PHYSICAL REVIEW B VOLUME 47, NUMBER 24 15 JUNE 1993-II

# Green functions in crystals and thin layers with long-range interactions

P. Zieliński
*Institute of Nuclear Physics, ulica Radzikowskiego 152, 31342 Kraków, Poland*

K. Żabińska
*Institute of Physics, Academy of Economics, Rynek Gł. 34, 31010 Kraków, Poland*

(Received 13 November 1992; revised manuscript received 1 February 1993)

The interactions between the lattice planes in planar lamellar crystalline systems in which the interatomic potentials are of electrostatic origin or in which they result from a coupling with elastic deformations show a distance dependence given by a series of exponentially decreasing functions. In the vicinity of the two-dimensional (2D) Brillouin zone and near the points of elastic instabilities the exponential decrease of some of the terms of the series is fairly slow. Two methods are presented which allow us to obtain closed expressions for the Green functions in such systems with and without surfaces regardless of the rate of the exponential decay. The first method, useful for exclusively exponential interactions, reduces the problem to the multiplication of matrices known from the theory for short-range interactions. The second method is adapted to systems having short- and long-range interactions at the same time and consists in introducing some additional degrees of freedom by which the range of the interactions becomes finite. Profiles of the order parameter at domain walls and surface relaxation in a crystal with short- and long-range interactions are calculated as first applications of the methods. A crossover between ferrodistortive and antiferrodistortive responses and anomalous localization of the response is found in systems with competing ferrodistortive and antiferrodistortive tendencies between the elasticity and the rotation-translation coupling. The transformation enabling the introduction of the additional degrees of freedom in the case of dipolar interactions is given.

## I. INTRODUCTION

Lamellar crystalline systems such as thin layers, superlattices, composites, etc. with planar and mutually parallel surfaces and interfaces consist of a number of atomic or ionic lattice planes which in most cases show a two-dimensional periodicity. The latter property allows any physical quantity to be expressed as a function of a two-dimensional wave vector $\mathbf{k}_\parallel$ parallel to the planes and of a discrete index $l$ labeling the lattice planes. In particular, the interactions of the constituent atoms or ions can be represented by a $\mathbf{k}_\parallel$-dependent energy matrix $H(\mathbf{k}_\parallel;l,l')$. The intraplanar matrix elements $H(\mathbf{k}_\parallel;l,l')$ for $l=l'$ are the two-dimensional Fourier transforms of the interactions of the atoms or ions belonging to the same lattice plane $l$. It has been shown that, in contrast to the three-dimensional case, the lattice sums involved in the intraplanar part of the energy matrix are unambiguous at every wave vector $\mathbf{k}_\parallel$ even for the long-range Coulomb interactions.[1,2]

The specific form of the Coulomb potential also implies the dependence of the interplanar matrix elements $H(\mathbf{k}_\parallel;l,l')$ on the separation of the planes of $|l-l'|$ in those systems, in which the constituent atoms or ions can be represented by distributions of electrostatic charges. The dependence is then expressed by a series of decreasing exponential functions. The simplest lattice sums showing this behavior correspond to the interaction of a lattice plane composed of pointlike charges with another single charge located out of the plane. Denoting by $\mathbf{R}_\parallel$ and $\mathbf{R}_\perp$ the coordinates of the single charge parallel and perpendicular to the plane, respectively, one can write the lattice sum as follows:

$$S_{\mathbf{k}_\parallel}=\sum_n \frac{e^{i\mathbf{k}_\parallel\cdot(\mathbf{R}(\mathrm{n})-\mathbf{R}_\parallel)}}{|\mathbf{R}(n)-\mathbf{R}_\perp-\mathbf{R}_\parallel|}=\frac{2\pi}{V_c}\sum_{\mathbf{K}_\parallel}\frac{1}{|\mathbf{K}_\parallel+\mathbf{k}_\parallel|}e^{-|\mathbf{K}_\parallel+\mathbf{k}_\parallel||\mathbf{R}_\perp|}e^{i\mathbf{K}_\parallel\cdot\mathbf{R}_\parallel}\,, \tag{1}$$

where $\mathbf{R}(n)$ are the nodes of the two-dimensional direct lattice and $\mathbf{K}_\parallel$ are the vectors of the corresponding reciprocal lattice. $V_c$ is the area of the unit cell of the direct lattice. If the single charge belongs to another lattice plane, the quantity $\mathbf{R}_\perp$ is just the separation of the planes. The apparent divergence of the term $\mathbf{K}_\parallel=\mathbf{0}$ at $\mathbf{k}_\parallel\rightarrow\mathbf{0}$ in Eq. (1) is removed whenever the lattice planes are electrically neutral. One can see that the term showing the slowest exponential decrease with distance corresponds to $\mathbf{K}_\parallel=\mathbf{0}$. In the limit $\mathbf{k}_\parallel\rightarrow\mathbf{0}$ this term describes a macroscopic electric field.

A similar exponentially decreasing dependence of the interplanar interactions on the separation of the planes has been shown to occur in lattices of fluctuating dipoles.[2] This case is of special importance, since it encompasses the dynamics of the ionic crystals. In Ref. 2 the detailed formulas have been given for the dipolar energy matrix, and it has been demonstrated that the neglect of the slowly decreasing term can lead to incorrect results such as, e.g., a nonexistent phase transition to an incommensurate phase. The formulas for the dipolar interactions of Ref. 2 are in fact related to Eq. (1) through appropriate derivatives. Analogously, an exponential char-

0163-1829/93/47(24)/16447(8)/$06.00

acter of the interplanar interactions can be derived for the systems of higher multipoles. It should, however, be kept in mind that this conclusion does not concern the interactions of induced multipoles such as the London dispersion forces.

Another important class of systems showing the interplanar energy described by a series of exponential functions are those where the orientational variables such as psuedospin Ising variables[3,4] or continuous variables represented by symmetry-adapted functions[5,6] are coupled to the elastic deformation of the lattice. The reason for the effective, lattice-mediated interactions then being of the exponential character lies in an analogous analytical form of the purely elastic Green functions.[7] The detailed derivation of the formulas for the interplanar lattice-mediated interactions are given in Sec. IV. When the system approaches an elastic instability the exponential decrease of the interplanar energies becomes fairly slow, which makes the range of the interactions effectively infinite.

The above review shows that in the most often encountered lamellar systems with long-range forces of electrostatic or elastic nature the interplanar interactions are given by a series of exponential functions of the separation of the lattice planes. Moreover, at some wave vectors $\mathbf{k}_\parallel$ in the electrostatic systems and near elastic instabilities the exponential decrease of these functions becomes so slow that approximations taking in the interactions of a limited number of neighboring lattice planes only are no longer valid. No attempts have been made till now, to the authors knowledge, to derive closed formulas for the Green functions in such systems. On the contrary, the existing Green-function techniques are based on a short range of the interplanar interactions.[8] In particular, the response theory due to Dobrzynski[9] offers a possibility of obtaining closed formulas for Green functions even in fairly complicated lamellar systems in which, however, the interplanar interactions do not go beyond the first neighboring planes.[10]

In the present work advantage is taken of the particular exponential form of the long-range interplanar interactions to derive relatively simple expressions for the corresponding bulk Green functions as well as for Green functions in similar systems with surfaces. The expressions are valid regardless of how slow the exponential decrease of the interactions might be. The definitions of the Green functions in terms of the energy matrix are given in Sec. II. Section III presents a method for evaluation of the Green functions in an infinite crystal and in a thin layer in which all the interplanar interactions have an exponential form. The principle of the method relies upon the observation that every exponential term in the energy matrix is an inverse of a tridiagonal matrix. This allows one to express the desired Green function in terms of the matrices known from the response theory for short-range interactions.[9] A method adapted to the systems possessing at the same time short- and long-range terms in the energy matrix is presented in Sec. IV. The method transforms the energy matrix to a short-range form at the expense of the introduction of additional degrees of freedom. Both methods are exemplified on simple systems. In Sec. V profiles of an orientational order parameter are calculated at the domain wall in a generalization of the model of Axel and Aubry[11] and Peyrard and Büttner.[12] Surface relaxation in a crystal with one short-range and one long-range term in the energy matrix is determined in Sec. VI using the additional degrees of freedom. In the Appendix we show the way in which the additional degrees of freedom needed in the method presented in Sec. IV can be constructed in the case of the dipolar energy matrix discussed in Ref. 2.

## II. THE ENERGY MATRIX AND THE GREEN FUNCTION

Regarding a crystal or a crystalline slab as a series of mutually parallel lattice planes labeled by an index $l$, one can express the lattice energy $E$ in terms of an energy matrix $H(\mathbf{k}_\parallel;l,l')$. The wave vector $\mathbf{k}_\parallel$ is parallel to the lattice planes and is a well-defined quantity or quantum number due to the two-dimensional periodicity of the system. The indices $l$ and $l'$ play the role of the matrix indices. The lattice energy then reads

$$E(\mathbf{k}_\parallel)=\tfrac{1}{2}\sum_{l,l'}u_l(\mathbf{k}_\parallel)H(\mathbf{k}_\parallel;l,l')u_{l'}(\mathbf{k}_\parallel)\ , \tag{2}$$

where $u_l(\mathbf{k}_\parallel)$ is a variable characterizing the state of the lattice plane $l$ at a given wave vector $\mathbf{k}_\parallel$. The variable can represent a translational displacement of atoms,[7] fluctuation of the spin or of the electron density, or, finally, an orientational probability of an orientationally disordered molecule.[13] For the sake of simplicity we shall first consider one-dimensional variables $u_l(\mathbf{k}_\parallel)$. The range of the sum in Eq. (2) can be infinite for the bulk crystal or finite when we deal with a thin layer. The explicit $\mathbf{k}_\parallel$ dependence of the quantities used in Eq. (2) will be dropped in what follows whenever it does not cause confusion.

Under some forces $f_l$, such as external fields or local forces due to the existence of the surfaces, the configuration $u_l$ of the variable of interest is given by the condition of minimum

$$\frac{\partial E}{\partial u_l}=f_l \tag{3}$$

or

$$u_l=\sum_{l'}G(l,l')f_{l'}\ , \tag{4}$$

where $G(l,l')$ is the Green function

$$\sum_{l''}G(l,l'')H(l'',l')=\delta_{ll'}\ . \tag{5}$$

The Green function is, therefore, a matrix inverse to the energy matrix. In the case of dynamical problems the static energy matrix $H(l,l')$ should be replaced by an analogous frequency-dependent dynamical matrix.[14] The Green function will then also depend on the frequency.

Explicit formulas for the Green functions in systems with surfaces and interfaces have been obtained assuming the range of interactions in the energy matrix $H(l,l')$ limited to the nearest-neighbor lattice planes, i.e., $H(l,l')=0$ except for $l'=l$ and $l'=l\pm1$ (Ref. 10) and to a given finite number $M$ of neighbors, i.e., $H(l,l')=0$ if $|l'-l|>M$.[15] In the following section we show a method for obtaining the Green functions in systems where the interactions are given by a series of exponentially decreasing functions.

## III. GREEN FUNCTIONS IN SYSTEMS WITH LONG-RANGE EXPONENTIAL INTERACTIONS

### A. Bulk green function

We assume the following form of the energy matrix:

$$\begin{aligned} H(l,l') &= \sum_{n=1}^{N} \varepsilon_n^{|l-l'|}\beta_n \exp(-\Gamma_n|l-l'|) \\ &\equiv \sum_{n=1}^{N} H_n \ , \end{aligned} \tag{6}$$

where $\varepsilon_n=\pm 1$. In order to find the Green function for the system with the interactions given by Eq. (6), it is useful to first solve the problem with only one term in the sum of Eq. (6), i.e., for $N=1$. When the number of the lattice planes is infinite one deals with the bulk crystal, which is also periodic in the direction perpendicular to the lattice planes. Then the Fourier transform of the interaction matrix $H_1(l,l')$ with respect to $\mathbf{k}_\perp$ can be found:

$$\begin{aligned} H_1(\mathbf{k}_\perp) &= \beta_1+\beta_1 \sum_{m=1}^{\infty} \varepsilon_1^m (e^{-\Gamma_1 m+ik_\perp m}+e^{-\Gamma_1 m-ik_\perp m}) \\ &= \beta_1 \frac{\sinh\Gamma_1}{\cosh\Gamma_1-\varepsilon_1\cos k_\perp} \ . \end{aligned} \tag{7}$$

Taking the inverse Fourier transform of the quantity $H_1^{-1}(k_\perp)$ (Ref. 15) one obtains the bulk Green function $G_1(l,l')$ for the system defined by Eq. (6) with $N=1$:

$$G_1(l,l')=\frac{1}{2\beta_1\sinh\Gamma_1}[2\cosh\Gamma_1\delta_{ll'}-\varepsilon_1(\delta_{ll'+1}+\delta_{ll'-1})] \ . \tag{8}$$

The tridiagonal form of the bulk Green function in this specific case is easily understandable in view of the fact that the Green function for the systems with the nearest-neighbor interactions, i.e., defined by a tridiagonal energy matrix, just has an exponentially decaying form.[16]

Analogously to Eq. (8), one can evaluate the bulk Green function $G_n(l,l')$ for every term $n=1,\ldots N$ entering the sum in Eq. (6). The commutator of every pair of these Green functions vanishes:

$$\sum_{l''=-\infty}^{\infty} G_n(l,l'')G_m(l'',l')=\sum_{l''=-\infty}^{\infty} G_m(l,l'')G_n(l'',l') \ . \tag{9}$$

This allows one to write down the bulk Green function $G(l,l')$ for the energy matrix Eq. (6) in a form resembling the inverse of a sum of $C$ numbers. Using matrix notation one has

$$\underline{G}\,\underline{H}=\underline{I} \ , \tag{10}$$

$$\underline{G}=\underline{R}^{-1}\prod_{m=1}^{N}\underline{G}_m \ , \tag{11}$$

where

$$\underline{R}=\sum_{n=1}^{N}\prod_{\substack{m=1\\ m\neq n}}^{N}\underline{G}_m \ . \tag{12}$$

The matrix $\underline{R}$ of Eq. (12) is symmetrical and has nonzero elements close to its diagonal only:

$$R(l,l')=0 \quad \text{if } |l-l'|>N \ . \tag{13}$$

The inverse $\underline{R}^{-1}$ of such a matrix has been already obtained as the bulk Green function for the systems with $N$ interacting neighboring lattice planes:[15]

$$\begin{aligned} R^{-1}(l,l') &= \frac{1}{R(0,N)} \\ &\quad\times\sum_{n=1}^{N}\frac{z_n^{|l-l'|+N}}{(z_n^2-1)\prod_{\substack{m=1\\ m\neq 1}}^{N}(z_n-z_m)(z_n-z_m^{-1})} \ , \end{aligned} \tag{14}$$

where $z_n$, $n=1,\ldots,N$ are the roots of the polynomial

$$R(l,l)z^N+\sum_{n=1}^{N}R(l,l+n)(z^{N+n}+z^{N-n}) \ , \tag{15}$$

with $|z_n|<1$ (see Refs. 15 and 14 for a detailed discussion). Equations (11) and (14) allow one to obtain the interesting bulk Green function as a simple matrix product. This is a consequence of the fact that the energy matrix [Eq. (6)] contains exclusively exponential terms.

### B. Ideal surfaces in systems with long-range exponential interactions

The bulk Green function [Eq. (11)] can in principle be used as the starting point in the surface response method of Dobrzynski.[9] Then, however, the infinite range of interactions would make the corresponding cleavage operator an infinite and thereby intractable matrix. A different scheme is, therefore, better in this case. In the first step we show that the Green function $g_1(l,l')$ for a slab of $L$ lattice planes and with the interactions given by the energy matrix $h_1(l,l')$ with only one exponential term [see Eq. (6)]

$$h_1(l,l')=H_1(l,l') \tag{16}$$

for $l,l'\geq 1$ and $l,l'\leq L$ and $h_1(l,l')=0$ otherwise is also given by a tridiagonal matrix. Indeed, the system of equations for the Green function $g_1(l,l')$,

$$\sum_{l''=1}^{L} g_1(l,l'')h_1(l'',l')=\delta_{ll'} \ , \tag{17}$$

is satisfied by the bulk Green function Eq. (8) for $l=2,\ldots,L-1$. The two remaining equations for $l=1$ and $l=L$ give

$$
\begin{aligned}
&g_1(l,l)=g_1(L,L)=\frac{e^{\Gamma_1}}{2\beta_1\sinh\Gamma_1}\;,\\
&g_1(1,2)=g_1(2,1)=g_1(L,L-1)=g_1(L-1,L)\\
&\qquad=G_1(1,2)=G_1(2,1)\;,
\end{aligned}
\tag{18}
$$

and

$$g_1(l,l')=G_1(l,l')$$

otherwise.

When there is more than one exponential term in the energy matrix Eq. (6), the evaluation of the slab Green function is similar. We shall illustrate this for $N=3$, i.e., for

$$\underline{h}=\underline{h}_1+\underline{h}_2+\underline{h}_3\;, \tag{19}$$

where the terms in Eq. (19) are defined analogously to that of Eq. (16) with the use of the bulk interactions [Eq. (6)]. Now one can state that

$$\underline{g}_1\underline{g}_2(\underline{h}_1+\underline{h}_2+\underline{h}_3)\underline{g}_3=\underline{\sigma}_{12}\underline{h}_1\underline{g}_3+\underline{g}_2\underline{g}_3+\underline{g}_1\underline{g}_3+\underline{g}_1\underline{g}_2\;, \tag{20}$$

where $\underline{\sigma}_{12}$ is the commutator

$$\underline{\sigma}_{12}=\underline{g}_1\underline{g}_2-\underline{g}_2\underline{g}_1\;. \tag{21}$$

The desired Green function is then

$$\underline{g}=\underline{h}^{-1}=\underline{g}_3(\underline{\sigma}_{12}\underline{h}_1\underline{g}_3+\underline{g}_2\underline{g}_3+\underline{g}_1\underline{g}_3+\underline{g}_1\underline{g}_2)^{-1}\underline{g}_1\underline{g}_2\;. \tag{22}$$

One can easily check that the products $\underline{g}_i\underline{g}_j$ form a matrix, which resembles the energy matrix in the slab with the interaction limited to next-nearest-neighbor lattice planes. The nonvanishing elements of the matrix $\underline{\sigma}_{12}\underline{h}_1\underline{g}_3$ lie in the stripe $l=1$, $l=2$, $l=L-1$, $l=L$, and $l'=1,\dots,L$. This form allows the Dobrzynski method[9] to be applied here, the response operator being a $4\times4$ matrix. An explicit expression for the matrix $(\underline{\sigma}_{12}\underline{h}_1\underline{g}_3+\underline{g}_2\underline{g}_3+\underline{g}_1\underline{g}_3+\underline{g}_1\underline{g}_2)^{-1}$ has been already discussed in Ref. 15. The last step is to insert this matrix into Eq. (22).

## IV. SYSTEMS WITH SHORT- AND LONG-RANGE INTERACTIONS

The method presented in the previous section allows one to derive a closed formula for the bulk Green function in a quasi-one-dimensional system with the interactions given by a finite series of terms showing an exponentially decreasing dependence on the distance. Here we shall demonstrate that the Green function can be also obtained in a closed form in systems where the long-range interactions coexist with some short-range forces. The present method stems from the observation that an exponential distance dependence is shown by the effective lattice-mediated interactions resulting from the elimination of the elastic degrees of freedom even if the purely elastic interactions have a short range. One can, therefore, expect that the introduction of some additional degrees of freedom to the system with initially long-range interactions may yield an equivalent system described by short-range interactions only.

Below we shall show how the elimination of the elastic degrees of freedom engenders a long-range effective interaction and how to use this piece of information to reduce the range of interactions in an initially long-range energy matrix. Analogously to the purely elastic case,[7] it is convenient to pass from the displacements $u_l$ to a strain variable $x_l=u_{l+1}-u_l$. Then the energy of the chain is

$$
\begin{aligned}
E&=\tfrac{1}{2}\sum_{l,l'=-\infty}^{\infty}[\sigma_lD(l,l')\sigma_{l'}+x_lS(l,l')x_{l'}+2x_lV(l,l')\sigma_{l'}]\\
&\equiv\tfrac{1}{2}\sum_{l,l'=-\infty}^{\infty}\mathbf{w}_l\underline{H}(l,l')\mathbf{w}_{l'}\;,
\end{aligned}
\tag{23}
$$

where the matrix $D(l,l')$ describes short-range direct interactions of orientational variables $\sigma_l$ and $\sigma_{l'}$, the matrix $S(l,l')$ the elastic interactions, and $V(l,l')$ their coupling. The variable $\sigma_l$ can be a spin variable or an orientational variable defined by symmetry-adapted functions.[5,13] All the above interactions can be arranged in a $2\times2$ matrix $\underline{H}(l,l')$:

$$
\begin{aligned}
&H_{11}(l,l')=D(l,l')\;,\\
&H_{22}(l,l')=S(l,l')\;,\\
&H_{12}(l,l')=H_{21}(l,l')=V(l,l')\;,
\end{aligned}
\tag{24}
$$

and the variables $\sigma_l$ and $x_l$ in a two-component vector $\mathbf{w}_l=(\sigma_l,x_l)$. The elimination of the elastic degrees of freedom follows from the condition for minimum

$$\frac{\partial E}{\partial x_l}=0\;, \tag{25}$$

which yields

$$x_l=-\sum_{l'l''=-\infty}^{\infty}G^e(l,l'')V(l'',l')\sigma_{l'}\;, \tag{26}$$

where $G^e(l,l')$ is the purely elastic Green function, i.e., $\sum_{l''=-\infty}^{\infty}G^e(l,l'')S(l'',l')=\delta_{ll'}$. With the expression Eq. (26) inserted into Eq. (23) one gets the effective orientational energy

$$E^{\text{eff}}=\tfrac{1}{2}\sum_{l,l'=-\infty}^{\infty}\sigma_l[D(l,l')-K(l,l')]\sigma_{l'}\;, \tag{27}$$

where

$$K(l,l')=\sum_{m,n=-\infty}^{\infty}V(n,l)G^e(n,m)V(m,l')\;. \tag{28}$$

In the simplest case showing a spatial dispersion[7] the elastic Green function reads

$$G^e(l,l')=\frac{1}{\beta_2}\frac{z_e^{|l-l'|+1}}{z_e^2-1}\;, \tag{29}$$

where $z_e$ is that root of the quadratic equation

$$z_e^2+z_e\frac{\beta_1+2\beta_2}{\beta_2}+1=0\;, \tag{30}$$

whose modulus is less than one. $\beta_1$ and $\beta_2$ are the force constants between first and second nearest neighbors, respectively, in the elastic part of the energy Eq. (23).[7] It follows from the general conditions for stability that

$$z_e = \varepsilon e^{-\Gamma} , \tag{31}$$

where $\Gamma > 0$ and $\varepsilon = \pm 1$, the sign of $\varepsilon$ being always opposite to the sign of the force constant $\beta_2$.[7]

For the sake of simplicity we shall only consider couplings $V$ of the orientational variable $\sigma_l$ with nearest-neighbor local strains, i.e., $x_l$ and $x_{l-1}$. Then two cases are possible depending on the symmetry of the local variable $\sigma_l$:

$$\begin{aligned} &\text{(i)}\;\; V(l,l-1) = V(l,l) = V_0 , \\ &\text{(ii)}\;\; V(l,l-1) = -V(l,l) = -V_0 . \end{aligned} \tag{32}$$

Case (i) corresponds to ferrodistortive and case (ii) to antiferrodistortive coupling. The explicit form of the effective energy matrix then is

$$\begin{aligned} H^{\text{eff}}(l,l') &= D(l,l') - K(l,l') \\ &= D(l,l') \mp \frac{V_0^2}{\beta_2} \delta_{ll'} \\ &\quad \pm \frac{V_0^2}{\beta_2} [\tanh(\Gamma/2)]^{\mp \varepsilon} \varepsilon^{|l-l'|} e^{-\Gamma|l-l'|} , \end{aligned} \tag{33}$$

where the upper sign corresponds to case (i) and the lower sign to case (ii) [Eq. (32)].

The last energy matrix [Eq. (33)] contains at the same time short- and long-range interactions. The Green function $G^{\text{eff}}(l,l')$ for the energy matrix $H^{\text{eff}}(l,l')$ [Eq. (33)] can be obtained in two ways. The first is to replace the short-range part by an approximate fast decreasing exponential term and proceed along the lines of Sec. III. The second way is to find the full Green function $G_{ij}(l,l')$, $i,j = 1,2$ for the coupled system with short-range interactions given by the energy matrix $H_{ij}(l,l')$ [Eq. (24)]. The latter Green function can be obtained exactly.[14] The element $G_{11}(l,l')$ then is equal to the desired Green function $G^{\text{eff}}(l,l')$:

$$G^{\text{eff}}(l,l') = G_{11}(l,l') . \tag{34}$$

The above reasoning indicates how to proceed in the case of the energy matrix given originally by, e.g.,

$$H(l,l') = D(l,l') + \beta \varepsilon^{|l-l'|} e^{-\Gamma|l-l'|} , \tag{35}$$

where the coefficients $\beta$ and $\Gamma$ are defined by the model. The exact Green function for this energy matrix can be obtained by introducing a new variable $x_l$ and the corresponding matrices $S$ and $V$ in such a way that

$$\beta \varepsilon^{|l-l'|} e^{-\Gamma|l-l'|} = -\sum_{m,n=-\infty}^{\infty} V(m,l) S^{-1}(m,n) V(n,l') . \tag{36}$$

In the present case this can be easily done knowing that the inverse of the exponentially decreasing energy matrix is given by Eq. (8). Consequently,

$$S(l,l') = -\frac{1}{2\beta \sinh\Gamma} [2\cosh\Gamma \delta_{ll'} - \varepsilon(\delta_{ll'+1} + \delta_{ll'-1})] \tag{37}$$

and

$$V(l,l') = \delta_{ll'} . \tag{38}$$

Now one has to find the Green function for the energy matrix Eq. (24) with the matrices $S(l,l')$ and $V(l,l')$ defined in Eqs. (37) and (38). As before, the desired Green function will be given by the element $G_{11}(l,l')$. In the above method the variable $x(l)$ has no physical meaning but it allows one to solve the problem of the Green function. Analogously, one can find the Green function in similar systems with surfaces. In the Appendix we transform the energy matrix for the dipolar interactions[2] to a sum of terms which are either of short range or have a short-range inverse which allows the present method to be applied.

## V. DOMAIN WALLS IN SIMPLE SYSTEMS WITH ROTATION TRANSLATION COUPLING

As an example of application of the formulas derived in previous sections we shall determine the profile of the orientational variable $\sigma_l$ at domain walls in systems described by the energy matrix given in Eq. (33). For simplicity we shall reduce the short-range part of the interactions to the local term $D(l,l') = W^2 \delta_{ll'}$, which in this kind of model can be understood as the inverse to a one-particle, generally temperature-dependent susceptibility. Taking the Fourier transform of the energy matrix Eq. (33) and using the result of Eq. (8) one easily finds that the resulting dispersion curve has its minimum at $k = 0$ in case (i), Eq. (32), and at $k = \pi$, i.e., at the Brillouin-zone boundary in the (ii) independently of the sign of $\varepsilon$. The dispersion curves correspond to the disordered phase in which $\langle \sigma_l \rangle = 0$ for every $l$. Whenever the only temperature dependence is involved in the local term $W^2$, cases (i) and (ii) imply an instability of ferrodistortive and antiferrodistortive character, respectively. In the ordered phase the average value $\langle \sigma_l \rangle = \sigma_l^0$ is nonzero. This can be modeled in the simplest way by replacing the term $W^2 \sigma_l^2 \delta_{ll'}$ in the energy matrix by $W^2(\sigma_l - \sigma_l^0)^2 \delta_{ll'}$. The lattice energy then is

$$E^{\text{eff}} = \tfrac{1}{2} \sum_{l,l'=-\infty}^{\infty} \sigma_l H^{\text{eff}}(l,l') \sigma_{l'} - W^2 \sum_{l=-\infty}^{\infty} (\sigma_l \sigma_l^0 - \tfrac{1}{2} \sigma_l^{02}) . \tag{39}$$

The desired configuration then is given by the Green function $G^{\text{eff}}(l,l')$, which is the inverse of the energy matrix $H^{\text{eff}}(l,l')$:

$$\sigma_l = W^2 \sum_{l'=-\infty}^{\infty} G^{\text{eff}}(l,l') \sigma_{l'}^0 . \tag{40}$$

To evaluate the Green function $G^{\text{eff}}(l,l')$ we shall apply the method described in Sec. III A. Thus the energy matrix $H^{\text{eff}}(l,l')$ with $D(l,l') = W^2 \delta_{ll'}$ will be treated as a sum of a one-particle term $\propto \delta_{ll'}$ and a term with an exponential dependence on the distance $|l-l'|$. The inverse matrices to both terms are a diagonal matrix $G_1(l,l')$ and a three-diagonal matrix $G_2(l,l')$, respectively, which allow the formula Eq. (11) to be easily applied. The resulting Green function is

$$G^{\text{eff}}(l,l')=\frac{1}{\left[W^2\mp\dfrac{V_0^2}{\beta_2}\right](z^2-1)}\times[1+z^2-2\varepsilon z\cosh\Gamma+(z^2-1)\delta_{ll'}]z^{|l-l'|}\ , \tag{41}$$

with the quantity $z$ following from the inversion of the tridiagonal matrix $R(l,l')=(G_1+G_2)(l,l')$:[16,7]

$$z=-A+\operatorname{sgn}(A)(A^2-1)^{1/2}\ , \tag{42}$$

where

$$A=\varepsilon\frac{-|\beta_2|W^2\cosh\Gamma+V_0^2}{W^2|\beta_2|\pm\varepsilon V_0^2}\ . \tag{43}$$

To ensure the stability of the system, a condition should hold that $|A|>1$ or

$$W^2>W_c^2=\frac{2V_0^2}{\beta_2}\frac{1}{\cosh\Gamma\mp\varepsilon}\ . \tag{44}$$

The value $W_c^2$ then corresponds to the critical temperature.

In the case of the ferrodistortive coupling (i) and of the ferrodistortive tendency of the elasticity, i.e., $\varepsilon>0$,[7] the quantity $z$ is positive in the whole range of stability. The response of the system to a pointlike perturbation then decreases exponentially with the distance from the perturbation. Similarly, at the antiferrodistortive coupling, i.e., in case (ii) and the antiferrodistortive tendency of the elastic terms, i.e., $\varepsilon<0$, the quantity $z$ is negative in the whole range of stability and the response is described by a damped oscillating curve. In the remaining cases a crossover value

$$W_s^2=\frac{V_0^2}{|\beta_2|} \tag{45}$$

exists at which the energy matrix Eq. (33) reduces to the purely exponential form. Then the response is localized at the nearest neighbors. Below the crossover value, i.e., $W_c^2<W^2<W_s^2$, the response is exponentially deceasing in case (i) and $\varepsilon<0$ and damped oscillating in case (ii) and $\varepsilon>0$. This complies with the character of the phase transitions indicated by the minimum of the respective dispersion curves. Above the crossover value, i.e., farther away from the phase transition, the types of the response in both cases are interchanged.

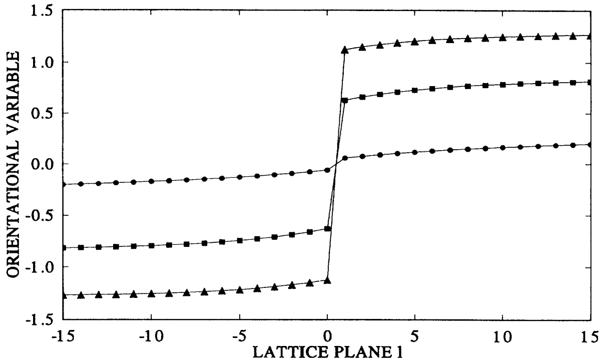

FIG. 1. Profiles of the orientational variable $\sigma_l$ at the ferrodistortive domain wall with ferroelastic coupling (i) [Eq. (32)] and ferrodistortive elasticity $\varepsilon=1$. Model parameters are $\beta_2=-1.0$, $V_0=0.2$, $\Gamma=0.2$, and $W_c^2=3.987$. Three curves (●), (■), and (▲) correspond to a lowering of temperature such that $W^2=5.0$, 15.0, and 30.0, respectively. The respective values of the parameter $z$ [Eq. (42)] are 0.915, 0.843, and 0.830.

The variation of the response manifests itself in the profiles of the order parameter $\sigma_l$ near to the domain walls. In Fig. 1 we show a ferrodistortive domain wall: $\sigma_l^0=-\sigma^0$ for $l=-\infty,\ldots,0$ and $\sigma_l^0=\sigma^0$ for $l=1,\ldots,\infty$ $(\sigma^0>0)$ in the system where both the coupling and the elasticity favor the ferrodistortive response, i.e., (i) and $\varepsilon=1$. One should remember that the increase in $W^2$ now corresponds to the lowering of temperature. The temperature dependence of the parameters of the model $\sigma^0$ and $W^2$ have been chosen so as to obtain the typical temperature dependence of the order parameter $\sigma_l\propto(T_c-T)^{1/2}$ at $l\to\infty$. The domain wall then behaves in a usual way and becomes narrower when we depart from the instability point. This is then the expected narrowing of the domain walls with decreasing temperature. In case (i) and $\varepsilon=-1$ the domain wall is particularly narrow at $W_s^2$. Below this value it has a typical ferrodistortive shape, whereas above this value it shows a damped oscillating profile as depicted in Fig. 2. In Fig. 3 we have shown a system (ii), $\varepsilon=1$, which in principle should undergo an antiferrodistortive phase transition. If, however, the transition is strongly of first order, a ferrodistor-

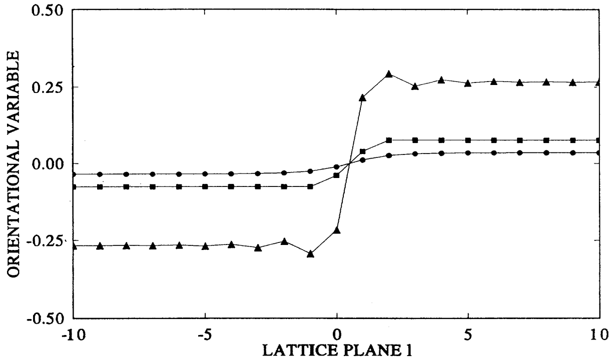

FIG. 2. Profiles of the orientational variable $\sigma_l$ at the ferrodistortive domain wall with ferroelastic coupling (i) [Eq. (32)] and antiferrodistortive elasticity $\varepsilon=-1$. Model parameters are $\beta_2=1.0$, $V_0=2.0$, $\Gamma=0.3$, $W_c^2=3.911$, and $W_s^2=4.0$. Three curves (●), (■), and (▲) correspond to a lowering of temperature such that $W^2=3.93$, 4.0, and 5.0, respectively. The respective values of the parameter $z$ [Eq. (42)] are 0.367, 0.0, and $-0.516$.

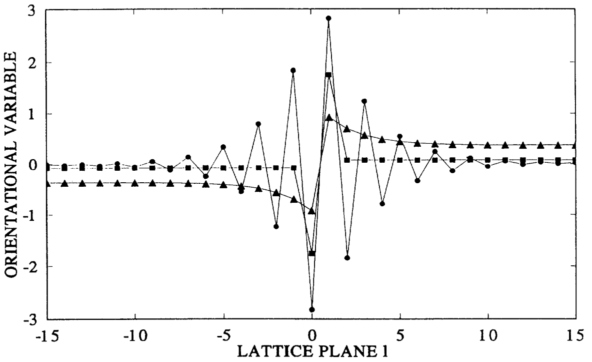

FIG. 3. Profiles of the orientational variable $\sigma_l$ at the ferrodistortive domain wall with antiferroelastic coupling (ii) [Eq. (32)] and ferrodistortive elasticity $\varepsilon=1$. Model parameters are $\beta_2=-1.0$, $V_0=2.0$, $\Gamma=0.3$, $W_c^2=3.911$, and $W_s^2=4.0$. Three curves (●), (■), and (▲) correspond to a lowering of temperature such that $W^2=3.915$, 4.0, and 6.0, respectively. The respective values of the parameter $z$ [Eq. (42)] are $-0.659$, 0.0, and 0.597.

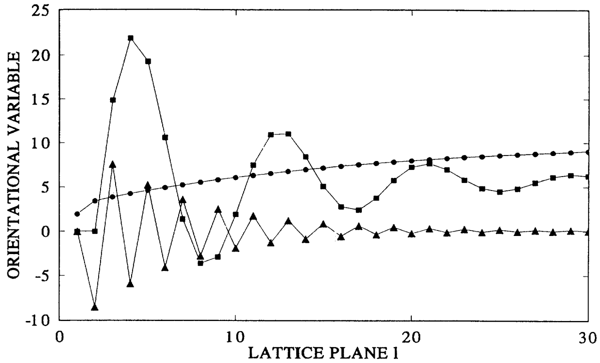

FIG. 4. Surface relaxation of the system described in Sec. VI under external field. The parameters of the model are the following: (●), $\beta=-1.0$, $\Gamma=0.2$, $a=1.2$, $a_1=1.5$, $b=-0.5$; (▲), $\beta=1.0$, $\Gamma=0.2$, $a=1.0$, $a_1=1.5$, $b=0.54$; and (■), $\beta=1.0$, $\Gamma=0.2$, $a=1.0$, $a_1=2.1$, $b=-1.12$. In the last case the competition between ferrodistortive short-range and antiferrodistortive long-range parts produces an incommensurate local distortion.

tive phase can also appear. The evolution of the respective domain wall with temperature or $W^2$ is shown in Fig. 3. Again a crossover between an antiferrodistortive and a ferrodistortive response is marked by a particularly narrow domain wall. The present model is a generalization of the model of Axel and Aubry[11] and Peyrard and Büttner.[12]

## VI. SURFACE RELAXATION IN A SYSTEM WITH SHORT- AND LONG-RANGE INTERACTIONS

The method consisting in the introduction of additional degrees of freedom as explained in Sec. IV will now be illustrated on a system described by the energy matrix given in Eq. (35) with $\varepsilon=1$ and

$$D(l,l')=a\delta_{l,l'}+b(\delta_{ll'+1}+\delta_{ll'-1})+(a_1-a)\delta_{l1}\delta_{l'1}\ , \qquad (46)$$

where $l,l'=1,\dots,\infty$. The last term of Eq. (46) describes a perturbation introduced by the surface to the energy matrix. We shall determine the profile of the variable $\sigma_l$ under a uniform field $f$ applied to the system for various parameters $\beta$, $\Gamma$, $a$, $a_1$, and $b$. The profile is given by the Green function $g(l,l')$:

$$\sigma_l=f\sum_{l'=1}^{\infty} g(l,l')\ . \qquad (47)$$

The Green function is now obtained as the element $\tilde{g}_{11}(l,l')$ of the $2\times2$ Green function $\tilde{g}$ calculated for the energy matrix defined by Eqs. (46), (24), (37), and (35) for $l,l'=1,\dots,\infty$ except for $S(1,1)$, which is $S(1,1)=-e^{\Gamma}/\{2\beta\sinh\Gamma\}$. The surface elements $a_1$ and $S(1,1)$ of the enlarged energy matrix define the cleavage operator of the Dobrzynski surface response theory,[9] which is now readily applicable. Figure 4 depicts the profiles [Eq. (47)] for the sets of parameters producing ferrodistortive, antiferrodistortive, and incommensurate local order near the surface.

## VII. CONCLUSION

Quasi-one-dimensional crystalline systems consisting of parallel lattice planes have been shown to exhibit an exponential distance dependence of the interplanar interaction parameters even in cases of slowly decreasing interatomic potentials. This particular form has allowed us to derive closed expressions for the Green functions in infinite crystals and in crystals with surfaces. Both presented methods, one for the interactions given by a series of exponential terms and the other adapted to the systems showing at the same time short- and long-range interactions, take advantage of the surface response theory due to Dobrzynski,[9] which has been till now applied only to short-range interactions models. The present methods seem to have a wide range of application whenever a short-range interplanar potential is a too-poor approximation, in particular in ionic crystals and in the materials undergoing structural phase transitions. The examples discussed in Secs. V and VI are only first illustration of the methods.

## ACKNOWLEDGMENTS

This work was partially supported by Grant No. 20182 91 01 from the Polish Committee for Scientific Research. Part of this work was done by one of the authors (P.Z.) during his stay at the University of Vienna supported by the Austrian "Ministerium für Wissenschaft und Forschung." The author thanks Professor Warhanek and his associates for their hospitality and help. The author also thanks Professor G. Benedek and L. Dobrzynski for their valuable remarks on the subject.

## APPENDIX

The energy matrix for dipolar systems[2] will now be transformed to the form that allows the method of Sec. IV to be applied. As follows from Ref. 2, the matrix contains a term corresponding to $\mathbf{K}_{\parallel}=0$ which decreases slowly with distance. This term will be denoted by $\underline{H}_l(l,l')$. The other terms of the energy matrix can be approximated by short-range interactions. Hence the matrix is

$$\underline{H}(l,l')=\underline{H}_s(l,l')+\underline{H}_l(l,l') ,$$

where $\underline{H}_s(l,l')$ involves short-range interaction only, whereas (see Ref. 2)

$$\underline{H}_l(l,l')=\underline{H}_{l1}(l,l')+\underline{H}_{l2}(l,l') ,$$

with

$$\underline{H}_{l1}(l,l')=\underline{D}_1(l,l')e^{-\Gamma|l-l'|} ,$$

$$\underline{H}_{l2}(l,l')=\underline{D}_2(l,l')\,\mathrm{sgn}(l-l')e^{-\Gamma|l-l'|} .$$

$$\underline{D}_1=\begin{bmatrix} D_{xx} & D_{xy} & 0 \\ D_{xy} & D_{yy} & 0 \\ 0 & 0 & D_{zz} \end{bmatrix} ,$$

$$\underline{D}_2=i\begin{bmatrix} 0 & 0 & D_{xz} \\ 0 & 0 & D_{yz} \\ D_{xz} & D_{yz} & 0 \end{bmatrix} .$$

Since the inverse to the energy matrix $\underline{H}_l(l,l')$ is not of a short range we introduce

$$\underline{H}_{l3}(l,l')=\underline{H}_{l4}(l,l')+\underline{H}_{l5}(l,l') ,$$

$$\underline{H}_{l4}(l,l')=\left[\begin{bmatrix} C & 0 & 0 \\ 0 & C & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & B \end{bmatrix} 2\cosh(2\Gamma)\right] e^{-\Gamma|l-l'|} ,$$

and

$$\underline{H}_{l5}(l,l')=-2[\sinh(2\Gamma)\delta_{ll'}+\delta_{ll'\pm 1}\sinh(\Gamma)]\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & B \end{bmatrix} ,$$

where the coefficients $C$ and $B$ are to be specified. One can prove that the inverse to the energy matrix

$$(\underline{H}_{l2}+\underline{H}_{l3})^{-1}$$

vanishes for $l,l'>3$ provided that

$$CB=-(D_{xz}^2+D_{yz}^2)/\{4\sinh^2\Gamma\} .$$

Now the initial energy matrix is

$$\underline{H}(l,l')=\underline{H}_s'(l,l')+\underline{H}_e'(l,l')+\underline{H}_n'(l,l') ,$$

where

$$\underline{H}_s'(l,l')=\underline{H}_s(l,l')-\underline{H}_{l5}(l,l') ,$$

$$\underline{H}_e'(l,l')=\underline{H}_{l1}(l,l')-\underline{H}_{l4}(l,l') ,$$

$$\underline{H}_n'(l,l')=\underline{H}_{l2}(l,l')+\underline{H}_{l3}(l,l') .$$

The terms $\underline{H}_e'(l,l')$ and $\underline{H}_n'(l,l')$ have inverse matrices of a short range, whereas the term $\underline{H}_s'(l,l')$ is itself of a short range. Introduction of additional degrees of freedom corresponding to $\underline{H}_e'(l,l')$ and $\underline{H}_n'(l,l')$ then allows for the application of the method of Sec. IV.

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