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Ground state of a two-dimensional lattice system with a long-range interparticle repulsion: Stripe formation and effective lowering of dimension

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It has been shown that particle ordering into stripes and effective lowering of dimension reside universally in the ground state of two-dimensional lattice systems with a long-range interparticle repulsion for any geometry of the host lattice and any physically reasonable *isotropic* pair potential. Examples are adatom systems and ensembles of self-localized charge carriers in layered or two-dimensional narrow-band conductors. On the basis of this fact a general analytical procedure has been formulated to describe fully the ground-state space structure of the above systems and the zero-temperature dependence of their filling factor on the chemical potential. The results obtained enable us to suggest that charge ordering into stripes revealed in copper-oxide superconductors can be caused solely by a long-range Coulomb hole-hole repulsion.

I. INTRODUCTION

The two-dimensional (2D) lattice systems with a long-range interparticle repulsion (LSLRIR) are of great interest as they have important physical applications. One of them is the adatom systems[1] with a sufficiently strong interaction between the particles and the substrate. Another field to apply the 2D LSLRIR model is a ‘‘frozen’’ charge carrier phase[2] (FCCP) that comes to existence in 2D or layered narrow-band conductors when electron or hole hopping is *suppressed* by a *long-range* mutual electron repulsion. This occurs for $t < \delta u = (a/\overline{r})\overline{u}$, where t is the electron/hole bandwidth, δu is the typical change in the energy of a narrow-band electron/hole as it hops between the host-lattice sites, a is the typical hopping range , $\overline{r}$ is the mean electron/hole separation, and $\overline{u}$ is the average energy per charge carrier. The FCCP differs principally from any known self-localized electron ensemble including a Wigner crystal.[2] The high-T_c cuprates, polycrystal electroceramic materials,[3] as well as some art 2D conductors[4–6] appear to be most favorable for 2D FCCP formation. The distinctive features of the FCCP are rooted in properties of its ground state (GS) at $t \ll \delta u$. In this limit the GS is much the same as that of the adatom systems.

As far as we know, neither the GS nor the thermodynamics of the 2D LSLRIR have been studied adequately. Here we offer a unified approach to the description of the GS of the 2D zero-bandwidth LSLRIR with an *isotropic* pair potential of the interparticle repulsion, $v(r)$ (r is the distance between interacting particles). The key point of our consideration is a *zero-temperature effective lowering of dimension (LOD)* — which we have revealed to underlie (*despite the pair potential isotropy*) the main GS properties of the 2D LSLRIR for (i) any filling factor, $\rho = N/\mathcal{N}$ (N and $\mathcal{N}$ are the total numbers of the particles and host-lattice sites, respectively, $N,\mathcal{N} \to \infty$); (ii) arbitrary geometry of the host lattice (with one site per cell); (iii) any physically reasonable $v(r) > 0$. We take the term LOD to mean that the GS of the 2D LSLRIR is a set of different effective one-dimensional (1D) LSLRIR whose ‘‘particles’’ are *periodic* stripes on the 2D host lattice. For each 1D system of the set there is its own ρ interval where this 1D LSLRIR represents the 2D one, the whole range, $0 \leqslant \rho \leqslant 1$, comprising all the intervals. The LOD enables us to offer a rigorous analytical procedure for the 2D LSLRIR GS description, using the results of the exact 1D LSLRIR theory.[7–9] Due to the LOD the GS with *irrational* ρ turns out to be incommensurable only in *one direction*.

II. HAMILTONIAN. *S* CRYSTALS

The Hamiltonian $\mathcal{H}$ of the system under consideration has the form

$$\mathcal{H}\{n(\vec{r})\} = \frac{1}{2} \sum_{\vec{r} \neq \vec{r}'} v(|\vec{r} - \vec{r}'|) n(\vec{r}) n(\vec{r}'), \tag{1}$$

where $\vec{r} = m_1 \vec{a}_1 + m_2 \vec{a}_2$ are radius vectors of the host-lattice sites, $m_{1,2}$ are integers, and $\vec{a}_{1,2}$ are host-lattice primitive translation vectors (PTV’s); below we put the host-lattice cell area, $|a_1 \times a_2|$, equal to unity, so that $\mathcal{N}$ is the dimensionless volume of the system; the occupation numbers of the host-lattice sites, $n(\vec{r})$ (microscopic variables), are assumed to be 0 or 1; the sum is taken over the whole host lattice; $v(r) = \tilde{v}(r)/r$ is an everywhere convex function with $\tilde{v}(r)$ tending to zero as r^{-2} or faster when $r \to \infty$. Otherwise $v(r)$ is arbitrary. This class of $v(r)$ covers both the FEP and the adatom systems.

Due to the *convexity* of $v(r) > 0$ there exists an infinite set of $\rho = 1/Q_j$ (Q_j are integers indexed by j in an increasing order) such that for each of them the GS particle configuration is a simple 2D crystal with one particle per cell (‘‘*S* crystal’’), i.e., $Q_j = |\det m^j_{\kappa\lambda}|$ are the *S*-crystals elementary cell areas, the integers $m^j_{\kappa\lambda}$ ($\kappa, \lambda = 1,2$) being components of the jth *S*-crystal PTV’s in the $\vec{a}_\lambda$ basis. [Violating the condition of $v(r)$ convexity can crucially change the GS configuration. For example, in the case of the boxlike $v(r)$ the GS configurations are not *S* crystals because of a clusterization of the particles.[10]] Our strategy is to derive the full description of the GS for any ρ, starting with consideration of small vicinities of $\rho=1/Q_j$. Since specific $m^j_{\kappa\lambda}$ are irrelevant to this reasoning, we drop the index j at Q and other characteristics of the S crystals for a while.

Owing to the discreteness of the considered system a macroscopically small change, ΔN or $\Delta\mathcal{N}$, in N or $\mathcal{N}$ (we mean that $\Delta N/N, \Delta\mathcal{N}/\mathcal{N}\to 0$ while $\Delta N/N^{1/2}, \Delta\mathcal{N}/\mathcal{N}^{1/2}\to\infty$ when $N,\mathcal{N}\to\infty$) produces only *isolated defects* in an S crystal, the space structure of the defects, and the energies of their formation, depending essentially on the ΔN or $\Delta\mathcal{N}$ sign. Therefore, the corresponding change, ΔE_g, in the GS energy E_g does not have an odd symmetry in $\Delta N,\Delta\mathcal{N}$,

$$\begin{aligned}\Delta E_g &= E_g(N\pm|\Delta N|,\mathcal{N}\pm|\Delta\mathcal{N}|)-E_g(N,\mathcal{N})\\ &=\pm\mu_\pm|\Delta N|\mp P_\mp|\Delta\mathcal{N}|,\end{aligned} \tag{2}$$

where the coefficients $\mu_\pm(Q)$ and $P_\pm(Q)$ are uniquely determined by the energies of defects formation and satisfy inequalities $\mu_-(Q)<\mu_+(Q)$ and $P_-(Q)<P_+(Q)$. Equation (2) shows that a given S crystal exists at any value of the chemical potential μ on the interval $[\mu_-(Q),\mu_+(Q)]$. Much the same, the interval of S-crystal existence in the pressure P is $[P_-(Q),P_+(Q)]$. The end points, $\mu_\pm$, $P_\pm$, are related by the equation

$$\mu_\pm=\overline{u}+P_\pm Q, \tag{3}$$

[$\overline{u}=\overline{u}(Q)$ is the S-crystal energy per cell], which follows immediately from the known zero-temperature thermodynamic identity,

$$\mu N=E_g+P\mathcal{N}. \tag{4}$$

Thus, in some vicinity of $\rho=1/Q$ the GS is bound to be a superstructure of the defects. Our next step is to find them.

III. ZERO-DIMENSIONAL DEFECTS AND THEIR COALESCENCE

Adding one particle to or removing one particle from an S crystal results in the formation of a zero-dimensional defect, ‘‘+ defecton’’ or ‘‘− defecton,’’ respectively. One can be inclined to think that δN should be identified exactly with the total number of ± defectons spatially separated, $\pm\mu_\pm$ being simply the energy of ± defecton formation, $\varepsilon^d_\pm$. However, this seemingly evident statement is actually incorrect due to a *coalescence* of defectons of the same ‘‘sign.’’ In other words, if the number $|\nu|$ of S-crystal particles removed $(\nu<0)$ or added $(\nu>0)$ is more than 1, there exists a *bound state* of $|\nu|$ ± defectons whose energy is less than $|\nu|\varepsilon^d_\pm$. We have revealed the coalescence by computation, using a ‘‘dipole’’ description of the GS with $\nu=\pm 1,\pm 2,\ldots$, which we have specially worked out for this purpose. It consists in the following.

At $\nu\neq 0$ the GS is a perturbed S crystal where, beside particles placed at host-lattice sites in the interstices of the S-crystal $(\nu>0)$ or empty S-crystal sites, ‘‘holes,’’ $(\nu<0)$, there are generally a certain number n_d of S-crystal particles displaced. An S-crystal site left by its particle can be considered as an ‘‘antiparticle’’ with the ‘‘charge’’ equal to the particle one in magnitude but opposite in sign. The pair ‘‘a particle displaced by a vector $\vec{\xi}$+its antiparticle located at an S-crystal site $\vec{r}$’’ can thus be considered to be a kind of a dipole (we will call it a ‘‘$\vec{r},\vec{\xi}$ dipole’’) which interacts with the interstitial particles/holes (IP/H’s) and other dipoles. The energy of the $\vec{r},\vec{\xi}$ dipole interaction with an IP/H (at $\vec{r}=0$) equals

$$u_{\vec{\xi}}(\vec{r})=(\operatorname{sign}\nu)[v(|\vec{r}-\vec{\xi}|)-v(|\vec{r}|)].$$

The energy of interaction between the $\vec{r},\vec{\xi}$ and $\vec{r}\,',\vec{\xi}\,'$ dipoles is

$$\begin{aligned}u_{\vec{\xi},\vec{\xi}'}(\vec{R})&=v(|\vec{R}+\vec{\xi}-\vec{\xi}\,'|)+v(|\vec{R}|)\\ &\quad -v(|\vec{R}+\vec{\xi}|)-v(|\vec{R}-\vec{\xi}\,'|),\end{aligned}$$

where $\vec{R}=\vec{r}-\vec{r}\,'$.

The IP/H’s, in turn, undergo a mutual repulsion and experience a ‘‘crystal’’ field, $u_{\mathrm{cr}}(\vec{r})$, which is the field produced at a point $\vec{r}$ by the ideal S crystal for $\nu>0$ and equals $-2\overline{u}$ for $\nu<0$. In the dipole terms the change in E_g at a given ν, $\delta E_g=\delta E_g(\nu)$, takes the form

$$\delta E_g(\nu)=\min(U_d+U_{\mathrm{ex}}+V_{\mathrm{rep}}+U_{\mathrm{cr}}). \tag{5a}$$

Here

$$U_d=\sum_{\alpha,i} u_{\vec{\xi}_i}(\vec{r}_{\alpha i}) \tag{5b}$$

is the energy of the IP/H-dipole interaction;

$$U_{\mathrm{ex}}=\sum_i \delta u_{\vec{\xi}_i}+\sum_{i<k} u_{\vec{\xi}_i,\vec{\xi}_k}(\vec{r}_{ik})>0 \tag{5c}$$

is the excitation energy of an S crystal at $\nu=0$, $n_d\neq 0$; $\delta u_{\vec{\xi}}\sim\overline{u}|\vec{\xi}|^2/Q>0$ is the energy of formation of a dipole with the displacement vector $\vec{\xi}$;

$$V_{\mathrm{rep}}=\sum_{\alpha<\beta} v(|\vec{r}_{\alpha\beta}|) \tag{5d}$$

is the energy of the mutual IP/H’s repulsion; $\vec{r}_{ab}\equiv\vec{r}_a-\vec{r}_b$; subscripts $i,k=1,\ldots,n_d$ and $\alpha,\beta=1,\ldots,|\nu|$ number the antiparticles’ and IP/H’s radius vectors, respectively;

$$U_{\mathrm{cr}}=\sum_\alpha u_{\mathrm{cr}}(\vec{r}_\alpha) \tag{5e}$$

is the IP/H’s energy in the above crystal field. The minimum is taken only with respect to the dipole variables, n_d, $\vec{r}_i$, $\vec{\xi}_i$, and $\vec{r}_\alpha$. Hence, the dipole approach allows us to work with only a few discrete variables. This facilitates considerably the (classic) Monte-Carlo computer simulation of the ± defectons [$|\nu|=1$, $\delta E_g(\pm 1)=\varepsilon^d_\pm$] and their coalescence at $|\nu|>1$.

The dipole approach offers a clear view of how the defecton bound state arises despite the fact that the defectons of the same sign repel each other, being widely spaced. In the GS the total dipole energy, $E_d(\nu)=U_{\mathrm{ex}}(\nu)+U_d(\nu)$, is negative despite the fact that $U_{\mathrm{ex}}>0$, so that for $|\nu|>1$ the GS space structure is governed by an interplay between $|U_d|$ and $V_{\mathrm{rep}}>0$. The IP/H dipole interaction gives the maximal gain

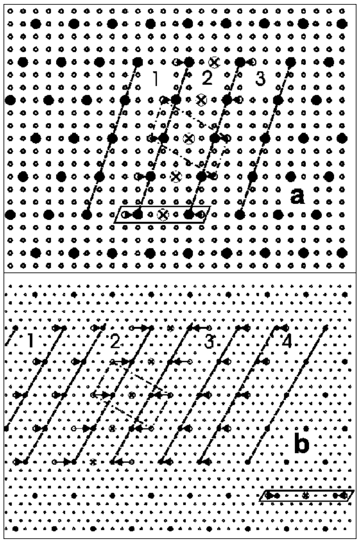

FIG. 1. The coalescence for square [(a), $Q=9$] and triangular [(b), $Q=16$] host lattices ($\nu=-5$). Here ○ denotes host-lattice sites, ● denotes particles, ⊙ denotes antiparticles, ⊗ denotes holes, → denotes dipoles, and solid boxes mark off a single defecton. The dash-dotted parallelograms mark off the dipole ''shells.'' The dotted lines show nucleation of the elementary stripes enumerated by 1,2, ... In case (a) boundary effects dominate the mutual repulsion of the unfinished − stripes; in case (b) the tendency to − stripes divergence is seen. Both configurations refer to the model potentials with $R\sim Q^{1/2}$.

in energy when *each* IP/H is embedded in a ''shell'' of four dipoles that are all attracted to it, the dipoles' antiparticles forming a parallelogram of a size $\sim\overline{r}\sim Q^{1/2}$. On the other hand, $U_{\rm ex}>0$ is as small as possible when the shells of neighboring IP/H's share some of their dipoles to reduce n_d. These requirements can all be fulfilled together only when the IP/H's are *aligned in a row*, the near-neighbor IP/H's being shifted relative to one another by the same *S*-crystal PTV with the modulus $\sim\overline{r}$ (Fig. 1). In such a case $|E_d(\nu)|$ is more than the magnitude of the dipole energy of $|\nu|$ infinitely separated defectons, $E_d^{\infty}=|\nu|E_d(\pm 1)$. The coalescence arises when the energy gain, $\Delta=|E_d(\nu)|-|E_d^{\infty}|$, exceeds $V_{\rm rep}$ of the row. Since $\Delta\sim|\nu|v(\overline{r})$ (the estimate holds for both small ρ and $\rho\sim 1$), this condition is met if $\tilde{v}(r)$ decreases not too slowly, or, more exactly, if

$$\gamma=\int_{\overline{r}}^{\infty} v(r)dr/\overline{r}v(\overline{r})\lesssim 1. \tag{6}$$

The computer simulation carried out with the model potential $v(r)\propto r^{-\beta}\exp(-r/R)$ over a wide range of the parameters, β,R, has shown that the condition $\gamma\lesssim 1$ is really the criterion of the coalescence for any $|\nu|$ (and any $\vec{a}_{1,2}$). It is this situation that is the subject for study from here on. It is of most frequent occurrence. The limiting case $\gamma\gg 1$ will be outlined in the next section.

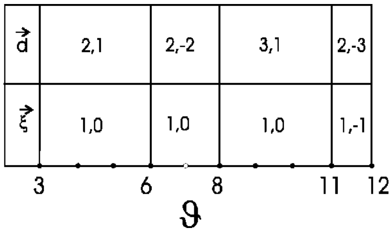

FIG. 2. The universality range of the ground state of 2D LSLRIR on a square host lattice ($3\leqslant\vartheta\leqslant 12$). The symbol ● marks off the *S*-crystal ϑ values. The symbol ○ at $\vartheta=7$ shows that the GS with this ϑ is not an *S* crystal but a mixture of native stripes of the neighboring *S* crystals ($\vartheta=6$ and $\vartheta=8$). The integers written out beneath the ϑ axis are the endpoints of the intervals over which all GS stripe structures share the same PTV $\vec{d}_{\pm}$ (''*director*''). The *S* crystals with these ϑ have different $\vec{d}_-$ and $\vec{d}_+$. The coordinates of the directors are shown in the upper row of the table. The pairs of integers in the lower row are the coordinates of the displacement vectors $\vec{\xi}_-$. All *S* crystals of the universality range share the same Q_j branch.

IV. STRIPE FORMATION AND THE LOWERING OF DIMENSION

A. Elementary 1D defects

It follows from the above results that with an infinite increase in $|\nu|$ the bound state of $|\nu|$ defectons is transformed into a periodic *stripelike* structure (Fig. 1). It consists of elementary substripes which, as will be shown below, repel each other. Therefore, it is *1D defects* of such a type that are expected to form the GS superstructure. They fall into the class of the simplest 1D defects. Generally, such a defect is a stripe of rarefaction or compression that arises when an *S*-crystal part adjacent to a line of particles with some *S*-crystal PTV, $\vec{d}$, is shifted as a whole relative to the other one by a host-lattice translation vector $\vec{\xi}$. Formation of n_s ($n_s\to\infty$, $n_s/N^{1/2}\to 0$) stripes of length L_s changes $\mathcal{N}$ by

$$\Delta\mathcal{N}=\pm n_s|\vec{d}\times\vec{\xi}|L_s,$$

where L_s is measured in units of $|\vec{d}|$. This produces the change in the system energy,

$$\Delta E=\varepsilon(\vec{d},\vec{\xi})|\Delta\mathcal{N}|,$$

the proportionality coefficient $\varepsilon(\vec{d},\vec{\xi})$ being given by the expression

$$\varepsilon(\vec{d},\vec{\xi})=|\vec{d}\times\vec{\xi}|^{-1}\sum_{n=1}^{\infty}\sum_{\vec{r}}{}' \, u_{\vec{\xi}}(\vec{r}-n\vec{f}), \tag{7}$$

where $\vec{f}$ is any *S*-crystal PTV other than $\vec{d}$; $\Sigma'_{\vec{r}}$ means summation over the *S*-crystal semiplane

$$\vec{r}=k\vec{d}+l\vec{f}, \quad -\infty<k<\infty, \quad -\infty<l\leqslant 0. \tag{8}$$

The GS is realized by the stripes with $\vec{d}=\vec{d}_-$, $\vec{\xi}=\vec{\xi}_-$ or $\vec{d}=\vec{d}_+$, $\vec{\xi}=\vec{\xi}_+$ which provide the minimum of $\varepsilon(\vec{d},\vec{\xi})$ for the case of rarefaction $[\varepsilon(\vec{d},\vec{\xi})<0]$ or of compression $[\varepsilon(\vec{d},\vec{\xi})>0]$, respectively. By analogy with ''− defectons'' or ''+ defectons'' we will call these stripes ''− stripes'' or ''+ stripes,'' respectively.

The absolute values of ± stripe formation energies per unit of stripe length,

$$\varepsilon_{\pm}=|\varepsilon(\vec{d}_{\pm},\vec{\xi}_{\pm})|, \tag{9}$$

are nothing but the coefficients $P_\pm$ [see Eq. (2)] associated with the elementary 1D defects. As follows from Eq. (3), the corresponding

$$\mu_\pm = \tilde{\varepsilon}_\pm \equiv \overline{u} + Q\varepsilon_\pm . \tag{10}$$

Lest there be a contradiction with the fact of the defecton coalescence, $\tilde{\varepsilon}_\pm$ and $\varepsilon^d_\pm$ are bound to satisfy inequalities

$$|\varepsilon^d_-| < \tilde{\varepsilon}_- < \tilde{\varepsilon}_+ < \varepsilon^d_+ . \tag{11}$$

To verify them we have computed $\varepsilon_\pm$, based on Eq. (7), for Q up to 150 in parallel to the Monte Carlo coalescence studies. The computation has shown that the inequalities are really the case for all $v(r)$ under consideration, i.e., for $v(r)$ which meet criterion (6).

When $Q \gg 1$ and $v(r)$ goes exponentially to zero over distances $R \ll \overline{r} \sim Q^{1/2}$, inequalities (11) become strengthened. In such a case they can be obtained by simple estimates. Since $|\vec{\xi}_\pm| \sim 1$, and, correspondingly, $|\vec{d}_\pm \times \vec{\xi}_\pm| \sim Q^{1/2}$, it follows from Eqs. (7) and (10) that $\tilde{\varepsilon}_\pm \sim Q^{1/2} R^{-1} \overline{u}$. On the other hand, $|\varepsilon^d_-| \sim \overline{u} \sim v(\overline{r})$. Therefore, $\tilde{\varepsilon}_- \gg |\varepsilon^d_-|$. As for ε^d_+, it is comparable to the minimum of the crystal field $u_{\rm cr}(\vec{r})$ (Sec. III). By virtue of the exponential decrease in $v(r)$ and the inequality $R \ll \overline{r}$ the ratio $\min[u_{\rm cr}(\vec{r})]/\overline{u}$ exceeds $Q^{1/2} R^{-1} \gg 1$ significantly, and hence, $|\varepsilon^d_+| \gg \tilde{\varepsilon}_+$.

Inequalities (11) together with the mutual repulsion of ± stripes of the same sign lead to the conclusion that the GS in a vicinity of $1/Q$ is a superstructure of ± stripes separated by ‘‘native’’ stripes of the unperturbed S crystal. These are pairs of neighboring S-crystal particle lines with PTV $\vec{d}_\pm$, i.e., they are shifted relative to one another by a vector $\vec{f}_\pm$ which is any S-crystal PTV satisfying the equation $|\vec{d}_\pm \times \vec{f}_\pm| = Q$, a ± stripe that is a pair of the particle lines with a relative-displacement vector $\vec{f}_\pm + \vec{\xi}_\pm$. Enumerating the ± stripes to, say, m, the equations of the particle lines bounding the mth ± stripe can be written in the form

$$\vec{r}^{\,(1)}_m(k) = k\vec{d}_\pm + l(m)\vec{f}_\pm + m\vec{\xi}_\pm , \tag{12a}$$

$$\vec{r}^{\,(2)}_m(k) = \vec{r}^{\,(1)}_m(k) + \vec{f}_\pm + \vec{\xi}_\pm , \tag{12b}$$

where $k = 0, \pm 1, \pm 2, \ldots$; the parameter $l(m)$ is the number of all particle lines parallel to $\vec{d}_\pm$ between the mth and zero ± stripes. The integer $l(m)$ can be considered as the ‘‘coordinate’’ of the mth ± stripe. The set of the integers $l(m)$ describes the GS space structure of the 2D LSLRIR fully as the system consisting of ± stripes and native stripes is invariant with respect to translation by $\vec{d}_\pm$. Therein lies the LOD.

B. The ground-state stripe superstructure

The GS set of the coordinates $l(m)$ is chosen such that the change in the system energy which is due to stripe formation in an S crystal,

$$E_s = \pm N_s^\pm \varepsilon_\pm + H_{\rm int} , \tag{13a}$$

is a minimum at a fixed number of ± stripes, $N_s^\pm$. Here $H_{\rm int} = H_{\rm int}\{l(m)\}$ is the energy of the interstripe interaction; it is the sum

$$H_{\rm int} = \sum_{m_2 > m_1} V^{ss}_{m_2 - m_1 - 1}(l_{m_2} - l_{m_1}), \tag{13b}$$

where the summation is taken over all ± stripes; $V^{ss}_m(l)$ is the generalized pair potential of the stripe-stripe interaction, namely, it is the interaction energy of two ± stripes with a coordinate difference l, between which there are $m = 0, 1, \ldots$ other ± stripes,

$$V^{ss}_m(l) = \sum_{n=0}^{\infty} U(\vec{F}_{l,m} + n\vec{f}_\pm), \quad \vec{F}_{l,m} = l\vec{f}_\pm + m\vec{\xi}_\pm ; \tag{14a}$$

$U(r)$ is the energy of interaction between a certain $\vec{r}, \vec{\xi}_\pm$ dipole and the infinite system of dipoles with the displacement vector $-\vec{\xi}_\pm$ whose antiparticles fill the semiplane (8) with $\vec{d} = \vec{d}_\pm$, $\vec{f} = \vec{f}_\pm$,

$$U(\vec{r}) = \sum_{\vec{r}_\pm}{}' u_{\vec{\xi}_\pm, -\vec{\xi}_\pm}(\vec{r} - \vec{r}_\pm). \tag{14b}$$

The symbol $\Sigma'_{\vec{r}_\pm}$ means summation over the semiplane just mentioned. Here and further on in the paper all energy quantities associated with stripes are energies per unit of stripe length.

To find the set of $l(m)$ that minimize $H_{\rm int}$, and thereby $\overline{\varepsilon}$, it is helpful to notice that the dipole-dipole interaction energy

$$u_{\vec{\xi}, -\vec{\xi}}(\vec{r}) = v(|\vec{r} - \vec{\xi}|) + v(|\vec{r} + \vec{\xi}|) - 2v(|\vec{r}|),$$

appearing in Eq. (14b), has the structure of the second-order finite difference. This suggests that $U(n\vec{f}_\pm)$ as a function of n is positive since $v(r)$ is a convex function. If $n \gg 1$, this is easy to see, taking into account that the considered $v(r)$ go to zero no slower than r^{-2}. Moreover, our computation has shown that $U(n\vec{f}_\pm)$ is a positive and monotonically decreasing function of n for *any* $n \geq 1$ provided $v(r)$ meets condition (6). For this reason potentials $V^{\rm ss}_m(l)$ are all positive and meet the convexity condition

$$V^{\rm ss}_m(l+1) - 2V^{\rm ss}_m(l) + V^{\rm ss}_m(l-1) > 0.$$

Consequently, (i) the ± stripes do repel each other, and (ii) due to the convexity of $V^{\rm ss}_m(l)$ integers $l(m)$ are arranged similar to the coordinates of particles of a 1D LSLRIR with a convex pair potential. Based on the line of argument of the 1D theory,[7–9] one can conclude that they obey the universal algorithm

$$l(m) = [m/c_\pm], \tag{15a}$$

where $[\cdots]$ is the integral part of a number, and

$$c_\pm = |\vartheta - Q|/\sigma_\pm = N_s^\pm / \mathcal{N}_s^\pm \tag{15b}$$

is the concentration of the ± stripes; $\vartheta = 1/\rho$; the integer

$$\sigma_\pm = |\vec{d}_\pm \times \vec{\xi}_\pm| \tag{15c}$$

equals the difference between the $\pm$ stripe and the native-stripe areas per unit of stripe length; $\mathcal{N}_s^{\pm}$ is the total number of the $\pm$ stripes and the native ones; the sign $-$ or $+$ in Eq. (15a) means that the expression describes a region of rarefaction, $\vartheta > Q$, or compression, $\vartheta < Q$, respectively. (In this connection it should be noted that the $\pm$ stripes are 2D analogues of the 1D dimers introduced by Hubbard.[7])

Of frequent occurrence is the situation that $\vec{f}_{\pm}$ can be chosen to be parallel to $\vec{\xi}_{\pm}$, i.e., $\vec{f}_{\pm}=(Q/\sigma_{\pm})\vec{\xi}_{\pm}$. (Particularly, this takes place necessarily if $\sigma_{\pm}=1$, and hence, $\vec{d}_{\pm}$ and $\vec{\xi}_{\pm}$ are both host-lattice PTV's.) In such a case both Eqs. (12a) and (12b) have the form

$$\vec{r}(k)=k\vec{d}_{\pm}+s\vec{\xi}_{\pm} \quad (k=0,\pm 1,\pm 2,\dots), \tag{16}$$

where s is a certain integer. This allows us to simplify the description of the GS, considering directly lines (16) as the ''particles'' of a 1D lattice system, the particle ''coordinates'' being s. As follows from Eqs. (15), such particles are arranged by the algorithm

$$s_m=[\overline{s}m], \tag{17}$$

where s_m is the coordinate of the mth line, $\overline{s}=\vartheta/\sigma_{\pm}$ is the mean line separation measured in units of $|\vec{\xi}_{\pm}|$.

C. Stable and metastable thermodynamic branches and first-order transitions

At $c_{\pm}=1$ $(\vartheta=Q\mp\sigma_{\pm})$ the algorithm (15) determines the crystal with one particle per cell built on PTV's $\vec{d}_{\pm}$ and $\vec{f}_{\pm}+\vec{\xi}_{\pm}$. Further, we call it the S^r crystal (rarefied S crystal, $c_{-}=1$) or the S^c crystal (compressed S crystal, $c_{+}=1$). If this structure is stable (i.e., the $S^{r,c}$ crystal is another S crystal) or metastable, the algorithm can be extended over the whole domain of $\pm$ stripe concentrations, $0\leqslant c_{\pm}\leqslant 1$, i.e., over the ϑ interval

$$\vartheta_c=Q-\sigma_{+}\leqslant\vartheta\leqslant\vartheta_r=Q+\sigma_{-}. \tag{18}$$

This follows from two intimately related plain statements that have been fully confirmed by our computation: (i) the above mechanism underlying the coalescence of zero-dimensional defects and the 1D defect formation holds for any space structure determined by the algorithm (15), i.e., irrespective of the $c_{\pm}$ value; (ii) the 1D defects resulting from macroscopically small variations in ϑ have the same PTV, $\vec{d}_{\pm}$, for all $c_{\pm}$.

It is evident that the S-crystal native stripes with the PTV $\vec{d}_{-}$ or $\vec{d}_{+}$ are also $+$ stripes of the S^r crystal or $-$ stripes of the S^c crystal, respectively. Vice versa, an S-crystal $-$ stripe or $+$ stripe is geometrically the same as an S^r- or S^c-crystal native stripe with the PTV $\vec{d}_{-}$ or $\vec{d}_{+}$. In view of this fact it does not matter whether one describes the GS space structure on the interval (18) in terms of the $\pm$ stripes of the S crystal or in terms of its native stripes. In the latter case $l(m)$ appearing in Eqs. (15) should be considered to be the ''coordinate'' of the mth native stripe, and $c_{\pm}$ should be replaced by the native-stripe concentration, $1-c_{\pm}$.

Due to (meta)stability of the $\mathrm{S}^{r,c}$ crystals the algorithm (15) holds also over ϑ ranges adjacent to both endpoints of the interval (18). For these ϑ Eqs. (15) determines a mixture of $-$ stripes and native stripes of the S^r crystal $(\vartheta>\vartheta_r)$ or that of $+$ stripes and native stripes of the S^c crystal $(\vartheta<\vartheta_c)$, the stripes being characterized by a new triple of vectors, $\vec{d}_r$, $\vec{f}_r$, $\vec{\xi}_r$ or $\vec{d}_c$, $\vec{f}_c$, $\vec{\xi}_c$, the analogs of $\vec{d}_{-}$, $\vec{f}_{-}$, $\vec{\xi}_{-}$ or $\vec{d}_{+}$, $\vec{f}_{+}$, $\vec{\xi}_{+}$ respectively. The concentration of new $\pm$ stripes, $c_{r,c}$, is related to ϑ by the expression

$$c_{r,c}=\frac{|\vartheta-\vartheta_{r,c}|}{\sigma_{r,c}}, \quad \sigma_{r,c}=|\vec{d}_{r,c}\times\vec{\xi}_{r,c}|.$$

In passing ϑ through the points $\vartheta_{r,c}$ the GS space structure changes continuously since $c_{r,c}$ goes to zero when $\vartheta\to\vartheta_{r,c}$.

Extending the algorithm (15) in the manner shown above over all possible ϑ, we obtain the branch of the (meta)stable zero-temperature states connected in continuity with the starting S crystal. Enumerating the S crystals by the index j (Sec. II) again, we will classify these thermodynamic branches by the elementary-cell areas Q_j of the starting S crystals and will name them Q_j branches. As follows from the definition, the energy of a Q_j-branch state as a function of ϑ, $E_j(\vartheta)$, is continuous. We have revealed that as a rule, a given Q_j branch is shared by several S crystals. On the other hand, there are inevitably intersections of different energy branches $E_j(\vartheta)$. What this means is that *zero-temperature first-order transitions (of a type of polymorphism) from one well developed stripe superstructure to another* occur at the intersection points. The first-order transitions take place irrespective of the geometry of the host lattice. (Examples are in Sec. VI.)

Summarizing the above reasoning, one can state that there are only two possibilities: the $(j+1)$th or $(j-1)$th means the S crystal whose numbers is $j+1$ or $j-1$, respectively; otherwise, there is a point of the first-order transition on the interval $[Q_j,Q_{j+1}]$ or $[Q_{j-1},Q_j]$.

Along with the Q_j branches there can exist the thermodynamic branches which, being *metastable* in vicinities of the points $\vartheta=Q_j$, become *stable* far from Q_j. Each state of such a ''pseudo-Q_j-branch'' is a mixture of native stripes of the jth S crystal and its elementary stripes of rarefaction or compression with PTV's other than $\vec{d}^{\,j}_{\pm}$, the energies of stripe formation, the stripe arrangement, and the energy of the state being determined by the expressions (9) and (13)–(15) if one replaces $\vec{d}_{\pm}$, $\vec{\xi}_{\pm}$ with the corresponding vectors. Thus, the GS energy dependence on ϑ comprises the stable portions of both Q_j branches and pseudo-Q_j branches.

To complete the description of the GS it should be also noted that the GS space structure with an arbitrary ρ is converted in that with the filling factor $1-\rho$ on mutual replacement of the particles by the empty host-lattice sites and vice versa. Correspondingly, $E_g(1-\rho)=E_g(\rho)+(1-2\rho)E_0$, where E_0 is the energy of the system at $\rho=1$. Therefore, it is sufficient to consider the range $\vartheta\geqslant 2$ only.

At $\vartheta=2$ the GS configuration can be envisioned as two geometrically equivalent sublattices with $\mathcal{N}/2$ sites, one of which is completely occupied by the particles and the other is empty, i.e., it is the S crystal with one empty host-lattice site per cell. The ± defectons of such an S crystal, irrespective of the host-lattice geometry and $v(r)$ form, are simply IP/H's, which do not coalesce as they do not have dipole surroundings. Despite this fact the IP/H's are arranged in a stripelike superstructure for deviation of ϑ from $\vartheta=2$ which is as small as is wished. This superstructure is fully described in terms of the above theory if one considers the sublattice just mentioned as the host lattice and the IP/H's as the particles, the filling factor being equal to $|1-2\rho|$. This special thermodynamic branch represents the GS over a ρ interval $[\rho_b,1-\rho_b]$, whose left end point ρ_b is more than 1/3. This is in accordance with the fact that the least inverse S-crystal filling factor for which the defecton coalescence occurs inevitably is found to be just $Q_j=3$.

D. A computation procedure to find the 2D LSLRIR ground state

The above analysis shows that the GS of the 2D LSLRIR is fully determined if the following quantities are known: (i) the PTV's $\vec{m}^j$ of the S crystals, (ii) the PTV's, $\vec{d}^j_\pm$, and the displacement vectors, $\vec{\xi}^j_\pm$, of the Q_j-branch ± stripes together with their pseudo-Q_j-branch analogs; and (iii) the set of first-order phase-transition points that are the only GS space-structure characteristics changing on infinitesimal variations in $v(r)$.

To cover both Q_j branches and pseudo-Q_j branches by computation it is appropriate to introduce the totality of the various stripe superstructures that are mixtures of the stripes of two types, $\vec{d},\vec{f}_1$ stripes and $\vec{d},\vec{f}_2$ stripes, and to obey the algorithm (15) where $c_\pm$ is replaced by their concentration, c_1 or c_2 $(c_1+c_2=1)$. The $\vec{d},\vec{f}_{1,2}$ stripes have the same PTV, $\vec{d}$, but different vectors, $\vec{f}_1$ or $\vec{f}_2$, of relative displacement of particle lines forming them. According to the definition, a given superstructure of $\vec{d},\vec{f}_{1,2}$ stripes has the inverse filling factor

$$\vartheta=c_1Q^{(1)},+c_2Q^{(2)}, \tag{19}$$

where integer $Q^{(1,2)}=|\vec{d}\times\vec{f}_{1,2}|$ is the area of the parallelogram built on the vectors $\vec{d},\vec{f}_{1,2}$. Computing the energy of the superstructure as a function of *independent* variables, $\vec{d}$, $\vec{f}_{1,2}$, and ϑ, on the basis of expressions Eq. (1), Eqs. (15) ($c_\pm\rightarrow c_1$or c_2), Eq. (19), and finding its minimum with respect to $\vec{d}$, $\vec{f}_{1,2}$, at a fixed ϑ, one obtains both the GS space structure, including the S crystals ($c_{1,2}=0$ or 1) and the GS energy $E_g(\vartheta)$.

Generally, $\vec{d}$ has the form $\vec{d}=k\vec{a}$, where $\vec{a}$ is a PTV of the host lattice, $k=1,2,\ldots$. For fixed $Q^{(1,2)}$ and $\vec{d}$, there are only k different $\vec{d},\vec{f}_{1,2}$ stripes. Another simplification is that it is in fact sufficient to bound the moduli of $\vec{d}$ components by values $\lesssim\vartheta^{1/2}$, while the area difference, $|Q^{(1)}-Q^{(2)}|$, can be chosen to be $\leqslant 3$. As a result, the computation does not take a lot of time even for big ϑ. Here we have considered the range $3\leqslant\vartheta\leqslant 100$.

E. The case $\gamma\gg 1$

In the limit $\gamma\gg 1$ the mutual repulsion of IP/H's dominates their attraction to the dipole surroundings, disrupting the row of IP/H's (Sec. III) at sufficiently big $|\nu|$. Consequently, the defecton coalescence fails for any S crystal, and it is separated ± defectons that constitute the GS superstructure in vicinities of $\vartheta=Q_j$. However, the LOD and stripe formation take place in the case $\gamma\gg 1$, too. This becomes clear if one takes into account that the ± defectons ensemble at $|\vartheta-Q_j|\ll 1$ can be considered as 2D LSLRIR, whose particles are the defectons on the S crystal that plays the role of the host lattice. For such a system criterion (6) is fulfilled since the mean defecton separation is large (it is $\sim|\vartheta-Q_j|^{-1/2}$), and the energy of a defecton-defecton interaction decreases at big distances by the same law as $v(r)$.

V. DEVIL STAIRCASE

For a rational concentration of ± stripes, $c_\pm=M/L$ (M,L are coprime integers, $M<L$), the GS stripe pattern determined by algorithm (15) is a 1D crystal with a cell of length L and with M ± stripes (''particles'') per cell. Correspondingly, for each triple of the basic vectors $\vec{d}_\pm,\vec{f}_\pm,\vec{\xi}_\pm$ associated with a given S crystal (we omit the index j in this section) the GS configuration with $c_\pm=M/L$ is a 2D crystal (L,M crystal, for short) whose elementary cell can be built on vectors

$$\vec{d}_\pm \quad\text{and}\quad \vec{F}_{L,M}=L\vec{f}_\pm+M\vec{\xi}_\pm \tag{20}$$

and contains L particles, the ϑ value of the L,M crystal being equal to $Q\mp\sigma_\pm M/L$. Similar to the S crystal case, the elementary defects arising in any L,M crystal on an infinitesimal decrease or increase in ρ are *stripes* of rarefaction (R stripes) or compression (C stripes) which are of *different* structure. For this reason the energies of R,C-stripe formation, $\varepsilon^r_{L,M},\varepsilon^c_{L,M}$ are different in magnitude, and hence each L,M crystal represents the GS over some finite μ or P interval, $[\mu^r_{L,M},\mu^c_{L,M}]$ or $[P^r_{L,M},P^c_{L,M}]$, the end points $\mu^r_{L,M}$, $P^r_{L,M}$ and $\mu^c_{L,M}$, $P^c_{L,M}$ being determined by $\varepsilon^r_{L,M}$ and $\varepsilon^c_{L,M}$, respectively. In other words, the GS dependence of $c_\pm$ on μ, P, much the same as for 1D LSLRIR,[7–9] is inevitably a devil staircase whose steps occur at all *rational* $c_\pm$, the stripe patterns of the L,M crystals forming a fractal structure.

The lengths of the devil-staircase intervals, $\Delta\mu_{L,M}=\mu^c_{L,M}-\mu^r_{L,M}$ and $\Delta P_{L,M}=P^c_{L,M}-P^r_{L,M}$, are related by the simple equation

$$\Delta\mu_{L,M}=\vartheta\Delta P_{L,M}, \tag{21}$$

which is an evident consequence of the identity (4). As has been shown in the Appendix, they can be expressed in terms of $v(r)$ explicitly. In the Appendix we have also described the structure of R,C stripes. The net result for $\Delta\mu_{L,M}$ is as follows:

$$\Delta\mu_{L,M}=\frac{L\vartheta}{\sigma_\pm}\sum_{n=1}^{\infty}n[V^{ss}_{nM}(nL+1)-2V^{ss}_{nM}(nL)+V^{ss}_{nM}(nL-1)]. \tag{22}$$

The positivity of the second-order finite difference in square brackets is provided by the convexity of $V^{ss}_m(l)$ mentioned in Sec. IV B.

Expression (22) can be transformed, in view of Eq. (14), to a form which is more convenient for calculations,

$$\Delta\mu_{L,M}=\frac{L\vartheta}{\sigma_\pm}\sum_{n=1}^{\infty} n[V(n\vec{F}_{L,M}+\vec{\xi}_\pm) - 2V(n\vec{F}_{L,M})+V(n\vec{F}_{L,M}-\vec{\xi}_\pm)], \tag{23}$$

where

$$V(\vec{r})=\sum_{k=-\infty}^{\infty} v(|k\vec{d}_\pm+\vec{r}|)$$

is the energy of interaction between a particle located at a site $\vec{r}$ and the particle line with the PTV $\vec{d}_\pm$ going through the site $\vec{r}=0$.

Expression (23) is still further simplified in the above-mentioned special (but widespread) case $\vec{f}_\pm \| \vec{\xi}_\pm$, which admits description in terms of lines (16) as the 1D ''particles,''

$$\Delta\mu=\mathcal{L}\sum_{n=1}^{\infty} n[V^{ll}(\mathcal{L}n-1)-2V^{ll}(\mathcal{L}n)+V^{ll}(\mathcal{L}n+1)]. \tag{24}$$

Here $V^{ll}(s)=V(s\vec{\xi}_\pm)$ is the pair potential of the line-line interaction (s is a difference of ''coordinates'' of interacting lines), $\mathcal{L}=(Q/\sigma_\pm)L\mp M$ is the length of the lines' pattern period measured in units of $|\vec{\xi}_\pm|$. Expression (24) can also be obtained immediately from the 1D LSLRIR theory[8,9] by substitution $V^{ll}(s)$ for the 1D pair potential.

Expressions (22)–(24) hold for all $M<L$, $M\neq 0,L$. They show that ratios $L^{-1}\Delta\mu(M/L)$ with different L,M but comparable $|\vec{F}_{L,M}|$ have the same order of magnitude. Particularly, it follows herefrom that irrespective of the M value devil-staircase step widths $\Delta\mu(M/L)$ go to zero as $Ld^2vr/dr^2|_{r=L}$ when $L\to\infty$.

VI. EXAMPLES

Here we demonstrate the above general results with 2D LSLRIR on triangular and square host lattices.

A. Triangular host lattice

All triangular lattices that can be built on a triangular host lattice are necessarily S crystals. This follows from the fact that the *absolute* energy minimum of a system whose particles are free to move is realized just by a *triangular* lattice. Such S crystals are ''p,q crystals'' with PTV's $p\vec{a}_1+q\vec{a}_2$ and $p\vec{a}_2+q\vec{a}_3$ (p,q are arbitrary integers, $\vec{a}_{1,2,3}$ is a triple of triangular-host-lattice PTV's which are equal in the modulus and form an angle of 120° with each other). Correspondingly, their $\vartheta=p^2+q^2-pq$. Using the procedure discussed in Sec. IV D, we have found that all 0,q crystals belong to the same Q_j branch (the main branch), which covers the range $4\leqslant\vartheta<\infty$. Their S′ crystals are S crystals, too. They occur at $\vartheta=q(q+1)$ $(2\leqslant q<\infty)$ and have PTV's $q\vec{a}_\kappa$, $(q+1)\vec{a}_\lambda$ ($\kappa,\lambda=1,2,3$; $\kappa\neq\lambda$). The stripe structures (15) have the same PTV, $q\vec{a}_\kappa$, for all ϑ of the interval $[q(q-1),q(q+1)]$, their $\vec{\xi}_\pm$ being $\pm\vec{a}_\lambda$ ($\kappa\neq\lambda$).

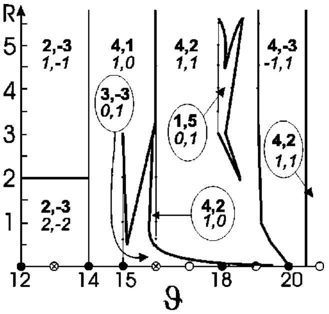

FIG. 3. The ground-state phase diagram for $v(r)=r^{-1}\exp(-r/R)$ on the ϑ,R plane $(12\leqslant\vartheta\leqslant 21)$. The symbols ● and ○ mean the same as in Fig. 2; the symbol ⊗ marks off the integer ϑ for which the GS is an S crystal only if R is not too small. The thin vertical line $\vartheta=14$ and the thin segments of the lines $\vartheta=15,16,18$ separate the regions with different directors and/or different $\vec{\xi}_\pm$ of the same Q_j branch. The lines of the first-order phase transitions are drawn boldly. The thin and bold lines together break up the whole R,ϑ region shown in the figure into subregions with their own directors and $\vec{\xi}_\pm$. The coordinates of the directors are boldfaced, those of $\vec{\xi}_\pm$ are in italic. Each director is also bound to be a PTV of one or another S crystal, namely, $(2,-3)=\mathrm{PTV}_{\vartheta=12}$; $(4,1)=\mathrm{PTV}_{\vartheta=14},\mathrm{PTV}_{\vartheta=15}$; $(3,-3)=\mathrm{PTV}_{\vartheta=15},\mathrm{PTV}_{\vartheta=18}$; $(4,2)=\mathrm{PTV}_{\vartheta=16},\mathrm{PTV}_{\vartheta=18}$; $(1,5)=\mathrm{PTV}_{\vartheta=18}$; $(4,-3)=\mathrm{PTV}_{\vartheta=20}$.

When both $p\neq 0$ and $q\neq 0$, Q_j branches of different p,q crystals are distinct. They do not have mutual intersections, but all intersect the main branch, the intersections occurring at rather small concentrations of the p,q-crystal ± stripes. In other words, the intervals of p,q-crystals stability ($p\neq 0$ and $q\neq 0$), and correspondingly, of main-branch metastability, turn out to be narrow.

The above classification of the triangular-host-lattice S crystals and Q_j branches is *universal* in the sense that it holds for any considered $v(r)$.

B. Square host lattice

This case is more complicated than the previous one since despite the fourfold symmetry the basic GS vector characteristics cannot be classified by a simple and general rule. For $\vartheta\leqslant 12$ the universality in the above sense takes place, i.e., the vector characteristics do not depend on $v(r)$. The GS structure over the universality region is shown in Fig. 2. For $\vartheta>12$ the universality fails. This is illustrated in Fig. 3 where the dependence of the GS vectors on the radius, R, of the screened Coulomb potential, $v(r)=\exp(-r/R)/r$, is presented for $12\leqslant\vartheta\leqslant 18$. With an increase in ϑ the phase diagram on the R,ϑ plane becomes more and more complicated. This suggests that in the limit $\vartheta\gg 1$ there exists an averaging procedure to reduce the description of the GS. This problem is beyond the scope of this paper.

VII. CONCLUSION

The above consideration shows that the particle ordering into stripes and the effective lowering of dimension reside in the 2D LSLRIR universally. It is a combination of the *discreteness* of particle positions with the long-range mutual particle repulsion and the *convexity* of $v(r)$ that is, in essence, the reason of the phenomenon. Extension of the above theory to disordered 2D LSLRIR leads to the conclusion that the coalescence of zero-dimensional defects and stripe formation caused by it take place in this case as well provided the disorder does not break a short-range order in the host lattice, the impurities or the host-lattice inhomogeneities only fracturing and pinning the stripes.

There are several fields of current interest wherein the 2D LSLRIR ground-state theory can find use.

(a) One field is research of charge stripes in high-temperature cuprate superconductors, which came to attention after being revealed with neutron scattering.[11] In the paper[11] this fact was interpreted in terms of the phase separation into an insulating region with an antiferromagnetic order and a metallic region with holes.[12] In our view, this is not the only way of how the charge stripes can occur: as follows from our present results, in 2D or layered narrow-band conductors *a long-range Coulomb interelectron or interhole repulsion* leads to stripe formation *by itself* if it gives rise to the FCCP mentioned in the Introduction. Since the criterion of FCCP existence given there is easily fulfilled in the cuprates (hole velocities in cuprates are less by an order of magnitude than Fermi velocities in the usual metals), taking into account the alternative, pure Coulomb, mechanism of stripe formation appears to be necessary in analyses of the experiments concerning the charge (hole) ordering into stripes.[13] The hole stripe superstructure of the Coulomb origin can manifest itself in the neutron experiments, affecting the antiferromagnetic spin order in cuprates. In this context it is noteworthy that direct studies of the La_2CuO_4 lattice carried out by the nuclear channeling[14] revealed a periodic stripelike superstructure of the oxygen atoms in Cu-O planes even at light doping.

(b) The effective lowering of dimension in a 2D FCCP is suggested to account for the interesting effect reported by Pepper,[4] which has not been explained to present. It lies in the fact that the resistivity of a conducting sheet that arises in a system metal – n-type GaAs – p-type GaAs at a certain combination of system parameters oscillates in the charge carrier density with a great amplitude, the oscillations minima occurring at *rational* ρ which are resolved in some simple series. There are strong reasons to suggest that the effect can be explained in a natural way in FCCP terms, taking into account a thermodynamic competition between the ± defectons and the thermally fractured ± stripes.

Recently we have shown that a FCCP can exist in polycrystalline nonlinear electroceramic materials (so-called posistors and varistors[3]). We expect that it is the above-mentioned interplay between FCCP defects of two topologically different types that underlies known, but as yet incomprehensible, conduction properties of nonlinear electroceramics.

(c) Interesting artificial systems to realize a conducting 2D LSLRIR are planar arrays of nanometer-size metal granules linked by organic molecule wires as tunnel junctions.[5,6] Such a 2D conductor differs from the FCCP in that there can be several electrons per granule. There are strong reasons to suggest that the above theory holds in this case, too, with a slight modification. Stripe formation caused by a mutual repulsion of electrons of different granules is anticipated to result in rather unconventional conduction in the granular systems. Particularly, due to charge arrangement into stripes the conductance of the granular film as a whole is expected to be highly sensitive with respect to a voltage *locally* applied.

We will discuss the issues mentioned in (a)–(c) in future papers, the immediate problem to study being the 2D LSLRIR low-temperature thermodynamics.

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APPENDIX A: THE LENGTHS OF THE DEVIL-STAIRCASE INTERVALS AND THE STRIPELIKE DEFECTS OF THE L,M CRYSTALS

It is somewhat more convenient to deal with $\Delta P_{L,M}$ than with $\Delta\mu_{L,M}$. To derive the expression for $\Delta P_{L,M}$ it is appropriate to consider what happens with a given L,M crystal as $N_s^\pm$ changes by a macroscopically small number, $\delta N_s^\pm$ $(|\delta N_s^\pm|/N_s^\pm \to 0, |\delta N_s^\pm| \to \infty)$, at a fixed $\mathcal{N}_s^\pm$, i.e., $|\delta N_s^\pm|$ ± stripes are removed from or added to the L,M crystal with adding or removing the same number of native stripes, respectively. In such a case the system volume changes by $\mp\,\delta N_s^\pm \sigma_\pm$ (per unit of stripe length) without a change in the number of the particles, and hence, the corresponding change in the ground-state energy, ΔE_g, has the form

$$\Delta E_g = \begin{cases} \Delta^c_\pm = \pm\,\delta N_s^\pm P^c_\pm \sigma_\pm & (\delta N_s^\pm = \pm\,\delta N_s,\ \text{rarefaction}) \\ \Delta^r_\pm = \pm\,\delta N_s^\pm P^r_\pm \sigma_\pm & (\delta N_s^\pm = \mp\,\delta N_s,\ \text{compression}), \end{cases} \tag{A1}$$

where $\delta N_s > 0$, so that $\Delta^c_\pm > 0$, $\Delta^r_\pm < 0$. Here and further on we drop the index L,M. The index ± at $P^{c,r}$ and other quantities relating to the L,M crystal is introduced to distinguish between the L,M crystals containing + stripes and those with − stripes.

As will be shown below, a change in $N_s^\pm$ by $\delta N_s^\pm = \pm\,\delta N_s$ or by $\delta N_s^\pm = \mp\,\delta N_s$ produces in the L,M crystal, C stripes, or R stripes, respectively, the number of C,R stripes being equal to

$$\delta N = L\,\delta N_s. \tag{A2}$$

Therefore,

$$\Delta^{c,r}_\pm = L\,\delta N_s \varepsilon^{c,r}_\pm$$

and

$$\sigma_\pm P^c_\pm = L\varepsilon^c_\pm, \quad -\sigma_\pm P^r_\pm = L\varepsilon^r_\pm. \tag{A3}$$

As is seen from the relation (A2) and expression (13a), $\varepsilon^{c,r}_\pm$ is the sum

$$\varepsilon^c_\pm = \varepsilon_\pm/L + \boldsymbol{\epsilon}^c_\pm > 0,$$

$$\varepsilon^r_\pm = -\varepsilon_\pm/L + \boldsymbol{\epsilon}^r_\pm < 0, \tag{A4}$$

where $\boldsymbol{\epsilon}^{r,c}_\pm$ is the change in H_{int} per R,C stripe.

From Eqs. (A3) and (A4) we obtain

$$\sigma_{\pm}\Delta P_{\pm}=L(\epsilon^{c}_{\pm}+\epsilon^{r}_{\pm}). \tag{A5}$$

Thus, the calculation of $\Delta P_{\pm}$ reduces to finding $\epsilon^{c,r}_{\pm}$. To do this we have to consider the perturbation of the L,M crystal stripe arrangement produced by the replacement $N_s^{\pm}\to N_s^{\pm}+\delta N_s^{\pm}$. Let it be, for definiteness, the L,M-crystal with $-$ stripes. As the $-$ stripe concentration changes by $\delta N_s^{-}/\mathcal{N}_s^{-}$, the algorithm (15) (with an accuracy of additions $\sim 1/N_s^2$) takes the form

$$l(m)=[mL/M-m/\mathcal{M}]=l^{(0)}(m)+\zeta(m), \tag{A6}$$

where $l_0(m)=[mL/M]$ describes the $-$ stripe arrangement in a L,M crystal,

$$\zeta(m)=[\{L/Mm\}-m/\mathcal{M}],$$

$\{\ldots\}$ is the fractional part of the number bracketed; $\mathcal{M}=MN_s^{-}/L\,\delta N_s^{-}$; in the macroscopical limit under consideration $|\mathcal{M}|\to\infty$ together with N_s^{-}. As is evident from Eq. (A6), it is the term $\zeta(m)$ that is responsible for the difference between the L,M crystal and that perturbed by the adding or removing of $-$ stripes.

First let δN_s^{-}, and hence $\mathcal{M}$, be negative (compression of the L,M crystal). Representing $m=0,1,\ldots,N_s^{-}$ in the form

$$m=kM+\tilde{m}$$

($k=0,1,\ldots$ enumerates the elementary cells of the L,M-crystal stripe pattern, $\tilde{m}=0,1,\ldots,M-1$ enumerates the $-$ stripes in a cell) and taking into account that $\{mL/M\}$ is a periodic function of m with the period M, we can write $\zeta(m)$ as

$$\zeta(m)=\zeta_k(\tilde{m})=[\{\tilde{m}L/M\}+\tilde{m}/|\mathcal{M}|+\phi_k], \tag{A7}$$

where

$$\phi_k=kM/|\mathcal{M}|.$$

As seen from this expression, $\zeta_k(\tilde{m})$ as a function of k changes for the first time as the phase ϕ_k, slowly increasing with an increase in k, becomes more than the greatest of the $\{\tilde{m}L/M\}$ values, namely, $(M-1)/M$. The second change happens as ϕ_k becomes more than the $\{\tilde{m}L/M\}$ value next to $(M-1)/M$, i.e., $(M-2)/M$, and so on. As the set of the $\{\tilde{m}L/M\}$ values consists of $0,1/M,\ldots,(M-1)/M$, a change in ϕ_k by 1 results in M changes of $\zeta_k(\tilde{m})$, i.e. $\zeta_k(\tilde{m})$ experiences altogether $L\,\delta N_s+\mathcal{O}(1)$ jumps as k runs from 0 to its greatest value, N_s^{-}/M. These occur at the points

$$k=k_1=K+\mathcal{O}(1),\quad k=k_2=2K+\mathcal{O}(1),\quad \ldots$$

($K=[\mathcal{M}/M^2]$) which are macroscopically far apart. Taking into account that $\tilde{m}/|\mathcal{M}|$ is negligible as compared with $\{\tilde{m}L/M\}$, we obtain from Eq. (A7)

$$\zeta_k\equiv 0,\quad k<k_1,$$

$$\zeta_k\equiv\zeta_{k_i}(\tilde{m}),\quad k_i\leqslant k<k_{i+1}\quad (i=1,2,\ldots). \tag{A8}$$

Here

$$\zeta_{k_1}(\tilde{m})=\delta_{\tilde{m}\tilde{m}_1},$$

$$\zeta_{k_2}(\tilde{m})=\delta_{\tilde{m}\tilde{m}_1}+\delta_{\tilde{m}\tilde{m}_2}, \tag{A9}$$

and so on. The quantity $\tilde{m}_i$ is the $\tilde{m}$ value for which $\{\tilde{m}L/M\}=1-i/M$ $(i=1,\ldots,M)$; δ_{ab} is the Kronecker delta.

Over the range $0\leqslant k<k_2$ the chain of expressions Eq. (A6)–Eq. (A9) is equivalent to the equation

$$l(m)=[mL/M+\theta(m-k_1M)/M], \tag{A10}$$

where $\theta(x)$ is the step function

$$\theta(x)=\begin{cases}1, & x\geqslant 0\\ 0, & x<0.\end{cases}$$

At the point $m_1=k_1M+\tilde{m}_1$ the function $\{mL/M\}+1/M$ equals zero, and hence, for $m\geqslant m_1$ we have $l(m)=l_0(m_1)+1+l_0(m-m_1)$, i.e., the mutual arrangement of $-$ stripes with $m>m_1$ remains unperturbed, coinciding with that for $0\leqslant m<k_1M$. Therefore, we have the following.

(i) The stripe pattern consisting of $\tilde{m}_1$ stripes with the numbers $k_1M,\ldots,k_1M+\tilde{m}_1$ and the native S-crystal stripes separating them is a *defect* of the L,M crystal of a discrete soliton type, the $-$ stripe positions in the defect being determined by the algorithm

$$l_m=\begin{cases}l_0(m), & k_1M\leqslant m\leqslant m_1-1\\ l_0(m_1)+1, & m=m_1.\end{cases}$$

(ii) For each jump of $\zeta_k(\tilde{m})$ there is a perturbation of the L,M crystal which is a L,M-crystal defect geometrically identical to that just described. It is clear that it is nothing but a *C stripe*.

(iii) The total number of C stripes produced by a decrease in N_s^{-} by $|\delta N_s^{-}|$ is really given by the expression (A2).

To find ϵ^{c}_{-} one can make use of the obvious fact that the replacement of $l_0(m)$ with $[mL/M+\varphi]$ (φ is an arbitrary constant) does not change the distances between $-$ stripes, resulting only in a cyclic permutation of $-$ stripes within each elementary cell of the L,M-crystal stripe pattern. Particularly, for $\varphi=1/M$ the cyclic permutation results from the shift of only *one* $-$ stripe per cell, its inner number, $\tilde{m}$ being equal to $\tilde{m}_1$, and its coordinate increasing by 1. Relating this fact to Eq. (A10), it is easy to conclude that the formation of one C stripe located, to say, in the elementary cell with $k=k_1$ increases (by one) only the distances between $-$ stripes with numbers $m=(k_1+n)M+\tilde{m}_1$ $(n=0,1,\ldots)$ and those with numbers $m=(k_1-n')M+\tilde{m}_1(n'=1,2,\ldots)$. In view of Eq. (13b) this gives for ϵ^{c}_{-} the expression:

$$\epsilon^{c}_{-}=\sum_{n=1}^{\infty}n[V^{ss}_{nM}(nL+1)-V^{ss}_{nM}(nL)]. \tag{A11}$$

The above argument can be applied for finding ϵ^{r}_{-} $(\delta N_s^{-}>0)$, too. To this end it is convenient to reverse the sign of m in Eq. (A6), replacing $-m/\mathcal{M}$ with $|m|/\mathcal{M}$ $(\mathcal{M}>0)$. By this means one can easily establish the space structure of R stripe. It is such that the R and C stripes adjacent to one another constitute an elementary cell of the L,M-crystal stripe pattern in which one $-$ stripe (with the inner number $\widetilde{m}_1$) is shifted by 1. Taking this into account and repeating the above calculations, we find

$$\epsilon_-^r=\sum_{n=1}^{\infty} n[V_{nM}^{ss}(nL-1)-V_{nM}^{ss}(nL)]. \tag{A12}$$

From Eqs. (A5), (A11), and (A12) we obtain finally

$$\Delta P_-=\frac{L}{\sigma_-}\sum_{n=1}^{\infty} n[V_{nM}^{ss}(nL+1)+V_{nM}^{ss}(nL-1)-2V_{nM}^{ss}(nL)]. \tag{A13}$$

This is equivalent to Eq. (22) due to Eq. (21).

The expression for ΔP_+ (the L,M crystal with + stripes) is derived just as it has been done for ΔP_-. The only thing that one has to bear in mind in this case is that the right-hand side of Eq. (A11) relates to ϵ_+^r, while ϵ_+^c is determined by the right-hand side of Eq. (A12).

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