

Coulomb disorder in periodic systems: Effect of unscreened charged impuritiesEdmond Orignac,^{1,*} Alberto Rosso,^{2,†} R. Chitra,^{3,‡} and Thierry Giamarchi^{4,§}¹*Laboratoire de physique théorique de l'École Normale Supérieure, CNRS UMR8549, 24, Rue Lhomond, 75231 Paris Cedex 05, France*²*Laboratoire de physique théorique et modèles statistiques, CNRS UMR8626, Bâtiment 100, Université Paris-Sud, 91405 Orsay Cedex, France*³*Laboratoire de physique théorique de la matière condensée, CNRS UMR7600, Université Pierre et Marie Curie, 4, Place Jussieu 75252 Paris Cedex 05, France*⁴*Université de Genève, DPMC, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*

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We study the effect of unscreened charged impurities on periodic systems. We show that the long-wavelength component of the disorder becomes long ranged and dominates static correlation functions. On the other hand, because of the statistical tilt symmetry, dynamical properties such as pinning remain unaffected. As a concrete example, we focus on the effect of Coulombian disorder generated by charged impurities on three-dimensional charge density waves with nonlocal elasticity. We calculate the x-ray intensity and find that it is identical to the one produced by thermal fluctuations in a disorder-free smectic-A phase. We discuss the consequences of these results for experiments.

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I. INTRODUCTION

The effect of quenched disorder on various condensed elastic systems is one of the fascinating problems in statistical mechanics. Examples of physical systems range from domain walls in magnetic and ferroelectric materials,^{1,2} contact lines of a liquid meniscus on a rough substrate,³ crack propagation,⁴ to vortex lattices in type-II superconductors,^{5,6} charge density waves (CDWs),^{7,8} and Wigner crystals.^{9–12} In these systems, the competition between elastic interactions which tend to impose some long-range order in the system and quenched disorder, leads to the formation of glassy phases. Two broad classes of elastic systems can be distinguished: random manifold systems such as domain walls, contact lines, and cracks, and periodic systems such as vortex lattices, charge density waves, and Wigner crystals. The latter are characterized by a long-range crystalline order in the absence of disorder and thermal fluctuations. For these systems, a crucial question is whether a weak disorder entirely destroys the crystalline order, or whether some remnants of the underlying periodic structure remain observable.

One of the earliest attempts to answer this question, was the pioneering work by Larkin¹³ on vortex lattices. Using a random-force model, he showed that due to the relevance of disorder in the renormalization group sense, long range order was entirely destroyed below four dimensions. Above four dimensions, long range order persists as disorder becomes irrelevant. A similar conclusion was reached by Sham and Patton for the case of a CDW with short-range elasticity,¹⁴ where, using an Imry-Ma approach,¹⁵ they concluded that long-range order was impossible in the presence of disorder below four dimensions. The problem of short-range disorder in periodic systems with short-ranged elasticity was reconsidered in Refs. 16–19. It was argued that the periodicity present in systems like CDWs and vortex lattices plays a pivotal role in determining the physics of the system in the presence of disorder. More precisely, it was shown that,

though the disorder is relevant below four dimensions, due to the underlying periodicity of the system a quasi-long-range order persisted for dimensions between 2 and 4. This is in stark contrast to the earlier results which predicted a total destruction of order. The resulting phase, nicknamed the Bragg glass phase, possesses both quasi-long-range order and metastability and glassy properties.^{18,19} It was further shown that the Bragg glass phase is stable to the formation of defects.^{19–22} Recent neutron scattering experiments on vortex lattices have furnished clear evidence for the existence of such a phase.²³

A complication arises in charged periodic systems due to the Coulomb repulsion, which renders the elasticity nonlocal.^{24–27} This nonlocal elasticity tends to rigidify the system, so that short-range-correlated disorder could be irrelevant in dimension smaller than 4.²⁸ For instance, within the random force model, the correlation function of the displacement in three dimensions displays a logarithmic growth indicating quasi-long-range order.^{24–26} In fact, when the periodic structure of the CDW is properly taken into account, the growth of the displacement correlation function is even weaker, increasing only as $\log[\log(r)]$ with the distance r .²⁹ A second complication arising from Coulomb interaction is that the disorder induced by charged impurities has long-range correlations. This type of disorder can exist in certain doped CDW materials³⁰ such as $K_{0.3}Mo_{1-x}V_xO_3$.

In this paper, we study the effect of the competition of the nonlocal elasticity produced by the Coulomb interaction with the long-range random potential resulting from the presence of charged impurities on the statics. The paper is organized as follows. In Sec. II, we introduce a decomposition of the Coulomb potential on the Fourier modes of the periodic structure. With this decomposition, we show that only the long-wavelength component of the random potential, i.e., forward scattering disorder, possesses long-range correlations. Using statistical tilt symmetry,³¹ we deduce that due to

the short-ranged nature of the backward scattering terms engendered by the disorder, the dynamical properties in the presence of charged impurities are not qualitatively different from those in the presence of neutral short-ranged impurities. In Sec. III, we consider the problem of the CDW system, and we derive the nonlocal elastic Hamiltonian. In Sec. IV, we derive the static displacement correlation functions and x-ray intensity of the CDW with charged impurities and we highlight the similitude of the latter to the x-ray intensity of smectic-A liquid crystals subjected to thermal fluctuations.³² In Sec. V, we discuss the experimental significance of our result and suggest that the smecticlike correlations should be observable in experiments on $K_{0.3}Mo_{1-x}V_xO_3$. Finally, we summarize the possible behavior of the static correlators in a pinned charge density wave according to the local or nonlocal character of elasticity and the presence or absence of charged impurities.

II. ELASTICITY AND DISORDER IN PERIODIC SYSTEMS

In this section, we discuss how Coulomb interactions affect elasticity and disorder in periodic systems. For a periodic elastic structure, the density can be written as

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot[\mathbf{r}-\mathbf{u}(\mathbf{r})]}, \quad (1)$$

where $\rho_0(\mathbf{r}) = \rho_0(1 - \nabla \cdot \mathbf{u})$ describes the density fluctuation arising from the long-wavelength deformation of the periodic structure and ρ_0 is the average density. In the second term, the vectors \mathbf{G} belong to the reciprocal lattice of the perfect periodic structure, and $\mathbf{u}(\mathbf{r})$ represents a slowly varying⁷² elastic deformation of the structure.¹⁹ The quantities $e^{i\mathbf{G}\cdot[\mathbf{r}-\mathbf{u}(\mathbf{r})]}$ describe fluctuations of the density on the scale of a lattice spacing. The low-energy physics of the periodic structure can be described in terms of a purely elastic Hamiltonian which has the generic form for isotropic systems

$$H_0 = \int_{\mathbf{r}} \frac{c}{2} (\nabla \mathbf{u})^2 \quad (2)$$

where c is the elastic coefficient and $\int_{\mathbf{r}}$ is a shorthand for $\int d^3\mathbf{r}$. This form can easily be generalized to anisotropic systems. Well-known examples of charged periodic structures are the Wigner crystal,^{9-11,33,34} charged colloidal crystals,³⁵ and charge density waves.³⁶⁻³⁸ In many charged systems, unscreened Coulomb interactions are present:

$$H_C = \frac{e^2}{8\pi\epsilon} \int_{\mathbf{r},\mathbf{r}'} \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \quad (3)$$

and strongly affect the elasticity and dispersion of the compression modes of the system. Moreover, in the presence of charged impurities, the original charge density on the lattice interacts with the charge impurity yielding:

$$H_{\text{dis}} = \frac{e^2}{4\pi\epsilon} \int_{\mathbf{r},\mathbf{r}'} \frac{\rho(\mathbf{r})\rho_{\text{imp}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \quad (4)$$

where ρ_{imp} denotes the impurity density. Using the decomposition of the density (1), we now show that the Coulomb

interactions fundamentally modify only the long-wavelength components of the elasticity and of the disorder energy.

To better handle the periodicity of the elastic structure, it is convenient to use the decomposition of the Coulomb interaction in terms of the reciprocal lattice vectors \mathbf{G} . In three dimensions, this decomposition reads

$$\frac{1}{4\pi|\mathbf{r}|} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2} = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} V_{\mathbf{G}}(\mathbf{r}) \quad (5)$$

where

$$V_{\mathbf{G}}(\mathbf{r}) = \int_{\text{BZ}} \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{(\mathbf{q} + \mathbf{G})^2}, \quad (6)$$

and \int_{BZ} indicates that the integral is restricted to the first Brillouin zone. It is straightforward to check that $V_{-\mathbf{G}}(\mathbf{r}) = V_{\mathbf{G}}^*(\mathbf{r})$. Using Eq. (5), the interaction term H_C can be rewritten as

$$H_C = \frac{e^2}{2\epsilon} \sum_{\mathbf{G} \neq 0} \int_{\mathbf{r},\mathbf{r}'} V_{\mathbf{G}}(\mathbf{r}-\mathbf{r}') e^{i\mathbf{G}\cdot[\mathbf{u}(\mathbf{r})-\mathbf{u}(\mathbf{r}')]} + \frac{e^2}{2\epsilon} \int_{\mathbf{r},\mathbf{r}'} V_0(\mathbf{r}-\mathbf{r}') \rho_0(\mathbf{r}) \rho_0(\mathbf{r}'). \quad (7)$$

Note that due to the slow variation of $\mathbf{u}(\mathbf{r})$, terms involving the oscillatory factors $e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}}$ can be dropped from the interaction. Let us first consider the term involving long-wavelength fluctuations of the density. Since we are interested only in the long-wavelength properties, we can replace the integration over the Brillouin zone in $V_0(\mathbf{r})$ by a Gaussian integration:

$$\int_{\text{BZ}} \frac{d^3\mathbf{q}}{(2\pi)^3} \rightarrow \int \frac{d^3\mathbf{q}}{(2\pi)^3} e^{-a^2\mathbf{q}^2}, \quad (8)$$

with the parameter a chosen so that $\pi/a \sim |\mathbf{G}_{\text{min}}|$, \mathbf{G}_{min} being the reciprocal lattice vector having the shortest length. In this case, $V_0(\mathbf{r})$ can be obtained indirectly by solving the Poisson equation with a Gaussian charge density and is found to be

$$V_0(\mathbf{r}) = \frac{1}{4\pi r} \text{erf}\left(\frac{r}{2a}\right). \quad (9)$$

In the limit $r \gg a$, we recover the known result $V_0 \sim 1/(4\pi r)$. Clearly, the nonoscillating component of the Coulomb potential remains long ranged and tends to rigidify the system.

It now remains to be seen whether the oscillating parts of the Coulomb interaction specified by $V_{\mathbf{G}}$ for \mathbf{G} are long ranged or not. We first note that the above trick of replacing the integration over the Brillouin zone by a Gaussian integral over the entire space is not applicable anymore, as it would introduce a spurious integration over a region where $\mathbf{G} + \mathbf{q} = \mathbf{0}$. This would result in an (incorrect) $1/r$ behavior of $V_{\mathbf{G} \neq 0}(r)$. To obtain a correct estimate for $V_{\mathbf{G}}$ we replace the integral over the Brillouin zone by

$$\int_{BZ} \frac{d^3 \mathbf{q}}{(2\pi)^3} \rightarrow \int \frac{d^3 \mathbf{q}}{(2\pi)^3} F_{BZ}(\mathbf{q}, \delta), \quad (10)$$

where $F_{BZ}(q, \delta)$ is an indefinitely derivable function with a compact support contained in the first Brillouin zone [see Appendix A for an explicit form of $F_{BZ}(q, \delta)$].⁷³ Obviously, for $\mathbf{G} \neq \mathbf{0}$, $F_{BZ}(q, \epsilon)/|\mathbf{q} + \mathbf{G}|^2$ is also an indefinitely differentiable function of compact support. A well-known theorem^{39,40} then shows that the Fourier transform of $F_{BZ}(q, \epsilon)/|\mathbf{q} + \mathbf{G}|^2$ is indefinitely differentiable and for $r \rightarrow \infty$ is $o(1/r^n)$ for any $n > 0$. This implies that the function $V_{\mathbf{G}}(r)$ is short ranged. Incorporating the above results in Eq. (7), we see that while the nonoscillating part of the Coulomb interaction modifies the long-wavelength behavior of the elasticity, rendering it nonlocal, the short-ranged nature of the oscillatory terms merely renormalizes the elastic coefficients. This is explicitly shown in Appendix B for the particular case of a CDW. The resulting nonlocal character of the elastic interactions modifies strongly the static and dynamic properties of the system.^{27,29,41,42}

To understand the nature of the interaction with the charged impurities, we use the above procedure to rewrite the random potential generated by the impurities as

$$U(\mathbf{r}) = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}} \rho_{\text{imp}}(\mathbf{q})}{\mathbf{q}^2},$$

$$= \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} U_{\mathbf{G}}(\mathbf{r}). \quad (11)$$

Using this in Eq. (4), the interaction of the system with the random potential is given by

$$H_{\text{dis}} = \frac{e^2}{\epsilon} \sum_{\mathbf{G} \neq \mathbf{0}} \int_{\mathbf{r}} U_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{G}\cdot\mathbf{u}(\mathbf{r})} + \frac{e^2}{\epsilon} \int_{\mathbf{r}} U_0(\mathbf{r}) \rho_0(\mathbf{r}). \quad (12)$$

In Eq. (12), the interaction of ρ_0 with the random potential U_0 is called forward scattering, and the terms containing $e^{i\mathbf{G}\cdot\mathbf{u}(\mathbf{r})}$ are called backward scattering. This nomenclature originates in the theory of electrons in one-dimensional (1D) random potential.⁴³ To calculate the disorder correlation functions, we consider the case of Gaussian distributed impurities where⁴⁴ $\overline{\rho_{\text{imp}}(\mathbf{G} + \mathbf{q}) \rho_{\text{imp}}(\mathbf{G}' + \mathbf{q}')} = (2\pi)^3 D \delta_{\mathbf{G}, -\mathbf{G}'} \delta(\mathbf{q} + \mathbf{q}')$, the parameter D measuring the disorder strength. Consequently, we find that for $\mathbf{G} \neq \mathbf{0}$

$$\overline{U_{\mathbf{G}}(\mathbf{r}) U_{-\mathbf{G}}(\mathbf{r}')} = D \int_{BZ} \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{(\mathbf{q} + \mathbf{G})^4}. \quad (13)$$

Using the same arguments as before, we infer that the correlations of $U_{\mathbf{G}}(\mathbf{r})$ are short ranged, as in the case of neutral impurities, for all \mathbf{G} except $\mathbf{G} = \mathbf{0}$. This implies that the backward scattering terms induced by disorder are short ranged and the treatment of these terms within the replica or the Martin-Siggia-Rose^{45,46} methods is identical to the case of neutral or screened impurities. However, the $\mathbf{G} = \mathbf{0}$ compo-

$$U_0(\mathbf{r}) = \int_{BZ} \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{\mathbf{q}^2} \rho_{\text{imp}}(\mathbf{q}), \quad (14)$$

manifests power law decay of the forward scattering correlations. This term however can be gauged out by the statistical tilt symmetry,³¹ and affects mainly the static properties of the periodic system. Typically, in periodic systems with both short-range disorder and local elasticity, the contribution of the forward scattering disorder can be neglected and it is the backward scattering that induces collective pinning and Bragg glass features like a quasi order in the static correlation functions. Here, we have shown that even in the case of long-range disorder, the backward scattering terms behave essentially like their short-ranged (neutral impurities) counterparts. However, the effect of the forward scattering terms on the correlation functions has to be studied carefully. In the next section, we show that in the case of charged impurities in a charge density wave system, the forward scattering term strongly modifies the static correlation. Finally, we remark that our decomposition of the elastic energy and the impurity potential is not exclusive to the Coulomb potential and is applicable to other long-range potentials. As a result, the conclusions of the present sections are expected to be valid for more general long-range potentials.

III. CHARGE DENSITY WAVES

In this section, we rederive the elastic Hamiltonian for a three-dimensional CDW with screened Coulomb interactions between the density fluctuations at zero temperature. We consider an incommensurate CDW, in which the electron density is modulated by a modulation vector Q incommensurate with the underlying crystal lattice. In this phase, the electron density has the following form:⁸

$$\rho(\mathbf{r}) = \rho_0 + \frac{\rho_0}{Q^2} \mathbf{Q} \cdot \nabla \phi(\mathbf{r}) + \rho_1 \cos[\mathbf{Q} \cdot \mathbf{r} + \phi(\mathbf{r})], \quad (15)$$

where ρ_0 is the average electronic density (see Appendix C for details). The second term in Eq. (15) is the long-wavelength density and corresponds to variations of the density over scales larger than Q^{-1} . The last oscillating term describes the sinusoidal deformation of the density at a scale of the order of Q^{-1} induced by the formation of the CDW with amplitude ρ_1 and phase ϕ .

In the absence of Coulomb interactions, the low energy properties of the CDW can be described by an effective Hamiltonian for phase fluctuations. For CDW aligned along the x axis, i.e., $\mathbf{Q} = Q\hat{x}$, this phase-only Hamiltonian reads⁴⁷⁻⁵⁰

$$H_0 = \frac{\hbar v_F n_c}{4\pi} \int_{\mathbf{r}} \left((\partial_x \phi)^2 + \frac{v_y^2}{v_x^2} (\partial_y \phi)^2 + \frac{v_z^2}{v_x^2} (\partial_z \phi)^2 \right), \quad (16)$$

where v_F is the Fermi velocity and n_c is the number of chains per unit surface that crosses a plane orthogonal to Q . The velocity of the phason excitations parallel to Q is $v_x = (m_e/m_*)^{1/2} v_F$ with m^* the effective mass of the CDW and m_e the mass of an electron. v_y and v_z denote the phason velocities in the transverse directions. A crucial observation

is that a deformation of $\phi(r)$ along Q produces an imbalance of the electronic charge density which then augments the electrostatic energy due to Coulomb repulsion between density fluctuations. We evaluate the contribution of Coulomb interactions screened beyond the characteristic length λ which accounts for the presence of free carriers. This length diverges in the limit $T \rightarrow 0$.^{51,52} The electrostatic energy takes the form:

$$H_C = \frac{e^2}{8\pi\epsilon} \int_{\mathbf{r}, \mathbf{r}'} e^{-|\mathbf{r}-\mathbf{r}'|/\lambda} \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \quad (17)$$

where we have assumed for simplicity an isotropic dielectric permittivity ϵ of the host medium.^{24,25,51,53,54} Due to the periodicity of the CDW system, we can use the decomposition of the Coulomb potential derived in Sec. II, obtaining

$$H_C = \frac{e^2 \rho_0^2}{8\pi\epsilon Q^2} \int_{\mathbf{r}, \mathbf{r}'} \partial_x \phi(\mathbf{r}) \frac{e^{-|\mathbf{r}-\mathbf{r}'|/\lambda}}{|\mathbf{r}-\mathbf{r}'|} \partial_x \phi(\mathbf{r}') + \frac{e^2 \rho_0^2}{2\epsilon} \int_{\mathbf{r}, \mathbf{r}'} [V_{-\mathbf{Q}}(\mathbf{r}-\mathbf{r}') e^{i[\phi(\mathbf{r})-\phi(\mathbf{r}')]} + \text{c.c.}]. \quad (18)$$

In Eq. (18), we have neglected the contribution of the higher harmonics of the CDW. Note that the oscillating terms, as discussed in Appendix B, only contribute to a renormalization of the coefficients in the short-range elastic Hamiltonian (16) and thus can be neglected. However, the contribution of the long-wavelength term has more dramatic effects and reads

$$H_C = \frac{e^2 \rho_0^2}{2\epsilon Q^2} \int_{BZ} \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{q_x^2}{\lambda^{-2} + q^2} |\phi(\mathbf{q})|^2. \quad (19)$$

It is interesting to note that Coulomb interactions generate a nonlocal elasticity, i.e., a q dispersion in the elastic constant.

The total Hamiltonian now reads

$$H_{\text{el.}} = H_0 + H_C = \frac{1}{2} \int \frac{d^3 \mathbf{q}}{(2\pi)^3} G^{-1}(\mathbf{q}) |\phi(\mathbf{q})|^2, \quad (20)$$

$$G^{-1}(\mathbf{q}) = \frac{n_c \hbar v_F}{2\pi} \left(\frac{q_x^2}{(q^2 + \lambda^{-2}) \xi^2} + q_x^2 + \frac{v_y^2}{v_x^2} q_y^2 + \frac{v_z^2}{v_x^2} q_z^2 \right)$$

where the length scale ξ is defined by

$$\xi^2 = \frac{n_c \hbar v_F}{2\pi e^2 \rho_0^2} Q^2 \epsilon. \quad (21)$$

Depending on the ratio λ/ξ , two regimes of behavior can be identified. (i) Short-ranged elasticity: when $\lambda/\xi \ll 1$ the Coulomb correction to the short-range elasticity is small even in the limit $q \rightarrow 0$ and hence can be neglected. (ii) Long-range elasticity: for $\lambda/\xi \gg 1$, the Coulomb correction to the short-range elasticity cannot be neglected. This regime is relevant at low temperatures, when the number of free carriers available to screen the Coulomb interaction is suppressed by the CDW gap.^{51,52} Mean field calculations show that this regime is obtained for temperatures $T < 0.2T_c$ where T_c is the Peierls transition temperature.⁵² In the following, we focus on regime (ii), and accordingly, we take $\lambda^{-1} = 0$ in Eq. (20).

IV. FORWARD SCATTERING

As discussed in Sec. I, the case of the short-ranged elasticity has been studied by various authors. For charged periodic systems with short-range disorder and a nonlocal elasticity generated by Coulomb interactions, it is known that the upper critical dimension is three for disorder and the displacement correlations grow as $B(r) = \log \log \Lambda r$.^{28,29} Here, we study the effect of the long-range disorder on the static correlations of a charged periodic system. Since, the backward scattering terms generated by such a disorder are short ranged, they lead to the same physics as that of short-ranged disorder with the corresponding nonlocal elasticity. These terms contribute a $\log \log r$ term to the displacement correlations. However, in this case a simple dimensional analysis shows that the forward scattering terms generate the leading contribution to the correlation functions. In the following, we calculate the contribution of the forward scattering disorder to the displacement correlation function in CDW.

A. Displacement correlation functions

The displacement correlation function is defined by

$$B(\mathbf{r}) = \overline{\langle [\phi(\mathbf{r}) - \phi(\mathbf{0})]^2 \rangle} = \frac{2}{L^6} \sum_{\mathbf{q}} \overline{\langle \phi(\mathbf{q}) \phi(-\mathbf{q}) \rangle} [1 - \cos \mathbf{q} \cdot \mathbf{r}]. \quad (22)$$

The calculation of the correlation induced by the forward scattering disorder is analogous to the calculation of Larkin for the random force model.¹³ Assuming an infinite screening length λ , the Hamiltonian reads:

$$H = H_{\text{el.}} + \frac{e^2}{4\pi\epsilon} \int_{\mathbf{r}, \mathbf{r}'} \frac{\rho_{\text{imp}}(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \quad (23)$$

Using Eq. (15) in Eq. (23), we obtain an expression of the form Eq. (12). Keeping only the forward scattering term we get

$$H = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \left(\frac{G^{-1}(\mathbf{q})}{2} |\phi(\mathbf{q})|^2 + \frac{i\rho_0 e^2 q_x}{Q\epsilon q^2} \rho_{\text{imp}}(-\mathbf{q}) \phi(\mathbf{q}) \right). \quad (24)$$

Shifting the field ϕ

$$\phi(\mathbf{q}) = \tilde{\phi}(\mathbf{q}) + \frac{e^2 \rho_0 i q_x G(\mathbf{q})}{Q\epsilon q^2} \rho_{\text{imp}}(\mathbf{q}), \quad (25)$$

brings the Hamiltonian (24) back to the form of Eq. (20). The average over disorder now yields

$$\begin{aligned} & \overline{\langle \phi(\mathbf{q}) \phi(-\mathbf{q}) \rangle} \\ &= \langle \tilde{\phi}(\mathbf{q}) \tilde{\phi}(-\mathbf{q}) \rangle + \frac{e^4 \rho_0^2 q_x^2 G(\mathbf{q})^2}{Q^2 \epsilon^2 q^4} \overline{\rho_{\text{imp}}(\mathbf{q}) \rho_{\text{imp}}(-\mathbf{q})} \\ &= L^3 \left(TG(\mathbf{q}) + \frac{e^4 \rho_0^2 q_x^2 G(\mathbf{q})^2}{Q^2 \epsilon^2 q^4} D \right) \end{aligned} \quad (26)$$

where $\langle \dots \rangle$ and $\overline{\dots}$ denote thermal average and disorder average, respectively. Equation (25) shows that even in the

presence of Coulombian disorder, the statistical tilt symmetry⁵⁵ is preserved. This implies that in the presence of backward scattering disorder, the forward scattering term can be gauged out by Eq. (25), and the contribution of the forward scattering disorder B^{FS} is simply added to the one obtained from the backward scattering disorder, B^{BS} .^{29,56} We conclude

$$B^{FS}(\mathbf{r}) = 2D \frac{e^4 \rho_0^2}{Q^2 \epsilon^2} \int \frac{d^3 q}{(2\pi)^3} \frac{q_x^2 G(\mathbf{q})^2}{q^4} [1 - \cos(\mathbf{q} \cdot \mathbf{r})]. \quad (27)$$

We want to evaluate this integral for the case of $v_y = v_z = v_\perp$. In the following we will use $q_\perp^2 = q_y^2 + q_z^2$. To obtain the asymptotic behavior of $B(\mathbf{r})$ for $r \rightarrow \infty$ we need to consider the $q \rightarrow 0$ limit of the integrand. The form of $G(\mathbf{q})$ suggests a scaling $q_x \sim q_\perp^2$ which then allows us to consider the integral

$$\begin{aligned} F(\mathbf{r}) &= \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{q_x^2}{[q_x^2 + (\xi' q_\perp^2)^2]} [1 - \cos(\mathbf{q} \cdot \mathbf{r})] \\ &= \frac{1}{16\pi \xi'} \left\{ \ln[1 + (\Lambda_\perp r_\perp)^2] + E_1\left(\frac{r_\perp^2}{4|x|\xi'}\right) + e^{-r_\perp^2/(4|x|\xi')} \right\}, \end{aligned} \quad (28)$$

where $\xi' = \xi v_\perp / v_x$, $r_\perp^2 = y^2 + z^2$ and Λ_\perp is a momentum cutoff. A study of the limits of this function for $r_\perp \rightarrow \infty$ and $|x| \rightarrow \infty$ shows that its asymptotic behavior is well described by

$$F(\mathbf{r}) \sim \frac{v_x}{16\pi v_\perp \xi} \ln\left(\frac{r_\perp^2 + 4(v_\perp |x| \xi / v_x)}{\Lambda_\perp^2}\right). \quad (29)$$

Therefore, we have for $r \rightarrow \infty$,

$$B^{FS}(\mathbf{r}) = \kappa \ln\left(\frac{r_\perp^2 + 4(v_\perp |x| \xi / v_x)}{\Lambda_\perp^2}\right). \quad (30)$$

where

$$\kappa = \frac{DQ^2 v_x}{16\pi \xi \rho_0^2 v_\perp}. \quad (31)$$

The full asymptotic correlation function is given by the sum of the forward scattering contribution, Eq. (30), and the backward scattering contribution given in Eq. (51) of Ref. 29 for the case of a short-range disorder and nonlocal elasticity:

$$B^{BS}(\mathbf{r}) = \log(\log\{\max[\Lambda|x|, (\Lambda r_\perp)^2]\}). \quad (32)$$

Obviously, the contribution of the backward scattering terms is subdominant and can be neglected.

B. Analogy with smectic-A crystals

We note that the result Eq. (29) can be obtained in the entirely different context of liquid crystals. If we consider a smectic-A liquid crystal, its elastic free energy reads⁵⁷⁻⁶⁰

$$\mathcal{F}_{el} = \int_{\mathbf{r}} \left(\frac{1}{2} B (\partial_z u)^2 + \frac{1}{2} k_{11} (\Delta_\perp u)^2 \right), \quad (33)$$

where u represents the displacement of the smectic layers, B is the compressibility, and k_{11} measures the bending energy

of the smectic layers. If we now assume a random compression force given by:

$$\mathcal{F}_{dis} = \int_{\mathbf{r}} \eta(\mathbf{r}) \partial_z u(\mathbf{r}), \quad (34)$$

$$\overline{\eta(\mathbf{r}) \eta(\mathbf{r}')} = D \delta(\mathbf{r} - \mathbf{r}'), \quad (35)$$

a straightforward calculation shows that the displacement correlation function $\overline{[u(\mathbf{r}) - u(\mathbf{0})]^2}$ is given by Eq. (29). Smectic-A crystals with disorder have been considered previously in Ref. 61 albeit with a different type of disorder coupling to $\nabla_\perp u$. This yields a displacement correlation function superficially similar to $F(\mathbf{r})$ with q_\perp^2 replacing q_x^2 in the numerator. The random compression force, which is not natural in the smectic-A context, is thus easily realized with charge density wave systems.

V. EXPERIMENTAL IMPLICATIONS

In the preceding sections, we have shown that the forward scattering terms generated by charged impurities lead to smecticlike order in a charge density wave material. A frequently used technique to characterize positional correlations in CDW systems is x-ray diffraction.⁶² In the present section, we provide a calculation of the x-ray intensity resulting from such a smecticlike order, and we provide a quantitative estimate of the exponent κ .

A. X-ray intensity

The intensity of the x-ray spectrum is given by⁶³

$$I(\mathbf{q}) = \frac{1}{L^3} \sum_{i,j} e^{-iq(R_i - R_j)} \langle f_i f_j e^{-iq(u_i - u_j)} \rangle. \quad (36)$$

u_i is the atom displacement from the equilibrium position R_i , f_i represents the total amplitude scattered by the atom at the position i and depends exclusively on the atom type. We consider the simple case of a disordered crystal, made of one kind of atom, characterized by the scattering factor $\bar{f} - \Delta f/2$, and containing impurities of scattering factor $\bar{f} + \Delta f/2$. Since we are interested in the behavior of the scattering intensity near a Bragg peak ($q \sim K$), we can use the continuum approximation.²⁹ In the case of the CDW, the lattice modulation is given by

$$u(\mathbf{r}) = \frac{u_0}{Q} \partial_x \{\cos[Qx + \phi(\mathbf{r})]\}. \quad (37)$$

It is well known that the presence of a CDW in the compound is associated with the appearance of two asymmetric satellites at positions $q \sim K \pm Q$ around each Bragg peak.⁶² The intensity profiles of these satellites give access to the structural properties of the CDW. For this reason a lot of work has been done to compute and measure these intensities.^{29,30,56,64,65} By expanding Eq. (36) for low $q(u_i - u_j)$, one finds an expression of the x-ray satellite intensity comprising a part I_d , which is symmetric under inversion around the Bragg vector K and a part I_a which is antisym-

metric under the same transformation.²⁹ The symmetric part is given by the following correlation function:

$$I_d(\mathbf{q}) = \bar{f}^2 q^2 \int_{\mathbf{r}} e^{-i\delta\mathbf{q}\cdot\mathbf{r}} \langle u(\mathbf{r}/2)u(-\mathbf{r}/2) \rangle, \quad (38)$$

and the antisymmetric part by

$$\frac{I_a(\mathbf{q})}{\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})} = 2q\Delta f \text{Im} \int_{\mathbf{r}} e^{-i\delta\mathbf{q}\cdot\mathbf{r}} \langle \rho_{\text{imp}}(\mathbf{r}/2)u(-\mathbf{r}/2) \rangle, \quad (39)$$

where $\delta q = (q-K) \sim Q$, and $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$ is the volume of the unit cell of the crystal. After some manipulations, Eq. (38) can be rewritten as

$$I_d(\mathbf{K} + \mathbf{Q} + \mathbf{k}) = u_0^2 \bar{f}^2 K^2 \int_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} C_d(\mathbf{r}),$$

$$I_a(\mathbf{K} + \mathbf{Q} + \mathbf{k}) = -\bar{f} K u_0 \Delta f \sqrt{\mathcal{N}D} \int_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} C_a(\mathbf{r}) \quad (40)$$

where \mathcal{N} is the number of impurities in the unit cell, and

$$C_d(\mathbf{r}) = \langle e^{i(\phi(\mathbf{r}/2) - \phi(-\mathbf{r}/2))} \rangle \quad (41)$$

$$= C_d^{\text{FS}}(\mathbf{r}) C_d^{\text{BS}}(\mathbf{r}), \quad (42)$$

$$C_a(\mathbf{r}) = \chi(\mathbf{r}) C_d(\mathbf{r}), \quad (43)$$

where $\chi(\mathbf{r})$ is defined by Eq. (33) of Ref. 29. It is easy to show, using this definition and the statistical tilt symmetry that $\chi(\mathbf{r})$ is independent of the forward scattering disorder. In Eq. (41), C_d^{BS} is the backward scattering contribution which has been obtained in Ref. 29, and C_d^{FS} is the forward scattering contribution, given by

$$C_d^{\text{FS}}(\mathbf{r}) = \left(\frac{\Lambda_{\perp}^{-2}}{r_{\perp}^2 + 4(v_{\perp}|x|\xi/v_x)} \right)^{\kappa}, \quad (44)$$

where we have used Eq. (30), assuming a Gaussian disorder. Using Eq. (32), one sees that the term C_d^{BS} gives only a logarithmic correction to Eq. (41). As a result, the symmetric structure factor I_d is dominated by the contribution of the forward scattering disorder. To obtain the structure factor, we Fourier transform Eq. (44) to obtain

$$I_d(\mathbf{q}) = \int d^2\mathbf{r}_{\perp} e^{i\mathbf{q}_{\perp}\cdot\mathbf{r}_{\perp}} \left(\frac{\Lambda_{\perp}^{-1}}{r_{\perp}} \right)^{2\kappa} \frac{r_{\perp}^2 v_x}{2\xi v_{\perp}} \times \int_0^{+\infty} \frac{du}{(1+u)^{\gamma}} \cos\left(\frac{|q_x| r_{\perp}^2 v_x}{4\xi v_{\perp}} u \right).$$

Using the relation

$$\int_0^{+\infty} \frac{du}{(1+u)^{\gamma}} \cos(\lambda u) = \frac{\lambda^{\gamma-1}}{\Gamma(\gamma)} \int_0^{+\infty} dv e^{-v\lambda} \frac{v^{\gamma}}{v^2+1} \quad (45)$$

we finally obtain

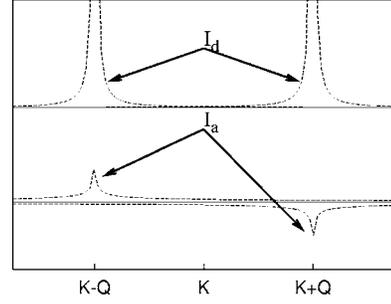


FIG. 1. A sketch of the x-ray intensity in a CDW with Coulomb elasticity and charged impurities for K, Q parallel to the chain direction. We have taken $\kappa=0.5$ in the expressions of I_a and I_d .

$$I_d(\mathbf{q}) = \frac{\pi(|q_x|\Lambda_{\perp}^{-1})^{\kappa-2}}{2^{2(\kappa-1)}\Gamma(\kappa)} \frac{\Lambda_{\perp}^{-\kappa-2}}{(\xi v_{\perp}/v_x)^{\kappa-1}} \times \int_0^{+\infty} dw \frac{w^{1-\kappa}}{w^2+1} e^{-w(\xi v_{\perp}/v_x)q_{\perp}^2/2|q_x|}, \quad (46)$$

so that $I_d(\mathbf{q}) \sim (|q_x|)^{\kappa-2}$ for $q_{\perp}^2(\xi v_{\perp}/v_x) \ll |q_x|$ and $I_d(\mathbf{q}) \sim (|q_{\perp}|)^{2(\kappa-2)}$ otherwise. The intensity $I_d(\mathbf{q}=0)$ is divergent for $\kappa < 2$ but is finite for $\kappa > 2$, i.e., for strong disorder. Next, we turn to the evaluation of I_a . From Ref. 29, we know that $\chi(\mathbf{r}) \sim 1/x$ when $x\xi \gg r_{\perp}^2$ and $\chi(\mathbf{r}) \sim 1/r_{\perp}^2$ when $|x| \xi \ll r_{\perp}^2$. This implies that I_a is subdominant in comparison with I_d . In particular, $I_a(\mathbf{q}) \sim (|q_x|)^{\kappa-1}$ for $q_{\perp}^2(\xi v_{\perp}/v_x) \ll |q_x|$ and $I_a(\mathbf{q}) \sim (|q_{\perp}|)^{2(\kappa-1)}$ otherwise. We illustrate the behavior of the x-ray intensities on Fig. 1.

We note that these intensities are remarkably similar to those of a disorder-free smectic-A liquid crystal³² at positive temperature. In fact, the expression of the exponent κ Eq. (31) is analogous to the expression (5.3.12) in Ref. 59, with the disorder strength D playing the role of the temperature $k_B T$ in the smectic-A liquid crystal.

B. Estimate of the exponent κ

Let us turn to an estimate of the exponent κ appearing in the intensities to determine whether such smecticlike intensities are indeed observable in experiments. To do this, we first need to determine whether Coulomb interactions are unscreened by comparing the screening length with ξ given by Eq. (21). This question is relevant only to a material with a full gap, in which free uncondensed electrons cannot screen charged impurities. A good candidate is the blue bronze material $K_{0.3}\text{MoO}_3$ which has a full gap, and is well characterized experimentally. We now evaluate the quantity ξ for this material. Using the parameters of Ref. 66:

$$n_c = 10^{20} \text{ chains/m}^2, \quad (47)$$

$$v_F = 1.3 \times 10^5 \text{ m s}^{-1}, \quad (48)$$

$$\rho_0 = 3 \times 10^{27} \text{ e}^{-}/\text{m}^3, \quad (49)$$

$$Q = 6 \times 10^9 \text{ m}^{-1}, \quad (50)$$

and a relative permittivity of $\epsilon_{K_{0.3}\text{MoO}_3} = 1$, so that ϵ in Eq. (21) is equal to the permittivity of the vacuum, we obtain ξ

TABLE I. The different cases with short-range and long-range random potential and elasticity. $\eta=1$ is the Bragg glass exponent (Ref. 68). κ is defined in Eq. (31).

Elasticity	Disorder	
	Short range	Long range
Local	$I_d(q) \sim q^{\eta-3}$	$I_d(q) \sim q^{-3}$
Nonlocal	Unphysical	$I_d(q_x) \sim q_x ^{\kappa-2}$ $I_d(q_\perp) \sim q_\perp ^{2(\kappa-2)}$

$\approx 5 \text{ \AA}$. Therefore, the screening length can be large compared to ξ at low temperature, and we expect that Coulombian effects will play an important role in this material. We can use this value of ξ to evaluate the exponent κ in Eq. (31). For the doped material $\text{K}_{0.3}\text{Mo}_{1-x}\text{V}_x\text{O}_3$, we find that the disorder strength can be expressed as a function of the doping and obtain

$$D = x(1-x) \frac{(\text{No. of Mo atoms/unit cell})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}. \quad (51)$$

This formula is derived in Appendix E. For the crystal parameters, $a=18.25 \text{ \AA}$, $b=7.56 \text{ \AA}$, $c=9.86 \text{ \AA}$, $\beta=117.53^\circ$,⁶⁷ with 20 molybdenum atoms per unit cell, and a doping $x=3\%$, the disorder strength $D=4.8 \times 10^{26} \text{ m}^{-3}$. Moreover, using the experimental bounds of the velocities, $3.6 \times 10^2 \text{ m s}^{-1} < v_\perp < 1.6 \times 10^3 \text{ m s}^{-1}$ and $v_x=3.7 \times 10^3 \text{ m s}^{-1}$, we find that κ is in the range 0.16–0.8. Therefore, the smecticlike order should be observable in x-ray diffraction measurements on this material.

VI. CONCLUSION

In this paper, we have introduced a decomposition of the disorder induced by charged impurities in terms of the reciprocal lattice vectors of a periodic charged elastic system. Using this decomposition, we have shown that only the long wavelength (forward scattering) component of the disorder was long-range correlated. Components with wave vectors commensurate with the reciprocal lattice of the periodic elastic system remain short ranged. The latter can thus be treated with the standard techniques developed for impurities producing short range forces.¹⁹ We find that only the forward scattering is affected by the long-range character of the forces created by charged impurities. Due to the statistical tilt symmetry, this implies that only the statics of the periodic elastic system is modified by Coulombian disorder. This has allowed us to obtain a full picture of the statics of three-dimensional charge density wave systems in the presence of charged and neutral impurities. The results are summarized in Table I. A remarkable result is that in the case of charged impurities in a system with unscreened Coulomb elasticity, the x-ray intensity turns out to be identical to that produced by thermal fluctuations in a smectic-A liquid crystal,³² with the disorder strength playing the role of an effective temperature. This behavior of the scattering intensity should be observable in the blue bronze material $\text{K}_{0.3}\text{MoO}_3$ doped with charged impurities such as vanadium.

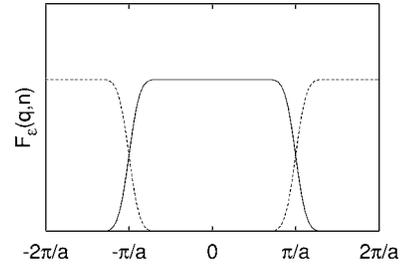


FIG. 2. The graph of the function $F_\delta(qa/\pi)$, of compact support for a value of $\delta=0.1$ (solid line). Dotted lines represent $F_\delta(qa/\pi \pm 2)$. We can graphically check the validity of Eq. (A3).

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APPENDIX A: DECOMPOSITION OF THE COULOMB POTENTIAL

In this appendix, we provide an explicit decomposition of the Coulomb potential using infinitely differentiable functions of compact support.⁶⁹ First, let us discuss a simple decomposition in 1D. We consider the function $F_\delta(x)$ (see Fig. 2) such that

$$F_\delta(x) = F_\delta(-x),$$

$$F_\delta(x) = \begin{cases} 1, & 0 \leq x \leq 1, \\ \frac{1}{2} \left[1 - \tanh\left(\frac{2(1-x)}{(x-1)^2 + \delta^2}\right) \right], & |x-1| < \delta, \\ 0, & x > 1 + \delta. \end{cases} \quad (A1)$$

It is easy to check that F_δ is continuous, infinitely differentiable, and that

$$\sum_{n=-\infty}^{\infty} F_\delta(x-2n) = 1. \quad (A2)$$

Applying this formula to a one-dimensional reciprocal space, we obtain

$$\sum_{n_x=-\infty}^{\infty} F_\delta\left(\frac{a}{\pi}\left(q - \frac{2\pi n}{a}\right)\right) = 1, \quad (A3)$$

i.e., we have constructed explicitly a partition of the unity.⁶⁹ The generalization to a cubic lattice in a three dimensional space is obvious:

$$\sum_{n_x, n_y, n_z=-\infty}^{\infty} F_{\delta}\left(\frac{a}{\pi}\left(q_x - \frac{2\pi n_x}{a}\right)\right) F_{\delta}\left(\frac{a}{\pi}\left(q_y - \frac{2\pi n_y}{a}\right)\right) \times F_{\delta}\left(\frac{a}{\pi}\left(q_z - \frac{2\pi n_z}{a}\right)\right) = \sum_{\mathbf{G}} F_{BZ}(\mathbf{q} - \mathbf{G}, \delta) = 1. \quad (\text{A4})$$

The function F_{δ}^{3D} has a compact support, and vanishes rapidly outside the Brillouin zone. Using this decomposition in Eq. (5) for fixed δ with δ sufficiently small, we avoid the oscillations induced by having a hard cutoff on the edge of the Brillouin zone.

APPENDIX B: CONTRIBUTION OF THE OSCILLATING COMPONENTS OF THE DENSITY TO THE ELASTIC HAMILTONIAN IN THE PRESENCE OF COULOMB INTERACTION

In this appendix, we calculate the contribution of the oscillating terms to the Hamiltonian of the charge density wave with unscreened Coulomb interactions, Eq. (17), and show that they only induce corrections to the short-range elasticity. Inserting the expression of the density, Eq. (15), in Eq. (7), the contribution of the oscillating component of wave vector Q is given by

$$H_C^{\text{osc}} = \frac{e^2 \rho_1^2}{2\epsilon} \sum_{\mathbf{n}, \mathbf{n}'} \int dx dx' V_Q(x - x', \mathbf{n} - \mathbf{n}') \times \cos[\phi(x, \mathbf{n}) - \phi(x', \mathbf{n}')], \quad (\text{B1})$$

where we have reestablished the discrete character of the transverse dimension \mathbf{y} . Both the intrachain ($\mathbf{n} = \mathbf{n}'$) and the interchain ($\mathbf{n} \neq \mathbf{n}'$) contributions are short ranged. Let us first consider the case of $\mathbf{n} \neq \mathbf{n}'$. We have to compute integrals

$$V_Q(x, \mathbf{n}) = \int \frac{d^3 q}{(2\pi)^3} F_{\delta}^{3D}(\mathbf{q}) \frac{e^{i(q_x x + \mathbf{q}_{\perp} \cdot \mathbf{n})}}{(Q + q_x)^2 + q_{\perp}^2}. \quad (\text{B2})$$

To evaluate the above integral in closed form, we need to make some approximations. Since F_{δ} vanishes for $Q + q_x = 0$, we can neglect q_x compared to Q in this integral. Then, we can extend the integration over the whole reciprocal space without encountering any singularity. The q_x integration produces a $\delta(x)$ function, and the q_{\perp} integration gives

$$V_Q(x, \mathbf{n}) = \frac{K_0(Q\sqrt{(n_y \ell_y)^2 + (n_z \ell_z)^2})}{2\pi} \delta(x), \quad (\text{B3})$$

where ℓ_y and ℓ_z are interchain spacings. Due to the exponential decay of the interchain interaction with the distance, it is justified to neglect interchain interactions beyond nearest neighbors. The logarithmic divergence in Eq. (B3) for $\mathbf{n} = \mathbf{0}$ is an artifact of the approximation we make when we integrate over the entire reciprocal space instead of the first Brillouin zone. A more refined estimate yields a finite, short-ranged intrachain contribution. The short range contribution in the electrostatic energy thus reads

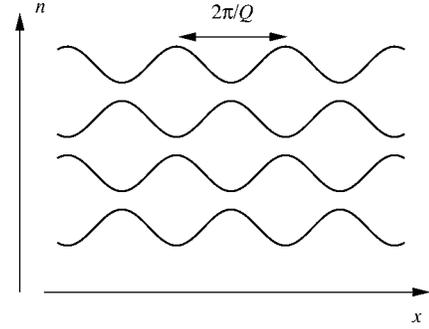


FIG. 3. The ground state of an array of CDWs coupled by a repulsive interaction.

$$H_C^{\text{osc}} = \sum_{\alpha=y,z} J_{\alpha} \int dx \sum_{\mathbf{n}} \cos[\phi(x, \mathbf{n} + \mathbf{e}_{\alpha}) - \phi(x, \mathbf{n})] + \sum_{\mathbf{n}} \int V_Q(x - x', 0) dx dx' \cos[\phi(x, \mathbf{n}) - \phi(x, \mathbf{n})], \quad (\text{B4})$$

where

$$J_{\alpha} = \frac{e^2 \rho_1^2}{2\pi\epsilon} K_0(Q\ell_{\alpha}). \quad (\text{B5})$$

In Eq. (B4), we expand $\cos[\phi(x, \mathbf{n}) - \phi(x', \mathbf{n})] \sim 1 - (x - x')^2 / 2 [\partial_x \phi(x, \mathbf{n})]^2$ to show that the backscattering term reduces to short-ranged elastic forces. Making $\phi(x, \mathbf{n}) = \bar{\phi}(x, \mathbf{n}) + n_y \pi + n_z \pi$, we can make the sign in front of J_{α} negative, and obtain the ground state for $\bar{\phi} = 0$. In its ground state, the CDW is out of phase on two nearest neighbor chains. This ground state is represented in Fig. 3. The excitations above this ground state are described by the Lagrangian (D3) derived in Appendix D.

APPENDIX C: ZERO-TEMPERATURE LIMIT OF THE CHARGE DENSITY IN A CDW

In the present appendix, we discuss the zero-temperature limit of the expression of the charge density in a CDW. Let us consider the form of the charge density in the presence of a nonuniform ϕ . It is given^{25,47,70,71} by the expression

$$\rho(\mathbf{r}) = \rho_0 + \frac{\rho_0 \bar{\rho}_c}{Q} \partial_x \phi(\mathbf{r}) + \rho_1 |\psi| \cos(Qx + \phi(\mathbf{r})) \quad (\text{C1})$$

where ρ_0 is the average electron density, ρ_1 is the condensate amplitude at $T=0$, $|\psi|$ takes into account the reduction of CDW order by thermal fluctuations ($|\psi|=1$ at $T=0$), the factor $\bar{\rho}_c$ takes into account the presence of noncondensed electrons⁷¹ at finite temperature (at $T=0$, $\bar{\rho}_c=1$) and $Q=2k_F$. Using the relation $k_F=(\pi/2)\rho_0$, valid in a one-dimensional system, one can see that this relation simplifies (at $T=0$) to

$$\delta\rho = \frac{\partial_x \phi}{\pi}. \quad (\text{C2})$$

The relation (C2) is well known in the bosonization treatment of one-dimensional interacting Fermi systems.⁴³ In the

paper, we consider temperatures very low compared to the Peierls transition temperature, and we take $|\psi|=1$, $\bar{\rho}_c=1$. This yields Eq. (15).

APPENDIX D: DERIVATION OF THE HAMILTONIAN OF A THREE-DIMENSIONAL CHARGE DENSITY WAVE

In this appendix, we provide a derivation of the Hamiltonian of a three dimensional CDW starting from the original Fukuyama one-dimensional description. The Lagrangian of a CDW in a single chain is given by⁴⁷

$$\mathcal{L} = \frac{\hbar v_F}{4\pi} \int dx \left(\frac{(\partial_t \phi)^2}{v_\phi^2} - (\partial_x \phi)^2 \right). \quad (\text{D1})$$

Obviously, this Lagrangian describes phason waves propagating with the velocity v_ϕ . v_F is the Fermi velocity of the electrons forming the CDW and ϕ is the phase of the CDW. We define an effective mass m^* by

$$\frac{v_F^2}{v_\phi^2} = \frac{m^*}{m_e} \quad (\text{D2})$$

where m_e is the electron mass.

In a three-dimensional CDW with screened Coulomb interactions, the chains are coupled by a backscattering interaction. The resulting Lagrangian reads

$$\begin{aligned} \mathcal{L} = & \frac{\hbar v_F}{4\pi} \sum_{\mathbf{n}} \int dx \left(\frac{(\partial_t \phi)^2}{v_\phi^2} - (\partial_x \phi)^2 \right) (x, \mathbf{n}) \\ & + \frac{1}{2} \sum_{\langle \mathbf{n}, \mathbf{n}' \rangle} J(\mathbf{n}, \mathbf{n}') \int dx \cos[\phi(x, \mathbf{n}) - \phi(x, \mathbf{n}')], \end{aligned} \quad (\text{D3})$$

where $J(\mathbf{n}, \mathbf{n}')$ is short ranged and is given by Eq. (B5). Expanding the cosines,

$$\begin{aligned} & \cos[\phi(x, \mathbf{n}) - \phi(x, \mathbf{n} + \mathbf{e}_y)] \\ & = 1 - \frac{[\phi(x, \mathbf{n}) - \phi(x, \mathbf{n} + \mathbf{e}_y)]}{2} + o(\nabla_y^2) \\ & = 1 - \frac{\ell_y^2}{2} (\partial_y \phi)^2 + o(\partial_y \phi)^2, \end{aligned} \quad (\text{D4})$$

and defining

$$\frac{\hbar v_F v_{y,z}}{4\pi v_\phi^2} = J_{y,z} \frac{\ell_{y,z}^2}{2}, \quad (\text{D5})$$

the Lagrangian in Eq. (D3) can be rewritten as²⁵

$$\mathcal{L} = \sum_{\mathbf{n}} \frac{\hbar v_F}{4\pi} \int dx \left(\frac{(\partial_t \phi)^2}{v_\phi^2} - (\partial_x \phi)^2 - \frac{v_y^2}{v_\phi^2} (\partial_y \phi)^2 - \frac{v_z^2}{v_\phi^2} (\partial_z \phi)^2 \right). \quad (\text{D6})$$

The sum over lattice sites in the transverse direction can be replaced by an integral, by writing

$$\mathcal{L} = \frac{\hbar v_F}{4\pi \ell_y \ell_z} \int_{\mathbf{r}} \left(\frac{(\partial_t \phi)^2}{v_\phi^2} - (\partial_x \phi)^2 - \frac{v_y^2}{v_\phi^2} (\partial_y \phi)^2 - \frac{v_z^2}{v_\phi^2} (\partial_z \phi)^2 \right). \quad (\text{D7})$$

The phason dispersion is now $\omega(\mathbf{q})^2 = v_\phi^2 q_x^2 + v_y^2 q_y^2 + v_z^2 q_z^2$. The momentum conjugate to ϕ is obtained by the usual relation

$$\Pi = \frac{\delta \mathcal{L}}{\delta(\partial_t \phi)} = \frac{\hbar v_F}{2\pi v_\phi^2 \ell_y \ell_z} \partial_t \phi, \quad (\text{D8})$$

yielding the Hamiltonian

$$\begin{aligned} H = & \frac{\hbar v_F}{4\pi \ell_y \ell_z} \int_{\mathbf{r}} \left(\frac{4\pi^2 v_\phi^2 (\ell_y \ell_z)^2}{\hbar^2 v_F^2} \Pi^2 + (\partial_x \phi)^2 \right. \\ & \left. + \frac{v_y^2}{v_\phi^2} (\partial_y \phi)^2 + \frac{v_z^2}{v_\phi^2} (\partial_z \phi)^2 \right). \end{aligned} \quad (\text{D9})$$

From the Hamiltonian Eq. (D9), it is straightforward to obtain the Debye-Waller factor associated with the zero-point fluctuations of the phase ϕ . In the isotropic case, $v_y=v_z=v_\phi$, one finds that $\langle \cos \phi(x) \rangle_{T=0} \sim e^{-C(m_e/m^*)^{1/2}}$, where $C \sim \pi/4$ is a dimensionless constant of order 1. Due to the smallness of the ratio $m_e/m^* \sim 10^{-2}$, the zero-point motion can be neglected, and the kinetic term $\propto \Pi^2$ in Eq. (D9) can be dropped. This leads to the Hamiltonian (16).

APPENDIX E: ESTIMATION OF THE DISORDER STRENGTH

Here, we give an estimation of the disorder strength D in doped $\text{KM}0_{1-x}\text{V}_x\text{O}_3$. We assume a binomial distribution of vanadium impurities on the molybdenum sites. The vanadium impurities carry an extra electron compared to the molybdenum ions. The resulting charge density fluctuation reads

$$\delta\rho(\mathbf{r}) = \sum_{i,\alpha} (x - \sigma_{i,\alpha}) \delta(\mathbf{r} - \mathbf{R}_{i,\alpha}), \quad (\text{E1})$$

where i is the index of the cell and α is the index of the molybdenum site in a given cell. $\sigma_{i,\alpha}=0$ if the site is occupied by a molybdenum ion, and $\sigma_{i,\alpha}=1$ if it is occupied by a vanadium impurity. By construction, the expectation value of $\delta\rho(\mathbf{r})$ is zero. We estimate the second moment of $\delta\rho(\mathbf{r})$ as

$$\begin{aligned} \overline{\delta\rho(\mathbf{r}) \delta\rho(\mathbf{r}')} & = \sum_{i,j,\alpha,\beta} \overline{(x - \sigma_{i,\alpha})(x - \sigma_{j,\beta})} \delta(\mathbf{r} - \mathbf{R}_{i,\alpha}) \delta(\mathbf{r}' - \mathbf{R}_{j,\beta}) \\ & = x(1-x) \sum_{i,\alpha} \delta(\mathbf{r} - \mathbf{R}_{i,\alpha}) \delta(\mathbf{r}' - \mathbf{r}), \end{aligned} \quad (\text{E2})$$

where we have used the property that $\overline{(x - \sigma_{i,\alpha})(x - \sigma_{j,\beta})} = \delta_{i,j} \delta_{\alpha,\beta} \overline{(x - \sigma_{j,\beta})^2}$. The expectation value of $\sum_{i,\alpha} \delta(\mathbf{r} - \mathbf{R}_{i,\alpha})$ is simply the number of molybdenum ions per unit volume, leading to the formula Eq. (51).

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