EXACTLY SOLUBLE PEIERLS MODELS

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Exactly soluble models for electrons on a deformable discrete chain are found. They include typical continuous Peierls models as special limits. The chain structure, electronic spectrum and thermodynamic functions in the ground state are found. The region of a nearly half filled band corresponding to the polyacetylene model is described in detail.

We consider a system of N molecules situated at arbitrary points x_n on a line L and N_e electrons, $N_e = \rho N$, $0 \leqslant \rho \leqslant 2$. The eigenfunctions $\psi_n = \psi_n(E)$ and the energy eigenvalues E for electrons are defined by a typical strong coupling hamiltonian

$$H\psi_n = c_n\psi_{n+1} + c_{n-1}\psi_{n-1} + v_n\psi_n = E\psi_n ,$$

$$c_n = c\exp[\alpha(x_n - x_{n+1})] , \quad x_{n+1} > x_n . \tag{1}$$

Here v_n are the on-site potentials and c_n are the integrals of tranfer among the nearest sites. Below, dimensionless units of energy ($c = 1$) and length ($\alpha^{-1} = 1$) are used. The ground state of the system has to be found by the minimization of the total energy functional

$$W\{c_n, v_n\} = \sum_{E<\mu} E\{c_n, v_n\} + NI_2\{c_n, v_n\} ,$$

$$I_2 = N^{-1}\sum_n (c_n^2 + v_n^2/2) , \tag{2}$$

over c_n, v_n at a given total length L

$$L = Na = -I_0\{c_n\} , \quad I_0 = x_1 - x_N = \sum_n \ln c_n ,$$

$$e^{-a} = \bar{c} . \tag{3}$$

Here μ is the chemical potential of the electrons, κI_2 is the potential of the intramolecular deformations v_n and that of the intramolecular repulsion which is supposed to be exponential in distance.

We shall distinguish the two models:

(i) $v_n \equiv 0$, $\delta W/\delta c_n = 0$;
(ii) $\delta W/\delta c_n = 0$, $\delta W/\delta v_n = 0$.

Model (i) is general enough to describe the Peierls effect due to the interaction of electrons with acoustical deformations of the lattice. Model (ii) also takes into account the effect of the on-site deformations, but it requires special adjustment for the coefficient of elastic deformations v_n, as can be seen from (2). This condition leads to the special degeneracy of model (ii) which displays itself, for instance, as the absence of solitons at $\rho \to 1$.

In the limit $\kappa\bar{c} \gg 1$ the displacements $u_n = x_n - na$ are small, $|u_n| \ll 1$, and model (i) becomes close to the Su–Schrieffer–Heeger model of polyacetylene [1]. Under the same condition this model may be approximated by one of the three typical continuum models depending on either $\rho \approx 1$, $|\rho - 1| \approx 1$ or $|\rho - 1| \ll 1$, or $\rho \ll 1$ (see refs. [2,3] for details).

In this paper we present the final results for the exact solution of model (i) and with less detail for model (ii). We shall also outline briefly the method of the solution. All the details are given in ref. [3].

In the ground state of model (i) the lattice $x_n = na + u_n$ is found to be an incommensurate doubly periodic structure. It may be considered as a superposition of the two shifted superlattices for odd and even numbers n with the periods $N_\rho = 2/|\rho - 1|$,

$$u_n = u(n - n_0) = \frac{1}{2}\ln\frac{\theta_4((n - n_0 - 1)/N_\rho + (-1)^n/\underline{4})}{\theta_4((n - n_0 + 1)/N_\rho + (-1)^n/\underline{4})} ,$$

$$\theta_4(v) = \theta_{\underline{4}}(v, \tau) , \quad \tau = iK'/K , \quad K = K(k) . \tag{4}$$

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Hereafter we follow the notations [4] adopted for the Weierstrass function $\theta_4(v, \tau)$, elliptical integrals K, K' and the functions $\mathrm{sn}\, u = \mathrm{sn}(u, k)$, etc. Note that n_0 in (4) is an arbitrary generally nonintegral number, so that the ground state is continuously degenerate relative to the translations of the superstructure in spite of the absence of the translational invariance in the energy functional (1), (2).

Deformations (4) are accompanied by the CDW defined as a local distribution of electronic density ρ_n:

$$\rho_n = 2 \sum_{E \leqslant \mu} |\psi_n(E)|^2 = \rho + \frac{N_\rho}{4} \frac{K'(k)}{K(k)} \frac{\partial}{\partial n_0} u(n - n_0). \tag{5}$$

The parameters $\tau = \tau(\rho)$ or $k = k(\rho)$ are determined from the selfconsistency equation

$$[K(r)/\mathrm{cn}\, u]\, \theta_4^2(0)/\theta_4^2(v) = \pi\kappa\bar{c}\,, \quad r = \mathrm{dn}\, u\,,$$
$$v = \tfrac{1}{2}|\rho - 1| \quad , u = K(k)|\rho - 1|\,. \tag{6}$$

The electronic spectrum at any $\rho \neq 0, 1, 2$ consists of three bands $(-E_m, -E_+)$, $(-E_-, E_-)$, (E_+, E_m). The chemical potential is situated in one of the gaps $(-E_+, -E_-)$ or (E_-, E_+) depending on whether $0 < \rho < 1$ or $1 < \rho < 2$. The band edges E_-, E_+, E_m are determined by the formula

$$E_m = 2\bar{c}\, \theta_3(v)\theta_4(v)/\theta_3(0)\theta_4(0)\,,$$
$$E_+/E_m = \mathrm{sn}\, u\,, \quad E_-/E_+ = k'/\mathrm{dn}\, u\,. \tag{7}$$

The energy of the ground state $W_0(\rho, a)$ per molecule is given by the formula

$$N^{-1}W_0 = \frac{K^2(r)}{\pi^2\kappa}\left[1 + \frac{\mathrm{sn}^2 u\, \mathrm{dn}^2 u}{\mathrm{cn}^2 u} - \frac{4}{3}\frac{E(r)}{K(r)} - \frac{\mathrm{sn}\, u}{K(k)} \frac{\theta_4'(1/2 - |\rho - 1|/2)}{\theta_4(1/2 - |\rho - 1|/2)}\right]. \tag{8}$$

The pressure $P(\rho, a)$ is

$$P = N^{-1}\left(\frac{\partial W_0}{\partial a}\right)_\rho = \frac{2K(r)}{\pi^2\kappa}\left[1 + \frac{\mathrm{sn}^2 u\, \mathrm{dn}^2 u}{\mathrm{cn}^2 u} - 2\frac{E(r)}{K(r)}\right]. \tag{9}$$

The parameters k, u, r in (7)–(9) have to be determined from relations (6).

In a weak coupling limit

$$\lambda_\rho = [\pi\kappa\bar{c}\cos(\tfrac{1}{2}\pi|\rho - 1|)]^{-1} \ll 1\,, \quad |\rho - 1| \gg \mathrm{e}^{-1/\lambda_1}.$$

We find from (6), (7) that

$$E_m \approx 2\bar{c}\,, \quad E_+/E_m \approx E_-/E_m \approx \sin(\pi|\rho - 1|/2)\,,$$
$$E_+^2 - E_-^2 = \Delta_\rho^2 \cos^2[\pi|\rho - 1|/2]\,,$$
$$\Delta_\rho = 8\bar{c}\exp(-1/\lambda_\rho)\,. \tag{10}$$

Relations (10) generalize the results for the continuum Peierls–Fröhlich models [2,5]. At $\rho(2 - \rho) \ll 1/\kappa\bar{c}$ we come to the limit [6] of isolated selftrapped states.

In the most interesting limit $|\rho - 1| \ll \mathrm{e}^{-1/\lambda_1}$ we have the dilute kink lattice. For the isolated kink we first find from (4) and (5)

$$u_{2n} = \frac{1}{2}\ln\frac{\mathrm{ch}[\alpha(n - n_0 - 1/2)]}{\mathrm{ch}[\alpha(n - n_0 + 1/2)]}\,, \quad u_{2n+1} = \mathrm{const.}\,,$$
$$\alpha = \tfrac{1}{2}\mathrm{e}^{-1/\lambda_1}\,,$$
$$\rho_{2n} - \rho = \tfrac{1}{2}[\mathrm{th}(\alpha(n - n_0)) - \mathrm{th}(\alpha(n - n_0 + \tfrac{1}{2}))]\,,$$
$$\rho_{2n+1} = \rho\,, \quad \sum_n \rho_{2n} = 1\,.$$

Note that every second site only is involved in the distortions and the charge concentration for an isolated kink. For the spectrum we find

$$E_m = 2\bar{c}\,, \quad E_+ \approx \Delta_1\,, \quad E_- \approx 4\Delta_1 \exp[-8\alpha/|\rho - 1|]$$
$$|\rho - 1| \ll \alpha\,. \tag{11}$$

In the same limit we can study relations (6)–(9), omitting the terms $\sim O(E_-/\Delta_1)$, which are exponentially small in distance $N_\rho = 2/|\rho - 1|$ between solitons. This approximation corresponds to the limit $k \to 1$, $|\tau| \sim |\rho - 1|$ in expressions (6)–(9). We find

$$rK(r)[(1 + r')/r]^{|\rho - 1|} = \pi\kappa\bar{c}\,, \tag{12}$$
$$w_0 = [K^2(r)/\pi^2\kappa][2 - r^2 - \tfrac{4}{3}E(r)/K(r) + 2r'|\rho - 1|]\,, \tag{13}$$
$$P = (2/\pi^2\kappa)K^2(r)[2 - r^2 - 2E(r)/K(r)]\,. \tag{14}$$

Using (12)–(14) we can find

$$w_0(\rho, a) = w_0(1, a) + E_s|\rho - 1| + \tfrac{1}{2}(\partial\mu/\partial\rho)_a(\rho - 1)^2 + \dots\,,$$
$$w_0(\rho, P) = w_0 + Pa = \tilde{w}_0(1, P) + E_s|\rho - 1|\,,$$

where $E_s = |\mu|$ is the soliton energy. Note that $(\partial\mu/\partial\rho)_P = O(\exp[-8\alpha/|\rho - 1|])$ like for the continuum model [5], while $(\partial\mu/\partial\rho)_a$ is finite at $\rho = 1$. Unlike

the earlier suggestions [9] we find $(\partial\mu/\partial\rho)_a > 0$. For a weak coupling we can calculate $E_s = 2\Delta_1/\pi$, $(\partial\mu/\partial\rho)_a = \Delta_1^2/\pi\lambda_1\bar{c}$.

Model (ii) can be described analogously. The qualitative difference is that in this case the electronic spectrum has only two bands (E_1, E_2), (E_3, E_4) and one gap (E_2, E_3), which lies at the Fermi level $E_2 < \mu < E_3$. Consequently model (ii) shows no singularity at $\rho = 1$. The method of the exact solution is based on the results [10] of the spectral theory for the discrete Schrödinger operators (1). All the details are described elsewhere [3]. The extrema of the functional (1), (2) are studied by making variations of the density of states for (1) in the space of the functionals $I_n\{c_n, v_n\}$ which are known as integrals of motion for the dynamics of the Toda lattice [11]. The two of them I_2 and I_0 appear explicitly in the energy functional (2). The exact integrability of our models is due to the fact that the energy functional depends only on the spectrum E and the integrals I_n for the operator (1).

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