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Multipolaron solutions of the Gross-Neveu field theory: Toda potential and doped polymers

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Exact, periodic multipolaron solutions are constructed for the Gross-Neveu (GN) field theory in one dimension for particles with N flavors. First we connect the appropriate GN equations with continuum models of Peierls distorted polymer chains. Then we utilize a relationship between the cnoidal wave solutions of the Toda lattice and the potential of a polaron lattice in polymers.

The existence and role of nonlinear excitations in an interacting one-dimensional (1D) electron-phonon system have been extensively studied in a variety of physical systems over the past decade. Of particular interest are solitons and polarons that are known to exist in polyenes [1–3], polyynes [4] and other related polymers. The single-soliton and single-polaron solutions in the continuum models (the Takayama–Lin-Liu–Maki [5] (TLM) model for *trans*-$(CH)_x$ and the Rice-Bishop-Campbell [4] (RBC) model for polyynes) can be obtained directly from the well-known results for the particle spectrum of the Gross-Neveu (GN) model [6]. This is possible, since a simple transformation [7] connecting the fermion fields in the polymer models with the GN model and the displacement field in the polymer with the scalar boson field in the GN model shows exact equivalence at an adiabatic level. If the two models are equivalent then their self-consistency conditions must also match. The GN model is known to be divergent in the ultraviolet region and requires a cutoff frequency Λ for renormalization. In the continuum models of the polymers, however, a precisely equivalent cutoff is introduced in a natural way by the finite width of the electron band. Thus the two self-consistency conditions can be shown to be equivalent. Furthermore, the number of different particle flavors N in the GN model corresponds to the total number of internal degrees of freedom in the polymer case.

In this way, any static solution obtained for the GN model can be carried over to the appropriate polymer continuum model and *vice versa*. Exact, periodic multisoliton solutions, or soliton lattices [8], are known for —$(A)_x$— and —$(AB)_x$— systems for $N=1$ (spinless fermions describing a spin-Peierls model [9]), $N=2$ (electrons with two spin states, such as in polyenes), and $N=4$ (including orbital degeneracy such as in polyynes). Bipolaron lattice solutions are known for $N=2$ in nondegenerate polyenes in the Brazovskii-Kirova [10] and other related models [11]. The polaron lattice has been studied analytically [12] within the TLM model ($N=2$) but there are no exact analytic solutions available for general N. Moreover, $N>2$ offers the possibility of multipolaron solutions with polaron charge varying from $Q=\pm e, \pm 2e, \ldots, \pm(N-1)e$. Specifically, a tripolaron lattice may exist in polyynes ($N=4$).

Our objective in this Rapid Communication is to construct analytic expressions for multipolaron lattice solutions for general N. Naturally, these nonlinear lattice solutions in polymer systems also constitute periodic solutions of the GN field-theory model in 1D. To attain our goal, we first establish an exact relationship between the cnoidal wave solution of the Toda lattice [13] and the order parameter associated with the polaron lattice. We emphasize here that this technique is not only straightforward but also applies to a wide class of potentials in order to obtain periodic (or "lattice") solutions. In addition, by way of this connection we have succeeded in bridging the gap between three seemingly disparate set of problems in physics, namely: (1) the classical-mechanics problem of a mass-spring chain with a nearest-neighbor nonlinear (exponential) interaction (the Toda lattice), (2) the quantum-mechanical problem of an interacting electron-phonon system in solid state (Peierls distorted polymers), and (3) the relativistic field theory problem of self-interacting fermions with an auxiliary scalar boson field (GN model).

The Lagrangian for the Gross-Neveu field theory in $1+1$ dimensions [14] is given by

$$L^{\mathrm{GN}}(x)=\sum_{\nu=1}^{N}\bar{\psi}^{\nu}(x)\left[i\gamma_{\mu}\frac{\partial}{\partial x_{\mu}}-g_{\mathrm{GN}}\sigma(x)\right]\psi^{\nu}(x)-\tfrac{1}{2}\sigma^{2}(x)\ ,$$

where $\psi^{\nu}(x)$ is a fermion field, $\psi^{\nu}(x)=(\psi_1^{\nu}(x),\psi_2^{\nu}(x))$, $\sigma(x)$ is a scalar boson field, and g_{GN} is the Gross-Neveu coupling constant. The summation index ν labels the particle type (or flavor). γ_{μ} ($\mu=0,1$) are the Dirac matrices ($\gamma_0=\sigma_3$, $\gamma_1=i\sigma_1$). If we consider the static solutions of the type $\psi^{\nu}(x,t)=e^{-i\varepsilon_n t}\psi^{\nu}(n;x)$ then the variation of $\bar{\psi}^{\nu}(x)$ gives ($x_0=t$, $x_1=x$)

$$\left[\varepsilon_n\gamma_0+i\gamma_1\frac{\partial}{\partial x}-g_{\mathrm{GN}}\sigma(x)\right]\psi^{\nu}(n;x)=0\ , \tag{1}$$

where ε_n is the nth eigenvalue. Equation (1) has exactly the structure of Bogoliubov–de Gennes equations [4,5] for the fermion fields $u(x)$ and $v(x)$ in the TLM ($\nu=1,2$) and RBC ($\nu=1,2,3,4$) continuum models.

The transformation $\psi_1^{\nu}(n;x)\to\frac{1}{2}[u_{\xi}(n;x)+v_{\xi}(n;x)]$, $\psi_2^{\nu}\to-(i/2)[u_{\xi}(n;x)-v_{\xi}(n;x)]$, $g_{\mathrm{GN}}\sigma\to\Delta$, and $x\to v_F x$ establishes an exact equivalence [7] of Gross-Neveu and polymer continuum models (TLM or RBC). Defining $f_{\xi}^{\pm}(x)=u_{\xi}(x)\pm iv_{\xi}(x)$ the analog of Eq. (1) in decoupled form for the polymers can be expressed as

$$\left[v_F^2\frac{\partial^2}{\partial x^2}+\varepsilon_{n,\xi}^2-\Delta^2(x)\pm v_F\frac{\partial}{\partial x}\Delta(x)\right]f_{n,\xi}^{\pm}(x)=0\ , \tag{2}$$

with an associated self-consistency equation

$$\Delta(x)=-2\lambda\pi v_F\left[\Delta(x)+\frac{v_F}{2}\frac{\partial}{\partial x}\right]\sum_{n,\xi}{}'\frac{|f^{+}_{n,\xi}(x)|^2}{2\varepsilon_{n,\xi}},$$

where λ denotes the dimensionless electron-phonon coupling constant and the sum is over occupied states excluding an $\varepsilon_{n,\xi}=0$ state.

The order parameter for a single polaron [4] is given by

$$\Delta_\theta(x)=\Delta_0-\Delta_0\sin(\theta)\left\{\tanh\left[\sin(\theta)\left[\frac{x+x_\theta}{\xi_0}\right]\right]-\tanh\left[\sin(\theta)\left[\frac{x-x_\theta}{\xi_0}\right]\right]\right\}, \quad (3)$$

where $\theta=\pi/2N(n+h)$, $\sin(\theta)=\tanh(2K_\theta x_\theta)=K_\theta\xi_0$, $v_F=\Delta_0\xi_0$, and n and h denote the number of electrons in the upper localized polaron level and the number of holes in the lower localized polaron level, respectively. The potential for a single polaron (bipolaron, tripolaron, etc.) in Eq. (2) thus becomes

$$V^{\pm}(x)=\Delta^2(x)\mp v_F\frac{\partial}{\partial x}\Delta(x)$$
$$=\Delta_0^2-2\Delta_0^2\sin^2(\theta)\mathrm{sech}^2\left[\sin(\theta)\left[\frac{x\mp x_0}{\xi_0}\right]\right]. \quad (4)$$

If we consider a lattice of polarons with a periodicity d then the lattice potential is given by the lattice sum

$$U^{\pm}(x)=\sum_{n=-\infty}^{+\infty}V^{\pm}(x-nd)$$
$$=\Delta_0^2-2\Delta_0^2\sin^2(\theta)\times\sum_{n=-\infty}^{+\infty}\mathrm{sech}^2\left[\sin(\theta)\left[\frac{x\mp x_\theta-nd}{\xi_0}\right]\right]. \quad (5)$$

To evaluate the infinite sum in Eq. (5) we first deduce a relationship between the Toda lattice potential $V_{\mathrm{TL}}(r_n)$ associated with a cnoidal wave [13] and the polaron lattice potential $U(x)$. The cnoidal wave is given by

$$-\frac{b/m}{(2K\nu')^2}V'_{\mathrm{TL}}(r_n)=\left[\mathrm{dn}^2(2\tilde{x}K)-\frac{E}{K}\right]=\left[\frac{\pi}{2K'}\right]^2\sum_{n=-\infty}^{+\infty}\mathrm{sech}^2\left[\frac{\pi K}{K'}\tilde{x}-\frac{\pi K}{K'}n\right]-\frac{\pi}{2KK'}, \quad (6)$$

where the Toda lattice potential [13] is given by

$$V_{\mathrm{TL}}(r_n)=\frac{a}{b}e^{-br_n}+ar_n,\quad ab>0,\quad r_n=x_{n+1}-x_n.$$

In Eq. (6) K, E, (and Π below) denote the complete elliptic integrals of the first, second, and third kind, respectively. $\tilde{x}=n/\lambda'\pm\nu't$, λ' and ν' being the wavelength and frequency, respectively, of a Toda chain with each particle having mass m. dn and sn and cn below are Jacobian elliptic functions with modulus k [and $k'=(1-k^2)^{1/2}$ below].

A direct comparison of Eqs. (5) and (6) leads to the following important relation between $V_{\mathrm{TL}}(r_n)$ and $U(x)$:

$$\frac{\Delta_0^2-U^{\pm}(x)}{2\Delta_0^2\sin^2(\theta)}=\left[\frac{2K'}{\pi}\right]^2\left[\frac{\pi}{2KK'}-\frac{b/m}{(2K\nu')^2}V'_{\mathrm{TL}}(r_n)\right], \quad (7)$$

where $-V'_{\mathrm{TL}}(r_n)$ is the force of the spring in the Toda chain when it is stretched by an amount r_n. Equation (7) not only connects the Toda lattice with doped polymers (polaron lattice) but also with the Gross-Neveu model (periodic multipolaron solutions) via the transformations mentioned before Eq. (2). Equation (7) should *not* be misconstrued as connecting a discrete problem (Toda lattice) with a continuum problem (polymer chains or the GN model). Instead, it only exploits the mathematical structure of Eq. (6), treating $\tilde{x}$ as a continuous variable. Note that the cnoidal wave $[\mathrm{dn}^2(2xk)-E/K]$ is also a solution of the Korteweg–de Vries (KdV) equation [15]. The KdV equation is a continuum equation. We also note that a discrete Su-Schrieffer-Heeger-like model was exactly solved [16] to obtain periodic solutions assuming an exponential (Toda-like) electron-phonon interaction.

Equations (6) and (7) lead to the following expression for the lattice potential:

$$U^{\pm}(x)=\Delta_{\mathrm{L}}^2(x)\mp v_F\frac{\partial}{\partial x}\Delta_{\mathrm{L}}(x)$$
$$=\Delta_0^2\left[2\sin^2(\theta_{\mathrm{L}})\mathrm{sn}^2\left[\sin(\theta_{\mathrm{L}})\left[\frac{x\mp x_{\mathrm{L}}}{k\xi_0}\right],k\right]+\left[1-\frac{2E'}{k^2K'}\sin^2(\theta_{\mathrm{L}})\right]\right], \quad (8)$$

where the lattice order parameter is given by

$$\Delta_{\mathrm{L}}(x)=\Delta_0 k\sin(\theta_{\mathrm{L}})\left[\frac{\mathrm{sn}(x^-)\mathrm{cn}(x^-)\mathrm{dn}(x^-)+\mathrm{sn}(x^+)\mathrm{cn}(x^+)\mathrm{dn}(x^+)}{\mathrm{dn}^2(x^-)-\mathrm{dn}^2(x^+)}\right],\quad d=\frac{2kK}{\sin(\theta)}\xi_{\mathrm{L}},\quad \xi_{\mathrm{L}}=\left[\frac{\pi}{2kK'}\right]\xi_0. \quad (9)$$

and

$$\mathrm{sn}\left[\frac{2x_{\mathrm{L}}}{k\xi_0}\sin(\theta_{\mathrm{L}})\right]=\frac{\sin(\theta_{\mathrm{L}})}{[k^2+k'^2(\theta_{\mathrm{L}})]^{1/2}},$$
$$\sin(\theta_{\mathrm{L}})=\left[\frac{2kK'}{\pi}\right]\sin(\theta),\quad x^{\pm}=\left[\frac{x\pm x_{\mathrm{L}}}{k\xi_0}\right]\sin(\theta_{\mathrm{L}}). \quad (10)$$

Note that the expression for the characteristic length ξ_{L} in the lattice problem will also emerge from the self-consistency condition as shown below. Equation (10) is an expression for the characteristic width x_{L} of a single polaron in the lattice problem as a function of k (doping). In the single-polaron limit ($k\to1$, $K\to\infty$, $d\to\infty$), Eqs. (8)–(10) reduce to Eqs. (3) and (4). Also, in the deconfinement limit [$\sin(\theta)\to1$, $x_\theta\to\infty$], known soliton lattice solutions (for $N=2,4$) are recovered. Within the context of the GN model Eq. (9) represents (N flavors of) self-interacting fermions in an inhomogeneous, periodic boson field. It is worth pointing out that Eq. (9) can be interpreted as a bound state of two soliton lattices shifted from each other by $2x_L$. Specifically,

$$\Delta_L(x) = \Delta_{SL}(x^-)\left\{\frac{\mathrm{dn}^2(x^-)}{\mathrm{dn}^2(x^-)-\mathrm{dn}^2(x^+)}\right\} + \Delta_{SL}(x^+)\left\{\frac{\mathrm{dn}^2(x^+)}{\mathrm{dn}^2(x^-)-\mathrm{dn}^2(x^+)}\right\},$$

where the factors in braces can be thought of as "binding weights." Similarly, Eq. (3) can be recast in the following form:

$$\Delta_\theta(x) = \Delta_0\tanh(x^-)\left\{\frac{\mathrm{sech}^2(x^-)}{\mathrm{sech}^2(x^-)-\mathrm{sech}^2(x^+)}\right\} + \Delta_0\tanh(x^+)\left\{\frac{\mathrm{sech}^2(x^+)}{\mathrm{sech}^2(x^-)-\mathrm{sech}^2(x^+)}\right\},$$

which shows a polaron to be a bound state of two solitons shifted from each other by $2x_\theta$ with the corresponding binding weights in the braces. Thus, it is evident that the lattice order parameter $\Delta_L(x)$ preserves the mathematical structure of $\Delta_\theta(x)$. This is (likely to be) a consequence of the reflectionless property of the potential $V(x)$, or in other words we are dealing with an integrable system.

Equation (2) with potential $U(x)$ given by Eq. (8) is a Lamé equation [8,11] of genus 1. The wave functions and eigenvalues $(f_{n,\xi}, \varepsilon_{n,\xi})$ can be obtained (with minor modifications) from Ref. [11]. In particular, the spectrum consists of four bands, namely, conduction, upper and lower polaron, and valence band. If E_C, E_U, and E_L denote the conduction-band edge, the upper edge and the lower edge of the upper polaron band, respectively, then the moduli k and k' of the elliptic integrals (or functions) can be expressed in terms of the band edges

$$k = \left[\frac{E_C^2 - E_U^2}{E_C^2 - E_L^2}\right]^{1/2}, \quad k' = \left[\frac{E_U^2 - E_L^2}{E_C^2 - E_L^2}\right]^{1/2}.$$

Explicit expressions for E_C, E_U, and E_L are given in Ref. [11]. Since the standard Gross-Neveu model has particle-hole (charge-conjugation) symmetry, $-E_C$, $-E_U$, and $-E_L$ correspond to the valence and lower polaron band, respectively.

Next, we explicitly check the self-consistency equation by using Lamé functions and the associated eigenvalues [11]. The solution given by Eq. (9) is found to be locally stable only if

$$E_U = E_C\,\mathrm{sn}\left[\frac{K(\tilde{k})}{k^2}\left[1-\frac{2}{\pi}\theta\right],\tilde{k}\right], \quad \tilde{k} = \frac{k' E_C}{E_U}. \quad (11)$$

Equation (11) is equivalent to the relation between ξ_L and ξ_0 and in the limit $k \to 1$ reduces to $E_p = \Delta_0 \cos\theta$, i.e., the localized single-polaron level, provided $\xi_L = (\pi/2kK')\xi_0$. In addition, when Eq. (11) holds, we obtain from the self-consistency condition a prescription for systematically taking the weak-coupling limit:

$$\frac{1}{N\lambda} = \frac{v_F}{\xi_L E_U}\left\{k^2 \Pi\left[\eta, \frac{E_C^2}{E_U^2}, \tilde{k}\right] - F(\eta,\tilde{k}) + \frac{1}{k}\left[1-\frac{2\theta}{\pi}\right]\left[K(\tilde{k})\left[1-\frac{k'^2}{\tilde{k}^2}\right] + \frac{k'^2}{\tilde{k}^2}E(\tilde{k})\right]\right\},$$

where $\eta = (E_U/E_C)\sin^{-1}\mathrm{sn}(K'-\delta,k')$. In the weak-coupling limit the arbitrary parameter $\delta \to 0$ corresponding to $\lambda \to 0$. $F(\eta,\tilde{k}), E(\eta,\tilde{k})$ below and $\Pi(\eta, E_C^2/E_U^2, \tilde{k})$ are the incomplete elliptic integrals of the first, second, and third kind, respectively. Furthermore, δ (and thus λ implicitly) is related to the upper momentum cutoff Λ (or the total bandwidth $2v_F\Lambda$) according to

$$\Lambda = \frac{\mathrm{sn}(K'-\delta,k')\mathrm{dn}(K'-\delta,k')}{k\xi_L \mathrm{cn}(K'-\delta,k')}.$$

The total energy of the polaron lattice relative to the polaron free ground state is given by

$$\frac{E^L}{L} = \frac{\Delta_0^2}{2\pi\lambda v_F}\left[1-\frac{4\sin^2(\theta)K'}{\pi K}\right] - \frac{N\Lambda}{\pi}(\Delta_0^2 + v_F^2\Lambda^2)^{1/2} + \frac{NE_U}{k\xi_L}\left[1-\frac{2}{\pi}\theta\right]\left\{E(\tilde{k}) - \left[\frac{E}{K}-1\right]\left[K(\tilde{k})\frac{E_C^2}{E_U^2} - \left[\frac{E_C^2}{E_U^2}-1\right]\Pi(k'^2,\tilde{k})\right]\right\}$$
$$- \frac{NE_U}{k\xi_L}\left\{\left[k^2 - (1-\tilde{k}^2)\left[1-\frac{E}{k'^2K}\right]\right]F(\eta,\tilde{k}) + \left[1-\frac{E}{k'^2K}\right]E(\eta,\tilde{k}) + \left[\frac{kv_F}{E_L\xi_L}\right]^2 \Pi\left[\eta,\frac{E_C^2}{E_U^2},\tilde{k}\right]\right\}.$$

Expansion of the above equation in the dilute limit to order k'^4 leads to a repulsive interaction between two polarons and can be calculated as in Ref. [11]. Moreover, the chemical potential μ can be shown to satisfy $E_U < \mu < E_C$, indicating that the polaron lattice is energetically the most favorable charged configuration.

Equation (7) and the solution given by Eqs. (9) and (10) provide a way to interpret phenomena encountered within the context of Gross-Neveu field theory, such as spontaneous dynamical symmetry breaking, mass generation, and negative-energy sea anomalies, in terms of phenomena in the solid state (Peierls distortion, fractional charge, consequences of valence-band phase shift) as well as in terms of Toda lattice (dual system, conserved quantities, discrete Hill's equation). In addition, the procedure described here can easily be extended to chiral GN field theory [17]. The Lagrangian for the latter is given by $\mathcal{L} = \mathcal{L}_{GN} - \frac{1}{2}g_{GN}^2\sum_{\nu=1}^{N}(\bar{\psi}^{(\nu)}\gamma_0\gamma_1\psi^{(\nu)})^2$, which has continuous chiral invariance $\psi \to e^{i\phi\gamma_0\gamma_1}\psi$ and no general charge conjugation symmetry. For $N=2$ this model has no stable polaron solution. However, stable soliton solutions exist; for $N>2$ the localized soliton levels are off-center in the energy gap. Therefore a soliton-lattice solution can readily be obtained in this case. Moreover, for $N>2$, stable polaron (and polaron lattice) solutions may well exist. Note that the $N=2$ chiral GN model also has an analog in solid state, namely, the incommensurate Peierls distorted system. Furthermore, it can be compared with the classical Heisenberg XY ferromagnet.

Another application of our procedure is obtaining multisoliton or multipolaron solutions of (AB)-type GN field theory with fermion fractionalization [18]. For $N=2$, single-soliton or -polaron solutions are known both field theoretically and in the solid state. The latter corresponds to a linearly conjugated diatomic polymer (Rice-Mele model [19]) which exhibits solitons with charge fractionalization into irrational numbers. Generalization of —(AB)— -type GN field theory for general $N(>2)$ is conceptually straightforward. The GN model corresponds to commensurability $M=2$ in the polymer case. Extension to general M requires nontrivial modification of the GN model. We also note that the known lattice solutions for the order parameter for liquid crystals [20], superconductors [21], Josephson junctions [22], and related solid-state systems can be obtained directly by our procedure.

Although we have obtained static multipolaron solutions, the present technique applies equally well to time-dependent solutions for polymers (but not in the GN model) and can possibly be linked to the Lamb ansatz [15]. Furthermore, this technique is implicitly related to the technique of inverse scattering and the potential $V(x)$ is related to the Bargmann potentials [15].

For $N=2$ our results can be compared with the analytical solution of Takahashi [12]. Since it is difficult to synthesize long chains of polyynes in the laboratory (small chains are believed to exist in the interstellar dust) as well as the —(AB)— -type polyynes, a comparison for $N=4$ results with experimentally doped systems is not possible at present. Solid-state realizations of $N>4$ field theories are yet to be found.

It is known that the nonlinear evolution equations that admit solitary-wave solutions also have spatially periodic exact solutions (or polycnoidal waves [23]). Equation (6) is a special case for a Schrödinger equation with a potential $V(x)=a+b\,\mathrm{sech}^2x$. We assert that exact periodic solutions also exist if the potential $V(x)=a+b\,\mathrm{sech}x$ or $V(x)=a+b\tanh x$. Specifically, using the method of Poisson summation [23] for elliptic functions, we have

$$\sum_{n=-\infty}^{\infty} \mathrm{sech}[\pi s(x-n)]=\frac{2K(s)}{\pi s}\mathrm{dn}(x)\ ,$$

$$\sum_{n=-\infty}^{\infty} (-1)^n\mathrm{sech}[\pi s(x-n)]=\frac{2k(s)K(s)}{\pi s}\mathrm{cn}(x)\ ,$$

$$\sum_{n=-\infty}^{\infty} (-1)^n\tanh[\pi s(x-n)]=\frac{2k(s)K(s)}{\pi s}\mathrm{sn}(x)\ ,$$

where $s=K(k)/K(k')$ and periodicity $d=\pi s$. In addition, various powers and combinations of $\tanh x$ and $\mathrm{sech}x$ can be summed in this manner in a Poisson sum. Whether the Schrödinger equation with such potentials [$V(x)$ or corresponding periodic potential $U(x)$] is exactly solvable remains to be seen. This procedure applies equally well to the solitonlike solutions of sine-Gordon, ϕ^4,ϕ^6 and related models as well as to the nonlinear Schrödinger equation [15].

In conclusion, we have obtained a simple technique with wide applicability for obtaining multipolaron solutions of (integrable) systems by connecting three problems belonging to very different physics disciplines.

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