Commensurability effects in the discrete Peierls model

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Pinning of a charge density wave is considered in the discrete Peierls model. Pinning is achieved by adding to the Hamiltonian of the previously considered Peierls model [S. A. Brazovskiĭ, I. E. Dzyaloshinskiĭ, and I. M. Krichever, Sov. Phys. JETP **56**, 212 (1982)] terms that violate the integrability. Analysis shows that, depending on the number ρ of electrons per ion and on the strength of the integrability-violating perturbation, two situations are possible, the so-called "devil's staircase" and stochastic extremals.

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1. INTRODUCTION

Commensurability effects and thermodynamic transitions between a commensurate phase and an incommensurate one were first considered by one of the authors[1] in his theory of magnetic helical structures or spin density waves (SDW). The analysis was carried out for the three-dimensional case, i.e., for a SDW that depends on one coordinate in three-dimensional space. In the molecular-field approximation, allowance for commensurability denoted in essence the influence of the anisotropy on the SDW. To describe SDW not far from the transition point it suffices to know only the angle φ of spin rotation in the helix. The effective free energy ("Hamiltonian") in relative units takes the universal form[1]

$$\mathcal{H}(f)=\int dx\left\{\frac{1}{2}\left(\frac{d\varphi}{dx}\right)^2-f\frac{d\varphi}{dx}-\alpha\sin^2\varphi\right\}, \tag{1.1}$$

where $\alpha(T)$ is the temperature-dependent anisotropy and f is the SDW wave vector at $\alpha=0$. Of course, f itself is also a function of temperature; it makes sense, however, to regard the energy (1.1) as a function of temperature [via $\alpha(T)$] and of the parameter f. An energy in the form (1.1) was considered first by Frank and Van der Merwe[2] in their theory of dislocations in a one-dimensional elastic chain of atoms on a crystalline substrate at absolute zero temperature.

The variational problem (1.1) is by now universally known. The ground states of the system are determined by the value of the parameter $\varkappa_0^2=2\alpha/f$. At $\varkappa_0<\pi/2$ (in particular, $f\gg\alpha$) the ground state is close to a simple helicoidal SDW with generally speaking irrational (in units of atomic spacing) period. This is the incommensurate phase. At $\varkappa_0\geqslant\pi/2$ the states φ are in the main independent of the coordinates ($\varphi=\pi/2$); this is the commensurate phase. The transition between the commensurate and incommensurate phases takes place in the region $\pi/2-\varkappa_0\ll\pi/2$. The SDW then degenerates into a lattice of solitons (dislocations in the terminology of Frank and Van der Merwe) with a period[1,2]

$$L=-\frac{4}{\pi f}\ln\left(\frac{\pi}{2\varkappa_0}-1\right). \tag{1.2}$$

The solitons interact in accord with the exponential law[1,2]

$$V_{int}\sim\exp\left(-{}^1/_4\pi fL\right). \tag{1.3}$$

The free energy has a rather weak singularity in $\varkappa_0$ (or in f; Ref. 1):

$$\mathcal{H}_{sing}\sim\frac{f-f_0}{\ln(f-f_0)},\qquad\frac{2\alpha(T)}{f_0}=\frac{\pi}{2} \tag{1.4}$$

at $f>f_0$ and $\mathcal{H}_{\text{sing}}=0$ at $f<f_0$.

It was also indicated in Ref. 1 that the a description with the aid of (1.1) of the action of the anisotropy on the SDW is a simplified one. Arguments were presented to show that $\mathcal{H}$ as a function of f has singularities much more nontrivial than (1.4); $\mathcal{H}(f)$ is in fact a function that is discontinuous at all points. Namely, its values at f with rational Miller indices $f=2\pi p/r$ (p and r are relatively prime integers) differ by a finite amount from an arbitrarily close irrational $f/2\pi$. The size of the spike (the pinning energy) is[1]

$$\mathcal{H}_{pinn}\sim\left(\frac{T_c-T}{T_c}\right)^{r/2} \tag{1.5}$$

at large r. By virtue of (1.5) the function $\mathcal{H}(f)$, being discontinuous everywhere, has a continuous derivative at all irrational f. (This situation was subsequently named the "devil's staircase").

It was also noted in Ref. 1 that since the pinning energy (1.5) is extremely small at large r, individual sections of the total devil's staircase can be in fact smoothed out. This situation is called the "harmless staircase."

The arguments in favor of the "diabolic character" of SDW were subsequently applied by one of us[3] to the charge-density waves produced in quasi-one-dimensional metals when acted upon by the Peierls-Fröhlich mechanism as a result of umklapp processes.

Far from transition point, a CDW is described approximately (in the three-dimensional case!) by the same Hamiltonian (1.1). Near the transition point, within the framework of the molecular-field theory, we must take into account, besides the coordinate dependence of the phase of the CDW also the inhomogeneity of its amplitude. This was first done by McMillan via numerical calculations.[4]

In the one-dimensional case, there is no molecular-field approximation for CDW and SDW. Therefore (1.1) loses the meaning of free energy and becomes the Hamiltonian (at $T=0$) of the CDW and SDW. The thermodynamics is determined by functional integration of the Gibbs distribution $\exp\{-\mathcal{H}(\varphi)/T\}$. Such calculations were first made by Brazovskiĭ and one of us[5] (see also Ref. 6). No phase transition

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exists in a one-dimensional system, as should be the case. At $\varkappa_0 < \pi/2$ the correlation radius R_c behaves at all temperatures as in the XY model:

$$R_c \sim 1/T, \tag{1.6}$$

thus indicating the absence of pinning (the CDW is a phason). At $\varkappa_0 > \pi/2$ R_c behaves in two ways. At $T > T_p$ (T_p is the characteristic pinning temperature) R_c retains the behavior of the XY model (1.6). With decreasing temperature, the XY regime gives way to the Ising regime at $T \sim T_p$:[1]

$$R_c \sim \exp(\text{const}/T), \tag{1.7}$$

and the phason acquires mass. The crossover is in fact the manifestation of the transition between the commensurate and incommensurate phases in the three-dimensional case.

The next decisive step in the study of commensurability effects (anisotropy for SDW, umklapp for CDW, substrate potential for elastic one-dimensional chains, etc.) was Aubry's discovery (a good review of Aubry's own results and of those by others is contained in his lecture[7]), who showed that $\mathscr{H}_0(f)$ has besides the devil's-staircase regime also stochastic regimes in which pinning occurs also for irrational values of $2\pi f$.

Aubry used mainly the known model of Frenkel' and Kontorovich.[8] Another model that admits of both regimes, the stochastic and the devil's staircase, is the three-dimensional anisotropic Ising model with allowance for nearest-neighbor interaction (called the ANNNI model). A good survey of the results obtained with this model is contained in Bak's article.[9]

We show below that both the devil's-staircase and the stochastic regimes occur in the exactly integrable discrete Peierls model, recently considered by Brazovskiĭ and us,[10] if a perturbation, no matter how small, is turned on and destroys the exact integrability. Of course, no pinning of a stationary CDW or of a soliton lattice is produced at all in the exactly integrable case, regardless of the parameter values.

2. THREE DIMENSIONAL GROUND STATE

We recall the formulation of an exactly solvable discrete Peierls model.[10] The electron spectrum is determined by the discrete Schrödinger equation

$$c_n\psi_{n+1} + c_{n-1}\psi_{n-1} = E\psi_n, \tag{2.1}$$

where $n = 0,1,\ldots,N-1$ numbers N ions with periodic boundary conditions $\psi_{n+N} = \psi_n$. The hop-over integral c_n (of course, again we have $c_{n+N} = c_n$) is expressed in the terms of the ion coordinates by the physically reasonable formula

$$c_n = \exp(x_n - x_{n+1}). \tag{2.2}$$

It is advantageous to introduce also the displacement of the n-th ion relative to its average coordinate na:

$$x_n = u_n + na. \tag{2.3}$$

Where possible, we always imply hereafter transition to the limit as $N \to \infty$. In this case, accurate to $O(1/N)$

$$N^{-1}\sum_x \ldots = \frac{1}{\pi}\int dp \ldots,$$

where p is the quasimomentum.[10] The equilibrium values of c_n are obtained by variation of the total energy $\mathscr{H}$ of the electrons and ions per ion. It is technically more convenient in this case to vary not at a fixed length of the string Na, but at a fixed pressure P:

$$\tilde{\mathscr{H}}(c_n, P) = \mathscr{H}(c_n, a) - PN^{-1}\sum_n \ln c_n$$
$$= \frac{1}{\pi}\int_{E<\mu} E\,dp - PN^{-1}\sum \ln c_n + W\{c_n\}. \tag{2.4}$$

In the case of interest to us, $W\{c_n\}$ is a linear combination of integrals $I_k\{c_n\}$ of the Toda chain[10] (see also Ref. 11):

$$I_0 = N^{-1}\sum \ln c_n, \quad I_2 = N^{-1}\sum c_n^2,$$
$$I_4 = N^{-1}\sum\left(c_n^2 c_{n-1}^2 + \frac{1}{2}c_n^4\right), \ldots. \tag{2.5}$$

We have

$$\tilde{\mathscr{H}}(c_n) = \mathscr{H}(c_n) - PI_0 = \frac{1}{\pi}\int_{E<\mu} E\,dp - PI_0 + \sum_{k=1}^{l} \varkappa_{2k} I_{2k}. \tag{2.6}$$

In this section we consider the case when only one invariant I_2 is retained in the sum in (2.6)

$$\tilde{\mathscr{H}} = \frac{1}{\pi}\int_{E<\mu} E\,dp - PI_0 + \varkappa I_2. \tag{2.7}$$

At absolute zero the integration in (2.7) is over the allowed bands up to the chemical potential μ of the electrons.

Equation (2.7) was exactly integrated in Ref. 10 and the energy $\mathscr{H}_0$ of the ground state was obtained. The results depend on the number ρ of electrons per ion. At $\rho = 1$ the electron spectrum consists of two allowed bands that are symmetric about zero energy,[2] see Fig. 1. It can be shown[10] that in integrable cases the chemical potential lies in the forbidden band for any number of invariants in (2.6). The lower band in Fig. 1 is therefore doubly filled:

$$\frac{2}{\pi}\int_{-E_m}^{-E_+} dp = \rho = 1. \tag{2.8}$$

The displacements u_n are in fact constant; there is only a classical Peierls shift of the odd ions relative to the even.

At $\rho \neq 0$ there are three allowed bands in the ground state, see Fig. 2. Moreover, it has been shown[10] that the extremals of (2.6) are potentials c_n with not more than $4l-1$ bands. At $\rho < 1$ the lower band is filled and the middle and upper one empty (2.8), while at $\rho > 1$ only the upper band is empty:

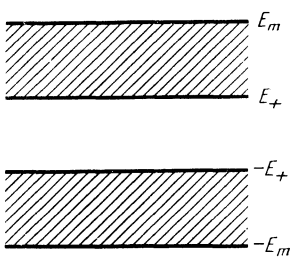

FIG. 1.

$$\frac{2}{\pi}\int_{-E_m}^{-E_+} dp=2-\rho, \quad \frac{2}{\pi}\int_{-E_-}^{E_-} dp=2(\rho-1). \tag{2.9}$$

There is no need to explain that in the exactly integrable cases there is no pinning (neither at $\rho = 1$ nor at $\rho \neq 1$). This statement is obviously valid at any number of invariants in (2.6). The ground state energy $\mathcal{H}_0(\rho)$ is a continuous function of all ρ, both rational and irrational. In Ref. 10 were analytically obtained the level density dp/dE, the displacements u_n, the wave functions ψ_n, and the electron charge density in the ground state. We note that the band widths are determined by the quantity $E_m \sim \exp(-a)$, where a is the average distance between ions.

Writing the elastic energy in the form $I_2(x_n - x_{n+1})$ implies a strongly correlated anharmonicity:

$$I_2=e^{-2a}+2e^{-2a}N^{-1}\sum_n (u_n-u_{n+1})^2$$

$$+e^{-2a}N^{-1}\sum_n\sum_{k=3}^{\infty}\frac{2^k}{k!}(u_n-u_{n+1})^k.$$

The correlation can be broken by introducing, e.g., a nonintegrable term of the form

$$\mathcal{H}_{n.i}=\lambda\varkappa N^{-1}\sum_n c_n, \quad \lambda\to 0. \tag{2.10}$$

If ρ is not too close to unity and $\lambda\to 0$ (a criterion follows) the nonintegrable increment (2.10) can be regarded as a small perturbation. This makes it easy to obtain the electron spectrum, u_n, ψ_n, and the increment $\Delta\mathcal{H}_0(\rho)$ to the ground-state energy in first order[3] in λ. In particular, it can be found, using the c_n previously obtained[10] for $\lambda = 0$, that the plot of $\Delta\mathcal{H}_0(\rho)$ vs the electron density ρ is a devil's staircase. At irrational ρ the sum over n in (2.10) is replaced by an integral and remains a continuous function of ρ (with only irrational points taken into account). At any rational ρ we have

$$|1-\rho|=p/r;$$

p and r are relatively prime integers, and a finite spike exists for $\Delta\mathcal{H}_0$. Its amplitude at large r is exponentially small:

$$\Delta\mathcal{H}_r\sim\lambda e^{-r\cdot\mathrm{const}}, \tag{2.11}$$

just as in Sec. 1 at finite temperatures. A proof of (2.11) is given in the Appendix.

Thus, the CDW is pinned at all rational ρ and is free at irrational ones (a zero mode exists). What is usually fixed, however, is not the number ρ of the electrons, but their chemical potential μ. The devil's staircase (2.11), just as the staircase in the Introduction, is differentiable at all the irrational points. We must therefore determine the standard chemical potential at irrational ρ:

$$\mu_{irr}=\frac{\partial\mathcal{H}_0}{\partial\rho}+\frac{\partial}{\partial\rho}\Delta\mathcal{H}_{irr}. \tag{2.12}$$

At rational ρ the chemical potential μ_r is simply the energy per particle:

$$\mu_r=\frac{\partial\mathcal{H}_0}{\partial\rho}+\frac{\partial}{\partial\rho}\Delta\mathcal{H}_{irr}+\Delta\mathcal{H}_r. \tag{2.13}$$

For a rational point p/r with large r the distance from the

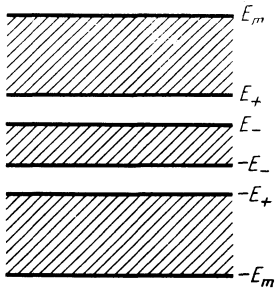

FIG. 2

"nearest" irrational point $\Delta\rho \sim 1/r^2$, therefore the difference

$$\mu_r-\mu_{irr}=\frac{\partial^2}{\partial\rho^2}(\mathcal{H}_0+\Delta\mathcal{H}_{irr})\Delta\rho+\lambda e^{-r\cdot\mathrm{const}}$$

is a smooth function of ρ at large r. This means that a devil's staircase that is differentiable with respect to ρ is found to be a harmless staircase as a function of the chemical potential, with all the ensuing simple and well known physical consequences.

The situation changes radically when the central band in Fig. 2 becomes narrow. This takes place as $\rho\to 1$. The number of states in this band tends to zero like $|\rho - 1|$, and the band width is[10]

$$2E_-\sim\exp\{-\mathrm{const}/|\rho-1|\}. \tag{2.14}$$

In the ensuing situation (see Ref. 10 for details) we have the discrete version described in the Introduction with a lattice of sparse solitons spaced $L \sim 1/|\rho - 1|$ apart and with the exponential interaction (1.3).

We consider the most interesting case

$$e^{-L}\ll\lambda\ll 1/L. \tag{2.15}$$

The action of the nonintegrable perturbation on the broad band can be separated separately from the action on the narrow one. Moreover, if we are not interested in a continuous dependence on ρ (more accurately on $|\rho - 1|$), the former can be neglected, the state with $\rho = 1$ can be chosen to be the unperturbed one, and the results of increasing $|\rho - 1|$ at fixed λ can be examined. To this end it suffices to know the solitons against the background of the picture of Fig. 1. This problem was solved in the continual variant by Brazovskiĭ[12] and by Su *et al.*[13] Appearance of each soliton decreases the number of delocalized states in the allowed bands of Fig. 1 by unity. A localized electronic state on a soliton appears instead. It was shown in the preceding paper[10] that the same picture is observed also in the discrete case, wherein the solitons are the standard solitons of the Toda chain (see Ref. 11), on each of which one or two electrons can be localized.

The energy of a soliton in the discrete version[10] at an effective weak coupling, say, is

$$E_{sol}=16\pi^{-1}\exp(-a-\pi\varkappa e^{-a}), \quad \pi\varkappa e^{-a}\gg 1.$$

Therefore the increment to the ground state energy at $\rho = 1$, due to the appearance of the free $|\rho - 1|$ soliton, is

$$\mathcal{H}_0(\rho)=\mathcal{H}_0(1)+E_{sol}|\rho-1|. \tag{2.16}$$

Under the conditions (2.15) the interaction between the solitons can be neglected in the first-order approximation. The nonintegrable perturbation (2.10) becomes a periodic poten-

tial, with a period $2a$, for the soliton (with center coordinate x_0):

$$\mathcal{H}_{n.i} \to \lambda U_{per}(x_0), \quad U_{per}(x_0+2a)=U_{per}(x_0). \tag{2.17}$$

The function U_{per} can be calculated by using the equations from Ref. 10. [For the potential (2.10) this is done in the Appendix.]

At small $|\rho - 1| \ll 1/a$ the number of solitons is small compared with the number of wells in the periodic potential (2.17). In the ground state all the solitons are then randomly distributed over the bottoms U_{min} and (2.16) goes over into

$$\mathcal{H}_0(\rho)=\mathcal{H}_0(1)+(E_{sol}+\lambda U_{min})\,|\rho-1|. \tag{2.18}$$

Finally, since the curvature of potential wells U_{per}, which is proportional to U_{min}/a^2, is very large, the electron levels localized on the solitons broaden into bands not on account of the displacement of the solitons from the positions U_{min}, but on account of interactions between the solitons, or else, equivalently, by the electrons of type (1.3) which are localized on them and are randomly dispersed over the minima of the potential (2.15).

The central regular band in Fig. 2 is thus transformed into a chaotic band of the impurity type.

The distribution in the energy E under $E_{\text{sol}} + \lambda U_{\text{min}}$ in this band is given by a Poisson distribution of the solitons over the distances L:

$$w(L)=\exp\{-L|\rho-1|\}. \tag{2.19}$$

Recognizing that

$$L=-C\ln(E_{sol}+\lambda U_{min}-E) \tag{2.20}$$

(C is a constant) we obtain ultimately

$$W(E)=(E_{sol}+\lambda U_{min}-E)^{-1+C|\rho-1|}. \tag{2.21}$$

The obtained filled chaotic band in the ground state and the random distribution (2.19) of the solitons correspond to the Aubry extremals[7] mentioned in the Introduction.

Just as in Aubry's work, in the stochastic regime there is no essential difference between rational and irrational ρ. In the rational case one selects out of the entire chaotic set of "points", i.e., of the levels in (2.21), a finite periodically passable set. Pinning takes place in both cases, as is evident from the fact that all the solitons together with the electrons localized on them land in the minima of U_{per}.

In the approximation linear in λ an unperturbed extremal remains, without significant change, an extremal also when the parameters ρ and λ correspond to the stochastic regime. The only difference is that in the stochastic regime such an extremal is known not to correspond to the absolute energy minimum but, as can be shown, is a local minimum. The last circumstance determines also the character of the conductivity in the stochastic regime. Obviously, standard Anderson localization exists in the stochastic impurity band and is preserved, in the one-dimensional case, also at all finite temperatures.[4] Conduction can set in therefore only on account of states that lie above the stochastic band. Such is precisely the already mentioned metastable state, which always exists at a fixed chemical potential. These states constitute an unpinned mode. The conductivity is determined mainly by the energy gap $\frac{1}{2}(U_{\text{max}} - U_{\text{min}})$:

$$\sigma \sim \exp\left[-\frac{\lambda}{2T}(U_{max}-U_{min})\right]. \tag{2.22}$$

3. MULTIBAND GROUND STATES

As already mentioned, when not only the invariant I_2, but several higher invariants $I_4, I_6, \ldots I_{2l}$ are retained in the exactly integrable Hamiltonian, the extremals (2.6) become multiband. Moreover, it was rigorously proved (see Appendix 2 of Ref 10) that at a finite number of invariants in (2.6) all (!) the extremals belong to the class of finite-band potentials. The maximum number of the allowed bands at a given l is equal to $4l - 1$. Of course,[10] all the states with smaller number of allowed bands remain extremal.

There are grounds for assuming, although we have no proof, that the absolute minimum of the functional (2.6) corresponds to an extremal with a maximum number of forbidden bands. When the number of such bands is large, and the combined width, proportional to $E_m \sim \exp(-a)$, of all the bands is fixed, a noticeable number of bands becomes narrow. If the number ν of states in such a narrow band is so small that its width becomes exponential, $\sim\exp(-1/\nu)$, it is transformed, as in the three-band case, into a sparse soliton lattice with period $L \sim 1/\nu$ and with exponential attraction $\sim\exp(-L)$ between the solitons. If the nonintegrable perturbation is not too small

$$e^{-1/\nu} \ll \lambda \ll \nu \ll 1, \tag{3.1}$$

a stochastic regime sets in already in first order in λ, just as in Sec. 2. To find the ground state we must again "collapse" all the bands that satisfy the condition (3.1) and consider the solitons corresponding to them against the background of the remaining several broad bands. Clearly, the procedure of finding the ground state will be an obvious generalization of the procedure described above for the three-band case.

Moreover, the corresponding periodic potential λU_{per} for the solitons can be again obtained analytically. The reason is that equations for ψ_n and c_n are known also in the multiband case[14] (see also Ref. 11). They are expressed in terms of the so-called multidimensional Riemann θ functions. Information on the latter can be found in the detailed review by Dubrovin[15] as well, in a more concise exposition, in Ref. 11.

We can finally consider also a converging infinite series in the invariants in (2.6). The number of allowed bands in the ground state becomes infinite. Moreover, since the combined width $\sim\exp(-a)$ is fixed, as already mentioned, the conditions (3.1) will be satisfied by an infinite number of bands at any fixed λ. Therefore, even in the approximation linear in λ we shall always have a stochastic regime. To obtain analytic expressions it is necessary to retain only a finite number of broad bands that do not satisfy the conditions (4.1), find all (!) the solitons against the background of the finite-band potential that remains after the collapse of the finite-band potential, calculate the corresponding periodic potential λU_{per}, etc. The exponential character of the conductivity is also conserved.

4. CONCLUSION

We have thus determined the ground state of the discrete Peierls model[10] with weak integrable perturbation.[5] There is no doubt that if the nonintegrable perturbation is not small, the number of allowed bands will be infinite in the ground state [with a total width $\sim\exp(-a)$]. The result is therefore the onset of qualitatively the same type of stochastic regime as described at the end of the preceding section for the case of an infinite number of invariants.

What happens with a three-band integrable state if account is taken of the nonintegrable perturbation (2.10) in an arbitrary order in λ in the case when λ does not satisfy the condition (3.1) for any of the bands? One can hardly doubt that even at $\lambda \ll \exp(-1/\nu)$ the number of bands in the ground state will be infinite. However, the number of states in the additional bands and the widths of the gaps that can appear in the old broad bands will be proportional to high powers of λ or will be exponentially small [$\sim\exp(-1/\lambda)$]. In this situation the entire thermodynamics will be determined by the first order in λ [by Eq. (2.11)], i.e., by the devil's staircase. On the other hand in the electronic spectrum and in the distribution of solitons corresponding to narrow bands there are preserved definite albeit numerically very small stochasticity elements described at the end of Sec. 3. Therefore pinning, although extremely weak, will take place also for an irrational number ρ of electrons.

APPENDIX

Let us prove (2.11). According to Ref. 10 the values of c_n with even n are given by

$$c_n=e^{-a}[\theta_4(v(n-n_0-1))\theta_3(v(n-n_0))/\theta_4(v(n-n_0+1))\theta_3(v(n-n_0+2))]^{1/2}. \tag{A.1}$$

Here θ_3 and θ_4 are standard θ-functions,[17]

$$v=\tfrac{1}{2}|\rho-1|, \tag{A.2}$$

n_0 is an arbitrary (noninteger!) constant—the coordinate of the soliton lattice. At odd n the values of c_n are given by (A.1) with the permutation $\theta_3 \rightleftarrows \theta_4$.

If ρ is rational,

$$|1-p|=p/r, \tag{A.3}$$

the sum (2.10) reduces to two sums of the type

$$\lambda e^{-a}\varkappa \frac{1}{r}\sum_{k=0}^{r-1} F\left(\frac{kp}{r}\right) \tag{A.4}$$

with F in the form

$$F(z)=\left[\frac{\theta_4(z-z_1)\theta_3(z-z_2)}{\theta_4(z-z_3)\theta_3(z-z_4)}\right]^{1/2}, \tag{A.5}$$

where $z_1,\ldots,z_4$ are real constants that are not equal to one another.

The entire functions $\theta_3(z)$ and $\theta_4(z)$ are periodic with a period 1 and quasiperiodic with period τ, where τ is the complex modulus of the θ function. The modulus of τ in our problem is pure imaginary, $\tau=i|\tau|$, and is expressed in terms ρ, a, and $\varkappa$ in Ref. 10. Finally $\theta_3(z)$ and $\theta_4(z)$ each have one zero in the parallelogram of the periods, at the respective points

$$\tfrac{1}{2}+\tfrac{1}{2}\tau,\quad \tfrac{1}{2}\tau. \tag{A.6}$$

We expand the periodic function $F(z)$ in a Fourier series

$$F(z)=\sum_{-\infty}^{\infty} F_l e^{-2\pi i l z}$$

and substitute this series in (A.4)

$$\frac{1}{r}\sum_{k=0}^{p-1} F\left(\frac{kp}{r}\right)=\sum_{l=-\infty}^{\infty} F_l \frac{1}{r}\sum_{k=0}^{r-1} e^{i2\pi l pk/r}. \tag{A.7}$$

The sum over k in the right-hand side of (A 7) is

$$\frac{1}{r}\sum_{k=0}^{r-1}\varepsilon_k{}^l,$$

where ε_k ($k=0,\ldots,r-1$) are the r-th roots of unity; we therefore have for (A.4)

$$F_0+\sum_{l=1}^{\infty}(F_{lr}+F_{-lr}). \tag{A.8}$$

Equation (A.8) solves the problem, with F_0 the smooth part of $\Delta\mathscr{H}_0$. The spikes $\Delta\mathscr{H}_r$ at large r are determined by the asymptotes of the Fourier coefficients

$$F_r=\frac{1}{2\pi}\int_0^1 dz F(z)e^{2\pi i z r}. \tag{A.9}$$

Since $F(z)$ of (A.5) is analytic on the real axis, the asymptotic form is exponential. The argument of the exponential is determined by the singular points of $F(z)$ in the complex plane, i.e., by the zeros of $\theta_3(z)$ and $\theta_4(z)$. The imaginary part of these zeros are all equal to $|\tau|/2$, therefore

$$F_r\sim\exp(-\pi|\tau|r),\quad F_{lr}\sim(-\pi|\tau|lr), \tag{A.10}$$

which agrees with Eq. (2.11) in the text.

Actually, (A.10) contains besides the exponential part also oscillating factors of the cos r type. To find them, the integrals in (A.9) must be calculated accurate to r-th power. Equations (2.11) with larger r, however, are of no physical interest inasmuch as in fact, as already indicated, the devil's staircase is incomplete and pinning takes place only at small r, where $\Delta\mathscr{H}_r$ must be calculated directly from Eqs. (A.1), (A.2), (A.4), and (A.5).

We calculate now the soliton potential U_{per} from (2.17). To this end we must find the modulus τ of the θ function as $|\rho-1|\to 0$. It follows from Eq. (2.4) of Ref. 10 that as $\rho\to 1$ the parameter also vanishes but the ratio $\delta=2|\tau|/|\rho-1|$ remains finite: it is the width of the soliton.[10] Using the imaginary Jacobi transformation,[17] we can rewrite Eq. (2.4) of Ref. 10 in the form

$$\frac{K(1/\operatorname{ch}\delta^{-1})}{\operatorname{ch}\delta^{-1}}=\frac{1}{g}\equiv\pi\varkappa e^{-a}, \tag{A.11}$$

where K is a complete elliptic integral.[17] In the case of weak coupling, $g\ll 1$, the soliton width δ is large[10]:

$$\delta=\tfrac{1}{4}e^{1/g}, \tag{A.12}$$

in the case of strong coupling, $g\gtrsim 1$, the soliton becomes narrower

$$\delta\approx 1/\ln \pi g,\quad g\to\infty. \tag{A.13}$$

As $\rho\to 1$, we obtain with the aid of the same imaginary Jacobi transformation for (A.1)

$$c_n = e^{-\alpha}\left[\frac{\mathrm{ch}((n-n_0-1)/\delta)}{\mathrm{ch}((n-n_0+1)/\delta)}\right]^{1/2}$$

for even n. For odd n we have

$$c_n = e^{-\alpha}\left[\frac{\mathrm{ch}((n-n_0+1)/\delta)}{\mathrm{ch}((n-n_0-1)/\delta)}\right]^{1/2}.$$

The periodic potential for the soliton is

$$U_{per}(n_0) = \varkappa e^{-\alpha}\sum_{m=-\infty}^{\infty}\left\{\left[\frac{\mathrm{ch}((2m-n_0-1)/\delta)}{\mathrm{ch}((2m-n_0+1)/\delta)}\right]^{1/2} + \left[\frac{\mathrm{ch}((2m-n_0)/\delta)}{\mathrm{ch}((2m-n_0-2)/\delta)}\right]^{1/2} - 2\,\mathrm{ch}\frac{1}{\delta}\right\}. \quad (A.14)$$

Its period is obviously equal to 2.

At $\delta \lesssim 1$ (strong or intermediate coupling) the series in (A.14) converges rapidly. On the contrary, in the physically more realistic weak-coupling case the soliton width is large and Eq. (A.4) is not convenient. The potential U_{per} must now be expanded in a Fourier series:

$$U_{per}(n_0) = \sum_{l=-\infty}^{\infty} U_l e^{i\pi l n_0}.$$

For U_{per} we obtain from (A.14)

$$U_l = \frac{1}{2}\varkappa e^{-\alpha} e^{i\pi l/2}\int_{-\infty}^{\infty} dz e^{il\pi z} F(z), \quad (A.15)$$

$$F(z) = \left[\frac{\mathrm{ch}((z-1/2)/\delta}{\mathrm{ch}((z+3/2)/\delta)}\right]^{1/2} + \left[\frac{\mathrm{ch}((z+1/2)/\delta)}{\mathrm{ch}((z-3/2)/\delta)}\right]^{1/2} - 2\,\mathrm{ch}\frac{1}{\delta}.$$

The integral in (A.15) is calculated with by shifting the contour into the complex plane. Its value is determined by the singular points of $F(z)$,i.e., by the points with $\mathrm{Im}\, z = i\delta\pi/2$:

$$U_l \sim \exp(-|l|\delta\pi^2/2).$$

It is clear that it suffices to retain in the Fourier series only the first two terms:

$$U_{per}(n_0) \approx 1/2(U_{max}+U_{min}) + 1/2(U_{max}-U_{min})\sin\pi n_0. \quad (A.16)$$

Here

$$U_{max} \approx U_{min} \sim \varkappa e^{-\alpha}/\delta, \quad U_{max} - U_{min} \sim \varkappa e^{-\alpha} e^{-\delta\pi^2/2} \quad (A.17)$$

with δ from (A.12).

[1)]We use the opportunity the note that R_c was calculated in the Ising model in Refs. 5 and 6 with exponential accuracy.
[2)]We recall (cf. Ref. 10) that the spectrum (2.1) is even.
[3)]See Sec. 4 concerning the actual possibility of expanding in powers of λ.
[4)]We disregard the finite conductivity due to inelastic scattering.
[5)]We have recently learned that Sinaĭ[16] has succeeded in finding a stochastic ground state in the Frenkel'-Kontorova model.

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