, y)$ by solving the linear integral equation

$$K(x, y) + F(x, y) + \int_x^\infty K(x, t) F(t, y)\, dt = 0. \tag{A.7}$$

Then the "potential"

$$V(x) \equiv \gamma_0(\sigma - \sigma_0) = \begin{bmatrix} g(\sigma - \sigma_0) & 0 \\ 0 & -g(\sigma - \sigma_0) \end{bmatrix}, \tag{A.8}$$

is given by the commutator

$$V(x) = [-i\gamma_5, K(x,x)], \tag{A.9}$$

where as usual $\gamma_5 = \gamma_0\gamma_1$. Further, the Dirac wave functions for given k follow from

$$f_\pm(x;k) = e_\pm(x;k) + \int_x^\infty K(x,y) e_\pm(k;y)\,\mathrm{d}y, \tag{A.10}$$

where $e_\pm(x;k)$ are (unnormalized) plane-wave solutions to the free Dirac equation for positive and for negative energy, respectively. Thus, with $\omega = +\sqrt{k^2+m^2}$,

$$e_+(x;k) = \begin{bmatrix} \dfrac{ik}{\omega - m} \\ 1 \end{bmatrix} \mathrm{e}^{+ikx}, \tag{A.11a}$$

$$e_-(x;k) = \begin{bmatrix} 1 \\ \dfrac{ik}{\omega - m} \end{bmatrix} \mathrm{e}^{+ikx}. \tag{A.11b}$$

Note that the solution in eq. (A.11b) is, as it should be, the same as that in eq. (2.12).

With this formal structure established, we can construct the static solutions explicitly. For the kink, there is only one bound state and it has $\omega_0 = 0$. Since $K_0 = m$, the matrix F becomes,

$$F(x,y) = c_0 \mathrm{e}^{-m(x+y)} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}. \tag{A.12}$$

For this simple kernel the integral equation (A.10) can be solved by algebraic means, with the result that

$$K(x,y) = \frac{-c_0 \mathrm{e}^{-m(x+y)}}{1+2z} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \tag{A.13}$$

where $z = c_0 \mathrm{e}^{-2mx}/2m$. Then from (A.8) and (A.9) we find that

$$g(\sigma - \sigma_0) = \frac{-4g\sigma_0 z}{1+2z}, \tag{A.14}$$

and hence, after a bit of algebra, that

$$\sigma = \sigma_0 \tanh(mx + \delta_0), \tag{A.15}$$

where $\tanh\delta_0 = (m - c_0)/(m + c_0)$. Clearly this translates into the "kink" Δ given by (3.2a). For the $\omega_0 = 0$ bound state – the "midgap" state $(CH)_x$ – one uses (A.10) with

$k = ik_0 = im$ and $\omega_0 = 0$ to find

$$\Psi_0(x) \equiv f_+(x; im) = \frac{c_0 e^{-mx}}{1+2z}\begin{pmatrix}1\\1\end{pmatrix}, \tag{A.16a}$$

which, after some algebra and normalization, becomes

$$\Psi_0(x) = (\tfrac{1}{4}m)^{1/2}\operatorname{sech}(mx+\delta_0)\begin{pmatrix}1\\1\end{pmatrix}, \tag{A.16b}$$

with δ_0 defined above; this translates into the u and v given by eqs. (3.2b) and (3.2c). The *negative* energy scattering states follow from (A.7) using (A.11b) and the transformation operator for the kink, given by (A.13). The result is

$$\Psi_-(x;k) \equiv f_-(x;k) = e^{ikx}\left[\begin{pmatrix}1\\ \dfrac{ik}{\omega-m}\end{pmatrix} - \frac{2mz}{1+2z}\frac{1}{m-ik}\begin{pmatrix}1+\dfrac{ik}{\omega-m}\\ 1+\dfrac{ik}{\omega-m}\end{pmatrix}\right], \tag{A.17a}$$

or, after some algebra and normalization

$$\Psi_-(x;k) = N_k e^{ikx}\begin{pmatrix}\tanh(mx+\delta_0) - \left(\dfrac{\omega+ik}{m}\right)\\ \tanh(mx+\delta_0) + \left(\dfrac{\omega-ik}{m}\right)\end{pmatrix}, \tag{A.17b}$$

where $N_k = im/2\omega\sqrt{2\pi}$. Again we see that this translates into the corresponding state–given by eqs. (3.2d) and (3.2e)–in $(CH)_x$.

For the "bag" or "polaron" excitation one starts with the form of F_{BS} for the case of bound states at both $+\omega_0$ and $-\omega_0$. Using (A.5) and (A.6) we see that this is

$$F(x,y) = c_0 e^{-K_0(x+y)}\begin{pmatrix}\alpha & \beta\\ \beta & \alpha\end{pmatrix}, \tag{A.18}$$

where $\alpha = 2m/(m-\omega_0)$ and $\beta = 2K_0/(m-\omega_0)$. Again the integral equation (A.7) reduces to an algebraic one. The explicit solution is

$$K(x,y) = \frac{-c_0 e^{-K_0(x+y)}}{D(x)}\begin{bmatrix}\alpha+\zeta(\alpha^2-\beta^2) & \beta\\ \beta & \alpha+\zeta(\alpha^2-\beta^2)\end{bmatrix}, \tag{A.19}$$

where $\zeta \equiv -c_0 e^{-2K_0 x}/2K_0$ and $D(x) \equiv [1+(\alpha+\beta)\zeta][1+(\alpha-\beta)\zeta]$. Applying

(A.9) gives

$$g(\sigma-\sigma_0)=\frac{-4\beta K_0\zeta}{D(x)}, \tag{A.20a}$$

which, after considerable algebra, can be reduced to the form

$$\sigma=\sigma_0-\frac{K_0^2}{\omega_0 g}\operatorname{sech}K_0[(x+x_0)+\delta_1]\operatorname{sech}K_0[(x-x_0)+\delta_1], \tag{A.20b}$$

with $\tanh K_0 x_0=(m-\omega_0)/K_0$ and $\tanh\delta_1=[K_0(m-\omega_0)-c_0\omega_0]/[K_0(m-\omega_0)+c_0\omega_0]$. Clearly this translates into the polaron form for Δ, given (for $\delta_1=0$) by (3.8a). The positive energy bound-state wave function follows from (A.10) with $k=ik_0$; the result is

$$\Psi_0(x)\equiv f_+(x;ik_0)=\frac{e^{-K_0x}}{D(x)}\begin{bmatrix}\beta\zeta(\frac{1}{2}\alpha-1)+\frac{1}{2}\beta\\ 1+\zeta(\alpha-\frac{1}{2}\beta^2)\end{bmatrix}, \tag{A.21a}$$

which, after a substantial amount of algebra and normalization to 1, reduces to

$$\Psi_0(x)=(\tfrac{1}{8}K_0)^{1/2}\begin{pmatrix}\operatorname{sech}[K_0(x+x_0)+\delta_1]+\operatorname{sech}[K_0(x-x_0)+\delta_1]\\ -\operatorname{sech}[K_0(x+x_0)+\delta_1]+\operatorname{sech}[K_0(x-x_0)+\delta_1]\end{pmatrix}. \tag{A.21b}$$

Again this translates into the correct result (taking $\delta_1=0$) for $(CH)_x$. Finally, the *negative* energy scattering solutions for the polaron excitation follow from (A.7) using (A.11b) and the transformation operator in (A.19). The result is

$$\Psi_-(x;k)\equiv f_-(x;k)$$
$$=e^{ikx}\left\{\begin{pmatrix}1\\ \dfrac{ik}{\omega-m}\end{pmatrix}-\frac{2K_0\zeta}{D(x)(K_0-ik)}\begin{pmatrix}\alpha+\zeta(\alpha^2-\beta^2)+\dfrac{ik\beta}{\omega-m}\\ \beta+\dfrac{ik}{\omega-m}\alpha+\zeta(\alpha^2-\beta^2)\end{pmatrix}\right\},$$

which, again after considerable algebra and normalization, can be reduced to

$$\Psi_-(x;k)=N_k' r e^{ikx}\begin{bmatrix}-ik+t_+\gamma+t_-\delta\\ \omega+m-t_+\gamma+t_-\delta\end{bmatrix}, \tag{A.22b}$$

with

$$N_k' = \frac{1}{\sqrt{2\pi}} \left(\frac{\omega - m}{2\omega\left(K_0^2 + k^2\right)} \right)^{1/2},$$

$$\gamma = \tfrac{1}{2} K_0 \left(1 - \frac{ik}{\omega - m} \right), \qquad \delta = \tfrac{1}{2} K_0 \left(1 + \frac{ik}{\omega - m} \right),$$

$$r = \frac{K_0 + ik}{K_0^2 + k^2}.$$

Again this result translates correctly – here into u_- and v_- quoted in (3.8d) and (3.8e) – into $(CH)_x$.

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