The essential role of surface pinning in the dynamics of charge density waves submitted to external dc fields

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Abstract. A charge density wave (CDW) submitted to an electric field displays a strong shear deformation because of pinning at the lateral surfaces of the sample. This CDW transverse pinning was recently observed but has received little attention from a theoretical point of view until now despite important consequences on electrical conductivity properties. Here, we provide a description of this phenomenon by considering a CDW submitted to an external dc electric field and constrained by boundary conditions including both longitudinal pinning due to electrical contacts and transverse surface pinning. A simple formula for the CDW phase is obtained in 3D by using the Green function and image charges method. In addition, an analytical expression of the threshold field dependence on both length and sample cross-section is obtained by considering the phase slip process. We show that the experimental data are well reproduced with this model and that bulk pinning can be neglected. This study shows that the dynamical properties of CDW systems could be mainly driven by boundary effects, despite the comparatively huge sample volumes.

1 Introduction

When a sufficiently large electrical current is applied to a charge density wave (CDW) system, a non-linear current may be induced [1,2]. This current has a periodic structure both in time [3] and space [4,5] and is believed to be due to a collective transport of charge based on a traveling periodic array of topological $2\pi$ solitons [6]. The CDW can be described as an elastic medium evolving under the application of an external electric field [7]. When this field exceeds a threshold value $E_{th}$, the CDW periodicity is broken and a soliton is created reducing the total elastic energy. This phase-slip mechanism [8,9] has been widely discussed in the literature as a thermally activated nucleation [10,11] or as a quantum process [12,13].

The sliding CDW phenomenon was extensively studied as a function of temperature [14], under a continuous laser photo-illumination [15] or as a depinning process induced by a short laser pulse excitation [16]. In all these phenomena, CDW pinning plays a fundamental role. The aim of this paper is to theoretically treat pinning effects as a whole including pinning at lateral surfaces when the CDW is submitted to an applied field and the incidence of this pinning on the threshold electric field $E_{th}$ as a function of sample dimensions.

There are two types of pinning at the sample boundaries. Longitudinal pinning due to the two electrical contacts along the CDW wavevector $2k_F$ has been observed by several techniques. At the contact position, the CDW phase is constant as a function of external current. Resistivity measurements show that the threshold field diverges with decreasing sample lengths in NbSe$_3$ [17,18] and in TaS$_3$ [19]. On the other hand, the consequence of longitudinal pinning under current leads to CDW compression/expansion in the vicinity of the two contacts as reported by X-ray diffraction [20,21] and transport measurements [22].

However, longitudinal pinning is not the only constraint applied to the CDW. Resistivity measurements have shown that transverse pinning at lateral sample surfaces may also play an important role since the threshold field $E_{th}$ diverges with decreasing sample cross sections in NbSe$_3$ [18,23] and in TaS$_3$ [24]. In a recent paper [25], transverse pinning was indeed observed at the local scale by scanning X-ray microdiffraction in NbSe$_3$. The CDW displays a large and continuous transverse deformation over an impressively large distance, spanning from one lateral surface to the other. This represents several tens of micrometers, which is 4 orders of magnitude larger than the CDW wavelength.

From a theoretical point of view, the threshold field $E_{th}$ has been mainly estimated by considering 1D models and the distance $L_x$ between the two electrical contacts. Feinberg and Friedel [7] proposed a phenomenological relation between $E_{th}$ and $L_x$ by considering CDW bulk impurity pinning. On the other hand, Batistic et al. [26]...
computed $E_{th}$ by considering longitudinal pinning and found a power law dependence $E_{th} \approx 2.55L_x^{-\alpha}$ where $\alpha = 1.23 \pm 0.05$. In this 1D model, $E_{th}$ drops to 0 for large $L_x$ in contradiction with experiments showing that $E_{th}$ converges to finite values [17]. We will show in the following that taking into account lateral surface pinning naturally leads to convergence towards finite threshold.

On the other hand, Borodin et al. [24] considered the effect of the sample cross-section and found a power law behavior $E_{th} \propto A^{-1/2}$ with $A = L_y \times L_z$.

In this article, we calculate $E_{th}(L_x, L_y, L_z)$ by taking into account both longitudinal and transverse pinning in the known 3D free energy [12, 27] by considering the phase-slip process and using the Green function and image charges methods.

2 Behavior of a CDW under electric field with contact and surface pinning

2.1 CDW phase equation, Green function, and image charges method

A CDW is described through its periodic charge modulation $\rho(r) = A(r) \cos(2k_F x + \phi(r))$ where $A(r)$ and $\phi(r)$ are respectively the CDW amplitude and phase with spatial dependence. In this paper, we only consider the evolution of $\phi$ under an applied electric field with component $E$ along the $x$ direction. The CDW behavior can be described by the following free energy considering only the phase variations:

$$\mathcal{F} = \int d^3r \left\{ C^{ij} \partial_i \phi_j + V_{imp}(\phi) - \eta E x \phi_x \right\}$$

$$\phi_i = \partial_i \phi, \quad \mathbf{r} \in \Omega \equiv \left\{ \mathbf{r} \in \mathbb{R}^3 | |\mathbf{r}| \leq L_i/2 \right\}$$

where $i, j = x, y, z$, $C^{ij} = c_xc_y \delta^{ij}$ with $c_x, c_y, c_z$ being the CDW longitudinal and transverse elastic coefficients, $L_x$ is the contact distance, $L_y$ and $L_z$ are the transverse sample lengths. We choose to consider a bulk impurity pinning potential $V_{imp}(\phi) = \omega_0^2 [1 - \cos(\phi)]$ with the pinning frequency $\omega_0$ often used in the literature [28, 29]. We will show in the following that this term can be neglected compared to the surface pinning effect. Finally, the last term corresponds to the interaction between the CDW and the applied electric field coupling the longitudinal gradient $\partial_x$ and the applied electric potential $E x$ where $\eta$ is a temperature dependent coupling coefficient [27].

While a randomly distributed bulk impurity pinning can break the CDW long range order [28, 30] X-ray diffraction experiment in NbSe$_3$ [25] showed a continuous CDW deformation over tens of micrometers. Furthermore, as measured in another X-ray diffraction experiment [20], the CDW wavevector variations are less than $0.25 \times 10^{-4} b^*$ below $E_{th}$, hence one can consider $\phi \ll 2\pi$ in the following and use a Taylor development of $V_{imp}(\phi) \approx \omega_0^2 \phi^2$. Above $E_{th}$, $2\pi$ solitons nucleate at the electrical contact, hence the phase solution is only correct in the linear current regime below $E_{th}$, which is the regime considered here.

Minimizing $\mathcal{F}[\phi]$ with the Euler Lagrange equation $\partial_i \partial^i \phi_x - \partial_x \phi = 0$ we obtain:

$$2 \left( c_x^2 \phi_{xx} + c_y^2 \phi_{yy} + c_z^2 \phi_{zz} \right) - \omega_0^2 \phi \approx \eta E. \quad (2)$$

The CDW longitudinal pinning at the two electrical contacts is taken into account by setting the phase at zero at $x = \pm \frac{L_x}{2}$ [7]. In addition, the transverse pinning observed in [25] is included in the model by considering boundary conditions at the lateral surfaces $y = \pm \frac{L_y}{2}$ and $z = \pm \frac{L_z}{2}$. The two types of pinning leads to the following constraints:

$$\phi(\mathbf{r}) = 0, \quad \forall \mathbf{r} \in \partial \Omega.$$ \hspace{1cm} (3)

By rescaling $x_j = c_j \sqrt{\frac{2}{3}} x_j'$, $L_j = c_j \sqrt{\frac{2}{3}} L_j'$ and $\omega^2 = c_x^2$, the phase equation (Eq. (2)) and the boundary conditions (Eq. (3)) become:

$$(\Delta' - \omega^2) \phi = E \quad (4)$$

with the Dirichlet conditions:

$$\phi(\mathbf{r}') = 0, \quad \forall \mathbf{r}' \in \partial \Omega'$$ \hspace{1cm} (5)

where $\Delta' = \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2}$ is the rescaled Laplacian operator.

Equation (4) is the screened Poisson equation that satisfies the uniqueness theorem as shown in Appendix B. Therefore, a solution to this differential equation can be computed by using the Green function and image charge method [31]. This technique is well established to solve electrostatic problems with boundary conditions. In our case, the source term is $+E$ inside the sample volume. The Green function satisfying the equation $(\Delta - \omega^2) G(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$ has a simple Lorentzian expression in Fourier space:

$$G(\mathbf{q}) = \frac{-1}{|\mathbf{q}|^2 + \omega^2}.$$ \hspace{1cm} (6)

There is no simple analytic solution fulfilling equation (4) with the boundary conditions (Eq. (5)) in 2D and 3D. We will show later that its resolution requires the use of the Green function and image charges method. As a first step, we describe the image charge construction in 1D before generalizing the procedure to the 2D and 3D cases.

2.2 The CDW phase in 1D, 2D, and 3D pinned by contacts and lateral surfaces

Equation (4) in 1D with $\phi \left( \pm \frac{L_x}{2} \right) = 0$ has an analytical solution:

$$\phi_{ana}(x') = \frac{E}{\omega^2} \left[ \cosh \left( x' \omega \right) - 1 \right].$$ \hspace{1cm} (7)
The final expression of the 2D CDW phase with contact and transverse surface pinning is the construction of the image charge density in 2D that is similar to the procedure used in 1D and is described in Appendix C. The phase solution from the Green function and image charge method reads:

\[
\phi(x') = -\frac{4E}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n \cos \left(\frac{(2n+1)\pi x'}{L_x'}\right)}{(2n+1)\left\{\left[\frac{(2n+1)\pi x'}{L_x'}\right]^2 + \omega^2\right\}}. \tag{8}
\]

This infinite sum converges quickly with \(n\), decreasing as \(\frac{1}{n^2}\). The contribution of the first term \((n = 0)\) and the first 100 terms \((n = 0 \text{ to } 99)\) is shown in Figure 1 and compared to the exact analytic expression (Eq. (7)). Note that equations (7) and (8) start to differ outside the sample boundary \(-\frac{L_x'}{2} < x' < \frac{L_x'}{2}\), which is not surprising since the two solutions have been defined to be valid in the sample limits.

The construction of the image charge density in 2D is similar to the procedure used in 1D and is described in Appendix C. The final expression of the 2D CDW phase with contact and transverse surface pinning is the following:

\[
\phi(x', y') = -\frac{16E}{\pi^2} \sum_{n_x, n_y=0}^{\infty} \frac{(-1)^{n_x+n_y}}{(2n_x+1)(2n_y+1)} \cos \left[\frac{(2n_x+1)\pi x'}{L_x'}\right] \cos \left[\frac{(2n_y+1)\pi y'}{L_y'}\right] \times \frac{1}{\left[\frac{(2n_x+1)\pi x'}{L_x'}\right]^2 + \left[\frac{(2n_y+1)\pi y'}{L_y'}\right]^2 + \omega^2}. \tag{9}
\]

This 2D CDW phase is shown in Figure 3b where we can observe a compression and a dilatation of the CDW period at the two electrical contacts induced by contact pinning. Furthermore, transverse surface pinning induces a shear effect with a curvature of the CDW wave fronts in the middle of the sample.

Note that the shear is strong when the compression–dilatation is weak and conversely, the curvature is almost zero when the compression and the dilatation are large as can be observed in Figures 2b and 2c. This feature is illustrated in Figure 3a where the transverse phase derivative \(\phi_{y'}\) is displayed as a function of the longitudinal phase derivative \(\phi_{x'}\). To get this figure, \(\phi_{x'}\) and \(\phi_{y'}\) have been calculated at each point \((x', y')\) in Figures 2b and 2c, and plotted as a 2D graph. From this graph and the 2D phase derivatives represented in Figures 2b and 2c, we observe that \(\phi_{y'}\) can be large only at positions where \(\phi_{x'}\) is low. This phenomenon is in agreement with X-ray diffraction experiments showing that the shear is ten times larger than the longitudinal dilatation–compression in the central part of the sample [25] and that the longitudinal deformation is largely close to the contacts [20,21]. In Figures 3c and 3d, we compare the calculated CDW shear in the middle part of the sample with the one measured in [25].

As detailed in Appendix A, the phase slip-process occurs at a given threshold field \(E_{th}\) when the strain along \(x\) \((\epsilon_{xx} = \frac{\partial \phi}{\partial x})\) exceeds a threshold value. The partial derivative \(\phi_{x'}\) is displayed in Figure 2b showing that the longitudinal strain is largely near the contact as observed by several experiments [20–22]. Moreover, the longitudinal
term only is a good approximation in the case $\frac{L_x}{c_x} \sim \frac{L_y}{c_y} \sim \frac{L_z}{c_z}$ and $\omega_0 \ll 1$ (see the 1D case in Fig. 1).

3 The threshold electric field $E_{th}$

3.1 $E_{th}$ as a function of electrical contact distance

As described in Appendix A, a soliton nucleates spontaneously whenever $\phi_x$ exceeds a threshold value $\phi'_c$. Therefore, the threshold electric field $E_{th}$ is defined by:

$$\phi_x \left( \frac{L_x}{2}, 0, 0; E_{th} \right) = \phi'_c. \quad (11)$$

Taking into account the derivative of $\phi(x', y', z')$ in 3D (Eq. (D.1) in Appendix D) where the longitudinal strain is maximum at $(x', y', z') = \left( \frac{L_x}{2}, 0, 0 \right)$. Making the reverse change of variable (Eqs. (4) and (5)) and using the following relation:

$$\sum_{n_x=0}^{\infty} \frac{1}{(2n_x + 1)^2 + a^2} = \frac{\pi}{4a} \tanh \left( \frac{\pi a}{2} \right), \quad (12)$$

we obtain the threshold field $E_{th}$ versus the sample dimensions $L_x$, $L_y$, $L_z$, and the bulk impurity pinning $\omega_0$:

$$E_{th} = \frac{\phi'_c \pi a c^2_x}{8\eta L_x} \sum_{n_y,n_z=0}^{\infty} \frac{(-1)^{n_y+n_z}}{(2n_y+1)(2n_z+1)\pi n_y n_z} \tanh \left( \frac{\pi n_y, n_z}{2} \right), \quad (13)$$

where we defined for ease of notation:

$$a_{n_y,n_z} = \frac{L_x}{c_x} \left( \left( \frac{2n_y + 1}{c_y} \right)^2 + \left( \frac{2n_z + 1}{c_z} \right)^2 \right)^{1/2} \quad (14)$$

Since $a_{n_y,n_z}$ is proportional to $L_x$, one can easily find the two limits. For small electrical contact distances $L_x \rightarrow 0$, using $\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} = \frac{\pi}{4}$ we find

$$\lim_{L_x \ll \gamma} E_{th} = \frac{4\phi'_c^2 c_x}{\pi} \frac{1}{L_x},$$

where

$$\gamma = \sqrt{\left( \frac{c_x}{\pi} \right)^2 + \left( \frac{c_y}{\pi} \right)^2 + \left( \frac{c_z}{\pi} \right)^2}.$$  

In this case, the threshold diverges as $1/L_x$ in agreement with the experiments as we will see later. On the contrary,
the threshold for longer samples:

\[
\lim_{L_x \gg \gamma} E_{th} = \frac{\phi_s^2 \pi^3 c_x}{8 \eta} \frac{1}{S(L_y, L_z)}
\]

with

\[
S(L_y, L_z) = \sum_{n_y, n_z=0}^{+\infty} \frac{(-1)^{n_y+n_z}}{(2n_y+1)(2n_z+1)} \times \frac{1}{\sqrt{\left[(2n_y + 1) \frac{x}{L_y}\right]^2 + \left[(2n_z + 1) \frac{z}{L_z}\right]^2 + \left(\frac{\pi}{2}\right)^2}}
\]

does not depend on \(L_x\) anymore. The threshold remains constant above a given contact distance even if \(\omega_0 = 0\). This last point is crucial, because it shows that the experimentally observed saturation of \(E_{th}\) is naturally reproduced by considering only surface and contact pinning, with no need of bulk pinning.

Equation (13) has been used to fit several transport measurements reporting the dependence of \(E_{th}\) on sample length in NbSe\(_3\) and TaS\(_3\) [17,19,32]. Equation (13) contains six free parameters \((c_x, c_y, c_z, \omega_0, \eta, \phi')\) assuming the crystal dimensions \((L_x, L_y, L_z)\) are known. Nevertheless, this too large number of free parameters can be significantly reduced to the four following parameters:

\[
\begin{align*}
    p_1 &= \frac{\phi_s^2 \pi^3 c_x}{8 \eta} \\
    p_2 &= \frac{L_y c_x}{\omega_0} \\
    p_3 &= \frac{L_z c_x}{\omega_0} \\
    p_4 &= \frac{\sqrt{2\pi} c_x}{\omega_0}
\end{align*}
\]

The expression of \(E_{th}\) with those parameters is given in Appendix E.

This number can be again reduced by making several assumptions. Despite the lack of data about the phason mode in NbSe\(_3\), the phason dispersion curve has been measured in K\(_{0.3}\)MoO\(_3\) [33] showing that the two transverse elastic constants are similar. We assume that it also the case in NbSe\(_3\) and set the constraint \(c_y = c_z\).

Furthermore, standard NbSe\(_3\) and TaS\(_3\) crystals display very elongated shapes, few millimeters long, tens of micrometers wide but only few micrometers thick. We thus assume \(L_y \gg L_z\) \((p_2 \ll p_3)\) and set \(p_2 = 0\) in the fit since the two contributions add up in the formula.

Furthermore, the bulk impurity frequency pinning \(\omega_0\) is a phenomenological parameter introduced in previous models [7] to explain why the threshold does not tend towards zero for large \(L_x\) distances. However, the impurity pinning \(\omega_0\) does not bring any crucial information in our model since the finite limit for large \(L_x\) is naturally obtained by the lateral surface pinning introduced here (see Appendix E). Therefore, impurity pinning frequency \(\omega_0\) is set to zero in the following.

The evolution of \(E_{th}\) as a function of \(L_x\) taken from reference [17] has been correctly fitted for different sets of free parameters (see Fig. E.1 in Appendix E). The overall \(E_{th}\) profile including its convergence towards a constant value for large \(L_x\) is well reproduced with \(\omega_0 = 0\), which confirms that the physical properties of sliding CDW is mainly driven by surface pinning effects and not by bulk pinning.

Within those assumptions, equation (13) correctly fits several measurements performed in different systems as in TaS\(_3\) [19] or in NbSe\(_3\) [17] as shown in Figure 4 despite our constraints \(p_2 = p_4 = 0\), showing that the phase-slip process combined with the transverse surface pinning can explain the non-linear CDW current measured in these materials. Finally, the electrical potential \(V_{th} = L_x \times E_{th}\) as a function of \(L_x\) taken from [32] is also fitted in the inset of Figure 4. The model also confirms the linear behavior of \(V_{th}\) for large contact distance.

A more systematic study knowing the exact sample dimensions \((L_y, L_z)\) would allow us to directly obtain the \(c_x/c_y\) and \(c_x/c_z\) ratios from resistivity measurements (the sample transverse dimensions are sometimes missing in the published data).

### 3.2 \(E_{th}\) as a function of the sample cross-section

Let us now study the effect of the sample cross section on \(E_{th}\) using our model. It is interesting to consider this dependence since the observed increase of \(E_{th}\) with decreasing cross sections cannot be explained by the bulk pinning frequency \(\omega_0\) alone. We use data from [24] of the threshold field as a function of the sample cross-section \(A = L_y L_z\) in small \(\alpha\)-TaS\(_3\) samples. The first \((2n_y + 1)\frac{x}{L_y}\) term in the expression of \(a_{n_y, n_z}\) equation (14) can be neglected since \(L_y \approx 10L_z \gg L_z\) \((A \approx 10L_z^2)\). As in the previous section, we assume \(c_y \approx c_z\) and the bulk impurity pinning is neglected \((\omega_0 = 0)\). It remains two free parameters are thus remaining, namely \(m_1 = \frac{\phi_s^2 \pi^3 c_x}{8 \eta L_x}, m_2 = \frac{c_x L_x \sqrt{2\pi}}{\omega_0}\) and the fitting function...
The increase of $E_{th}$ for decreasing cross sections cannot be reproduced by bulk impurity pinning but is correctly described by considering only surface pinning. This adjustment with cross sections is the best illustration that the pinning volume plays little, if any role, in the CDW transition temperature ($T_s^c = 70–75$ K) $15$ K above the bulk transition ($T_{c_{bulk}} = 59$ K), indicating a different CDW amplitude between surface and bulk.

Several explanations were given in the literature for the origin of surface pinning in CDW system. Feinberg and Friedel proposed a CDW frontal pinning in the case of rough sample surfaces or, as a second mechanism, a condensation of electrons near the surface if the CDW wavefronts are not perpendicular to the sample transverse surfaces [7,46].

The diffraction measurements showing a systematic and identical pinning over so large distances [25], however, tend to show that surface pinning is not due to extrinsic surface defects but rather to the intrinsic nature of CDW. As proposed by Yetman and Gill [18] and in [47], this effect could be associated to a commensurate CDW pinned to the crystal lattice at the surface in contrast to an incommensurate CDW in the bulk. Gammie et al. measured the surface CDW modulation in TaS$_3$ to be approximately at the commensurate value $4c_0 \times 10b_0$ [48] where $c_0$ and $b_0$ are the crystal lattice parameters. Brun et al. measured by STM the CDW wavevector in Rb$_{0.3}$MoO$_3$ at the commensurate value $q_{cdw} = \pm 0.25b^* + (a+2c)^*$ [49]. Finally, several STM measurements from the literature indicate a surface CDW wavevector in NbSe$_3$ at $q_{cdw} = 0.24b^*$ [37–39] close to the commensurate value $0.25b^*$. Unfortunately, the error bars of $q_{cdw}$ are not indicated, hence, to our knowledge, no experimental evidence can either support or deny this assumption yet mainly because the surface local probes lack the desired $q$-resolution.

### 4 Conclusion

In conclusion, we provide here an analytical expression for the CDW phase and threshold field, when the system is submitted to an applied current and constrained by

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**Fig. 5.** The experimental threshold $E_{th}$ (blue dots) versus the sample cross section in small α-TaS$_3$ samples from [24]. The fit using equation (16) (red line) correctly reproduces the whole behavior especially the increase of $E_{th}$ for decreasing cross sections and the asymptotic constant value for large cross sections (no bulk pinning is used in the fit).

reads:

$$E_{th, \text{fit}}(A, \{m_1, m_2\}) = m_1 \frac{1}{\sum_{n_y,z=0}^{+\infty} (-1)^{n_y+n_z} \tanh \left( \frac{\pi a_{ny,nz}}{2} \right)} (16)$$

with

$$a_{ny,nz}^{fit} = m_2 \frac{2(n_z+1)}{\sqrt{A}}. (17)$$

Our model with $\omega_0 = 0$, $c_y = c_z$ and $L_y \gg L_z$ correctly fits the experimental data (see Fig. 5) especially the two extreme cases, the threshold increase for small cross sections and the finite asymptotic value for large cross sections.

The increase of $E_{th}$ for decreasing cross sections cannot be reproduced by bulk impurity pinning but is correctly described by considering only surface pinning. This adjustment with cross sections is the best illustration that the pinning volume plays little, if any role, in the CDW deformation under current.

It can also be noted that the critical strain is reached at larger fields for smaller cross sections. Due to surface pinning, part of the elastic energy induced by the deformation goes into the transverse shear, thus the longitudinal strain becomes smaller than in the case of a free CDW on the transverse surfaces.

### 3.3 Discussion

We have shown in this article that the macroscopic properties of a CDW can be more surface than bulk dependent especially in thin samples, in particular due to transverse pinning that was either neglected or little considered until now. However, this conclusion raises the question of macroscopic samples depending so much on it surfaces. Why is the bulk CDW phase so closely associated to boundary conditions?

The surfaces of many CDW systems have been studied especially by STM. The CDW phase is present at the top layer and can display a perfect long range order over hundreds of nanometers, like in the quasi-1D Rb$_{0.3}$MoO$_3$ [34], K$_{0.8}$Mo$_6$O$_{17}$ [35], TaS$_3$ [36], NbSe$_3$ [37–39] and in the quasi-2D TbTe$_3$ [40,41] and 1T-TaS$_2$ [42]. Moreover, several groups observed a surface CDW using grazing incident X-ray diffraction in NbSe$_2$ [43] and K$_{0.3}$MoO$_3$ [44].

The surface and volume properties of CDW materials may be different but are, however, systems dependent. Although similar CDW properties were reported at the surface and in the bulk of K$_{0.3}$MoO$_3$ by grazing-incidence X-ray diffraction [44] (the $T_{c_{sdw}}$ and the order parameter remain identical), this is not the case in other compounds in which the CDW phase in the bulk is different from the surface [45] like in TbTe$_3$, on which a second CDW phase along the $a$ axis is measured by STM [41]. In NbSe$_3$, the surface transition was measured at a temperature larger by $1.4 \pm 0.6$ K from the one measured in the bulk. In NbSe$_3$, Brun et al. [37] measured a surface CDW transition temperature ($T_s^c = 70–75$ K) $15$ K above the bulk transition ($T_{c_{bulk}} = 59$ K), indicating a different CDW amplitude between surface and bulk.
boundary conditions including transverse surface pinning as observed in a recent experiment [25]. The threshold field $E_{th}$ is obtained from the 3D phase as a function of the sample dimensions and the phase slip process. We show that the CDW deformations appear at larger fields when surface pinning is taken into account, which leads to an increase of threshold fields for small samples. The solution correctly describes the threshold field $E_{th}$ measured in several CDW systems as a function of both, lengths and sample cross sections.

In addition, this study shows that bulk impurity pinning, usually introduced in theoretical models as a phenomenological parameter to better fit the data, is not necessary to predict the threshold dependence on the sample dimensions. This threshold field behavior can be explained by the only means of pinning from lateral surfaces without consideration of bulk properties. On the other hand, in the case of thick samples, it seems that bulk impurity pinning still has to be taken into account to predict the temperature dependence of $E_{th}$ [50].

The CDW dynamics for thin samples is surprisingly mainly controlled by surface effects and less by the volume, despite the comparatively large volume scales. This strong boundary effect between surfaces tens of micrometers apart cannot occur without an extraordinary long-range order of the CDW. This effect is consistent with the experiment reported in [25] that observes a continuous deformation of the CDW wave fronts spanning a distance of 4 orders of magnitude larger than the CDW wavelength.

This study also raises the question on the origin of the strong surface pinning effect. As discussed in the text, surface pinning is most probably an intrinsic property of CDW systems and could be related to the loss of incommensurability at the surface. In this framework, the impressive CDW deformation under field would then be a consequence of a coexisting incommensurate CDW in the volume with commensurate CDW at the surfaces.

The model proposed in this paper highlights the importance of surface effects on sliding properties. The surface state is undoubtedly an important parameter to explain the threshold evolution under mechanical strain [51]. Finally, we show here that surface pinning must be taken into account to correctly describe the threshold field and thus the soliton nucleation at the electrical contact. If transverse pinning plays a significant role for the threshold, it could also be an important parameter to determine the soliton propagation in the sample. Pinning of the soliton could explain the CDW hysteresis effect with current [52–54] as well as the observed decrease of the transverse CDW satellite peak width measured in diffraction [47,55] and a complete theoretical study of this propagation including surface pinning is necessary.

**Author contribution statement**

The four authors contributed to the CDW phase solution and the comparison with resistivity experiments from the literature. E.B., V.L.R.J., and D.L.B. participated in the experiment presented in Figure 3. All four authors contributed to the writing of the paper.

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**Appendix A: Description of the phase-slip process**

In this section, we describe the phase-slip process defining the electric field threshold equation (11). As discussed in the introduction, solitons, transporting charges from one contact to the other, are created at the electrical contact when the field exceeds $E_{th}$. However, due to the topology of these $2\pi$ Sine-Gordon phase solitons [56], they cannot nucleate without destroying the CDW order and the CDW amplitude needs to locally drop to zero. The least energetic way to create a soliton is through a phase vortex ring, also referred to as a CDW dislocation loop [7], which appears spontaneously under strain and increases in size until it vanishes on the sample surface, leaving behind it a soliton. This is the so-called phase-slip process that we describe here, starting from the phase vortex configuration.

A CDW phase vortex is shown in Figure A.1a in which the phase $\phi(r)$ increases by $2\pi$ when following the green path around the vortex center. In order to avoid an infinite $\phi$ derivative in the center, meaning an infinite elastic energy, the CDW amplitude $A$ drops exponentially to zero at the center as shown in the vertical axis of Figure A.1a. Due to its topological property, a vortex configuration can only be created in the CDW volume as a vortex–antivortex pair, where an antivortex is a vortex of opposite chirality. The vortex and antivortex nucleate at the same position and then split in two to create a CDW phase configuration as illustrated in Figure A.1b where the vortex centers are schematized as black dots and the $\phi$ value in color. The $\phi$ profile through the vortex–antivortex configuration contains a $2\pi$ phase shift (see Figs. A.1b and A.1c). Hence, every atomic chain located in between the vortex and the antivortex have a CDW soliton. This vortex–antivortex nucleation is the least energetic way to create topological $2\pi$ solitons in the CDW bulk.

The generalization in 3D is a vortex ring as presented in Figure A.2 where the CDW phase $\phi$ is shown by a color gradient. This ring corresponds to a continuous vortex–antivortex pairs configuration where the 2D case in Figure A.1b corresponds to a section of the 3D case in the plane $(x,y,z=0)$. Each atomic chain inside this ring contains a CDW soliton as in the 2D case (Figs. A.1b and A.1c). The vortex ring induces a phase gradient leading to the elastic energy [47]:

$$E_{ring}(d) \propto 4\pi^2d\ln\left(\frac{d-\xi}{\xi}\right) - \pi^2d^2\phi_x \quad (A.1)$$

where $d$ is the vortex diameter and $\xi$ the CDW coherence length. As the vortex center radius is $\xi$, the ring energy is not defined for a diameter $d \leq 2\xi$. The elastic energy $E_{ring}$ without strain ($\phi_x = 0$) is shown as function of the diameter $d$ in blue in Figure A.3a. We observe that...
Fig. A.1. (a) 2D topological phase vortex where the CDW amplitude $A$ corresponds to the vertical axis while the CDW phase $\phi$ is displayed in color gradient. Following the green arrow path, $\phi$ increases by $2\pi$. (b) Vortex–antivortex pair configuration. (c) $\phi$ profile along the black dashed line in (c) showing that a topological $2\pi$ soliton is present on each atomic chain inside the vortex–antivortex pair.

$E_{\text{ring}}$ is always positive and increases for large $d$, thus the vortex ring cannot nucleate spontaneously in a CDW at equilibrium. However, this is no more the case under an external electric field inducing a CDW longitudinal strain $\phi_x \neq 0$ (see Fig. 2b). The ring energy decreases in the presence of a non-zero $\phi_x$ as shown in Figure A.3a and for large ring size ($d \gg \xi$) $E_{\text{ring}}$ is negative and the ring nucleation becomes favorable.

However, if $\xi\phi_x < 2$ (blue, orange, and green curves in Fig. A.3a), the energy derivative at smallest ring diameter $\frac{\partial E_{\text{ring}}}{\partial d}(d = 2\xi)$ is positive, hence an energy barrier forbids the ring to increase to larger diameters and to nucleate. Yet, as $\phi_x$ increases, $\frac{\partial E_{\text{ring}}}{\partial d}(d = 2\xi)$ decreases linearly as shown in Figure A.3b until it becomes negative for $\xi\phi_x > 2$, hence the energy barrier disappear and the ring nucleates spontaneously. As shown in the violet curve in Figure A.3b, for $\phi_x > 2/\xi$, $E_{\text{ring}}$ is always decreasing, therefore the diameter $d$ increases until the ring reaches the sample borders and vanishes, leaving behind a topological $2\pi$ soliton on each atomic chain at the electrical contact. This phenomenon is the “phase-slip process”.

We see from this argument that the ring nucleates where the longitudinal derivative $\phi_x$ is maximum, i.e. at the electrical contact and as far as possible from the lateral surface in $(x = L_x/2, y = 0, z = 0)$ with our model (see Figs. 2b and D.1b). The soliton nucleation with the appearance of the non-linear CDW current occurs when the applied electric field is such that the phase longitudinal derivative is larger than a critical value $\phi_x(L_x/2, 0, 0) > \phi_c \equiv 2/\xi$, hence defining the threshold field equation (11).

Finally, we considered here the strain to be constant locally, that is $\phi_x$ is constant in the calculation of $E_{\text{ring}}(d)$ shown in Figure A.3. This approximation is correct since the typical length of the derivative variation is of the
order of the sample dimensions $L_x, L_y, L_z$ as observed in Figure 2b. Since $E_{\text{ring}}$ reaches a large negative value for $d \gg \xi$ and $\phi_x(\frac{L_x'}{2}, y, z) \geq 0 \ (\forall y, z)$, the spatial variation of the CDW strain will not prevent the ring size to spontaneously increase.

Appendix B: Uniqueness theorem

The image charges method is often used to solve electrostatic problems with boundary conditions by adding charges strategically placed to enable the Laplace equation to be more easily solved. This method is valid in electrostatic since the Poisson equation satisfies the uniqueness theorem regarding the solutions gradient (electric field). The use of the image charge method in our case with contacts and surface pinning is justified if the inhomogeneous screened Poisson equation (4) also satisfies this theorem.

Let us consider two different solutions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ of equation (4) both satisfying the boundary conditions equation (5) and the difference $\psi = \phi_1 - \phi_2$ that must be zero if the solution is unique. This phase difference $\psi$ fulfill the homogeneous screened Poisson equation alongside with the Dirichlet conditions (Eq. (5)):

$$\left(\Delta - \omega^2\right)\psi = 0. \quad (B.1)$$

The only solution to this equation is the trivial solution $\psi = 0$ since in this case the Laplacian is negative definite while $\omega^2 > 0$ [57]. In the following, we show a step by step demonstration of this trivial solution. Let us consider the relations:

$$\nabla (\psi \nabla \psi) = (\nabla \psi)^2 + \psi \Delta \psi = (\nabla \psi)^2 + \omega^2 \psi^2 \quad (B.2)$$

where equation (B.1) is used in the second line. By integrating equation (B.2) over the CDW sample volume $\mathcal{V}$ and using the divergence theorem one finds:

$$\int_{\mathcal{V}} \nabla (\psi \nabla \psi) = \int_{\mathcal{V}} \left[(\nabla \psi)^2 + \omega^2 \psi^2\right] d^3 \mathbf{r}$$

$$\int_{\partial \mathcal{V}} \psi \nabla \psi = \int_{\mathcal{V}} \left[(\nabla \psi)^2 + \omega^2 \psi^2\right] d^3 \mathbf{r} \quad (B.3)$$

where the surface $\partial \mathcal{V}$ corresponds to the CDW boundaries. Since $\psi$ satisfies equation (5), $\psi = 0$ on the boundaries and the left-hand side of equation (B.3) is therefore, zero. Each squares term on the right-hand side must be zero to vanish the integral. Hence $\psi(\mathbf{r}) = 0 \ (\forall \mathbf{r})$, proving the unicity of the solution.

Appendix C: Step-by-step construction of the image charge and CDW phase solution in 1D and 2D

A step-by-step construction of the image charge density, for the 1D case, satisfying $\phi(\pm \frac{L_x'}{2}) = 0$ is shown in Figure C.1. The first step is to consider a uniform source term $+E$ in the bulk of the sample (the red line in Figure C.1a where the source density is $\rho_0(x') = E \times \Pi \left(\frac{x'}{L_x'}\right)$ where $\Pi$ is the gate function defined $\Pi(x) = \Theta(\frac{L_x}{2} - |x|)$ with $\Theta$ being the Heavyside function.

The second step is to consider an “anti-mirror” located at $x' = -\frac{L_x'}{2}$ to create an artificial negative image charge density $-E$ located in the region $-\frac{3L_x'}{2} < x' < -\frac{L_x'}{2}$ that fulfills the boundary condition $\phi(-\frac{L_x'}{2}) = 0$ as shown in Figure C.1b. At the end of this step, the total charge density is $\rho_b(x') = \rho_0(x') - E \times \Pi \left(\frac{x'+L_x'}{2}\right)$.

In order to satisfy the second boundary condition $\phi(\frac{L_x'}{2}) = 0$, the procedure has to be repeated by adding two additional image charge densities, $-E$ at $-\frac{L_x'}{2} < x' < \frac{3L_x'}{2}$ and $+E$ at $\frac{3L_x'}{2} < x' < \frac{5L_x'}{2}$ as shown in Figure C.1c. However, while this new charge density impose $\phi(\frac{L_x'}{2}) = 0$, the first boundary condition is lost since $\phi(-\frac{L_x'}{2}) \neq 0$ (see Fig. C.1c). Therefore, we must repeat the process back and forth between the left and right side of the sample until reaching an infinite periodic total charge density $\rho(x')$ shown in Figure C.1d, which can be expressed by the infinite sum:

$$\rho(x') = \sum_{p=-\infty}^{+\infty} \rho_{\text{unit}}(x' - p2L_x') \quad (C.1)$$

where the density of the unit cell $\rho_{\text{unit}}$ (see the grey rectangle in Fig. C.1d) reads:

$$\rho_{\text{unit}}(x') = E \left[ -\Pi \left(\frac{2}{L_x'} \left(x' + \frac{3L_x'}{2}\right)\right) + \Pi \left(\frac{x'}{L_x'}\right) \right.$$

$$\left. -\Pi \left(\frac{2}{L_x'} \left(x' - \frac{3L_x'}{2}\right)\right) \right] \quad (C.2)$$

![Fig. C.1. The uniform charge density $+E$ in the CDW system used in the image charge method (see Eq. (4)) is displayed as a red line for $x' \in [-\frac{L_x'}{2}, \frac{L_x'}{2}]$ while the negative image charges are displayed in blue. (b), (c), and (d) present the step-by-step construction of the image charge density array described in this Appendix.](image-url)
The phase is the space convolution \( \phi(x') = [G \ast \rho](x') \), which is easier to express in Fourier space as a product \( \phi(q) = G(q) \times \rho(q) \). The Fourier transform of the unit cell of periodic array, its Fourier transform is an infinite sum:

\[
\rho_{\text{unit}}(q) = E \frac{8}{q} \sin^2 \left( \frac{qL_x}{4} \right) \sin \left( \frac{qL'_x}{4} \right) \tag{C.3}
\]

and since the total charge density \( \rho(x') \) is an infinite periodic array, its Fourier transform is an infinite sum:

\[
\rho(q) = \rho_{\text{unit}}(q) \pi \left( \frac{qL_x}{4} \right) \sum_{h=\infty}^{+\infty} \delta(q - h \frac{\pi}{L_x}) \tag{C.4}
\]

Finally, the phase solution is the inverse Fourier transform of \( G(q)\rho(q) \). One finds an infinite sum that can be simplified using first \( \rho_{\text{unit}}(h \frac{\pi}{L_x}) = \rho_{\text{unit}}(h \frac{\pi}{L_x}) \) and then \( \rho(2n \frac{\pi}{L_x}) = 0 \) and \( \rho((2n+1) \frac{\pi}{L_x}) = \frac{4EL_x(2n+1)}{\pi(2n+1)} \). We finally obtain the following expression for the CDW phase in 1D:

\[
\phi(x') = -\frac{4E}{\pi} \sum_{n=0}^{+\infty} (-1)^n \cos \left[ \frac{(2n+1)\pi x'}{L_x} \right] \left[ \frac{(2n+1)\pi x'}{L_x} \right]^2 + \omega^2 \tag{C.5}
\]

The construction of the image charge density in 2D is similar to the procedure used in 1D. The CDW sample of size \( L'_x \times L'_y \) has a uniform charge density \( +E \) and an infinite array of periodic image charges is built to fulfill the boundary conditions \( \phi(\pm \frac{L'_x}{2}, 0) = \phi(\pm \frac{L'_x}{2}, \pm \frac{L'_y}{2}) = 0 \) (see Fig. C.2). The Fourier transform of the unit cell of the two-dimensional periodic density is:

\[
\rho_{\text{unit}}(q_x, q_y) = E \frac{64}{q_x q_y} \sin \left( \frac{q_x L'_x}{2} \right) \sin^2 \left( \frac{q_x L'_x}{4} \right) \times \sin \left( \frac{q_y L'_y}{2} \right) \sin^2 \left( \frac{q_y L'_y}{4} \right) \tag{C.6}
\]

Appendix D: The CDW phase deformation in 3D

Following the same procedure as in 1D (Eq. (8)) and in 2D (Eq. (9)), the solution of the CDW phase submitted
to an electric field with Dirichlet conditions in 3D reads:

$$
\phi(r') = \frac{-64E}{\pi^3} \sum_{n,y,z=0}^{+\infty} \frac{(-1)^{n_y+n_z+n_x}}{(2n_x+1)(2n_y+1)(2n_z+1)} \cos \left[ \frac{(2n_x+1)\pi x'}{L_x} \right] \cos \left[ \frac{(2n_y+1)\pi y'}{L_y} \right] \cos \left[ \frac{(2n_z+1)\pi z'}{L_z} \right] \\
\times \left[ \frac{(2n_x+1)\pi x'}{L_x} \right]^2 + \left[ \frac{(2n_y+1)\pi y'}{L_y} \right]^2 + \left[ \frac{(2n_z+1)\pi z'}{L_z} \right]^2 + \omega^2
$$

The corresponding phase profile $\phi(r')$ is shown in Figure D.1a in the 3D volume of the sample. The phase is zero at the sample boundaries as expected while $\phi$ varies mostly in the middle of the sample. The longitudinal derivative $\phi_x'$ is close to zero in the middle of the sample and reaches its maximum at the electrical contact where the phase slip occurs (see Fig. D.1b). One can also observe that $\phi_x'$ drops to zero at the transverse surfaces along $y$ and $z$. Therefore, as considered in the main text, the phase slip occurs where $\phi_x'$ is maximum, at $(x', y', z') = (L_x'/2, 0, 0)$.

### Appendix E: Fitting procedure for the 3D threshold field $E_{th}$ versus the length $L_x$

In this section, we describe the procedure used to fit the expression of the threshold field given in equation (13) from the experimental resistivity measurements [17,19,32]. As discussed in the main text, four free parameters are used

$$
\{p_1, p_2, p_3, p_4\} = \left\{ \frac{\phi_0^3 \pi^3 c_x^2}{8\eta}, \frac{c_y}{L_y c_x}, \frac{c_z}{L_z c_x}, \frac{\omega_0}{\sqrt{2\pi c_x}} \right\}
$$

with:

$$
E_{th}^{fit_{L_x}}(L_x, \{p_1, p_2, p_3, p_4\}) = \frac{p_1}{L_x} \sum_{n_y,z=0}^{+\infty} \frac{(-1)^{n_y+n_z+n_x}}{(2n_y+1)(2n_z+1)(2n_x+1)} \tan \left( \frac{\pi a_{n_y,n_z}}{2} \right)
$$

with

$$
\left( a_{n_y,n_z}^{fit_{L_x}} \right)^2 = [(2n_y+1)p_2L_x]^2 + [(2n_z+1)p_3L_x]^2 + (p_4L_x)^2
$$

We fit $E_{th}$ as a function of $L_x$ from Prester et al. [17] for different choices of parameters. As a first step, we fit the data by using the four parameters $\{p_1, p_2, p_3, p_4\}$ (see the red curve in Fig. E.1). The data are correctly fitted but the covariance matrix has large diagonal as well as non-diagonal elements showing correlation between parameters, especially between $p_2$ and $p_3$ (see Eq. (E.2)).

As discussed in the main text, the characteristics of $E_{th}$ can be reproduced without the need of $\omega_0$. Without bulk pinning ($\omega_0 = p_4 = 0$), the global $E_{th}$ profile with $L_x$ is also well reproduced (see the yellow curve in Fig. E.1).

In addition, the two transverse elastic constants $c_y$ and $c_z$ are assumed to be the same, as in K$_{0.3}$MoO$_3$ [33]. Furthermore, the standard NbSe$_3$ dimensions allow us to set $L_y > L_z$ leading to $p_2 \ll p_3$. By using only two free parameters $\{p_1, p_2 = 0, p_3, p_4 = 0\}$, our model can still correctly reproduce the overall behavior of the experimental $E_{th}$ (see the blue line in Fig. E.1).

### Appendix F: Convergence of the $E_{th}$ expression

The double sum used in the expression of $E_{th}$ reads (where we set $\omega_0 = 0$ as in the fits of Figs. 4 and 5)

$$
S(k_1, k_2) = \sum_{n_y,z=0}^{+\infty} \frac{(-1)^{n_y+n_z}\tanh(\frac{\pi a_{n_y,n_z}}{2})}{(2n_y+1)(2n_z+1)a_{n_y,n_z}},
$$

with

$$
a_{n_y,n_z}^2 = [(2n_y+1)k_1]^2 + [(2n_z+1)k_2]^2
$$

and $k_1 = \frac{L_x}{L_y} \frac{c_y}{c_x}$ and $k_2 = \frac{L_x}{L_y} \frac{c_z}{c_x}$. We evaluate here the error made on $S$ when a finite number of terms is used in the sum.

For large $k_1$ and $k_2$ values, the hyperbolic tangent term tends towards one and the double series converges as an alternating sign inverse square $\sim \frac{(-1)^n}{(2n+1)^2}$. However, in the other limit ($k_1, k_2 \ll 1$), the first order expansion of $\tanh$ gives:

$$
\lim_{k_1, k_2 \ll 1} S(k_1, k_2) = \frac{\pi}{2} \sum_{n_y,z=0}^{+\infty} \frac{(-1)^{n_y+n_z}}{(2n_y+1)(2n_z+1)},
$$

that converges much slower as an alternating sign inverse linear convergence. In the following, we will study the sum convergence in this specific case knowing that $S(k_1, k_2)$ converges much faster for the other cases. The relative
Relative error $E_{\text{limit},N,N}$ (Eq. (F.5)) made in the numerical approximation of equation (F.1) in the limit case $k_1 = k_2 = 0$ and taking into account the first terms for which $n_y, n_z \leq N$, both equal to $N_y = N_z = N$. The contribution of the first $N = 63$ terms is necessary to have less than 1% relative error.

The relative error considering the first $N_y$ and $N_z$ terms in the double sum

$$S_{\text{limit},N_y,N_z} = \sum_{0 \leq n_y \leq N_y \atop 0 \leq n_z \leq N_z} \frac{(-1)^{n_y+n_z}}{(2n_y+1)(2n_z+1)}$$

(F.4)

can be written as:

$$E_{\text{limit},N_y,N_z} \equiv \left| \frac{S_{\text{limit},\infty,\infty} - S_{\text{limit},N_y,N_z}}{S_{\text{limit},\infty,\infty}} \right|
= \left| 1 - \left[ 1 + \frac{2}{\pi} (-1)^{N_y} \Phi \left( -1, 1, \frac{3}{2} + N_y \right) \right]
\times \left[ 1 + \frac{2}{\pi} (-1)^{N_z} \Phi \left( -1, 1, \frac{3}{2} + N_z \right) \right] \right|$$

(F.5)

where $\Phi(z, s, a)$ is the Lerch transcendent function [58,59]. This relative error $E_{\text{limit},N,Y}$ for $N_y = N_z = N$ is shown in Figure F.1. The sum up to the 63th term both in $n_y$ and $n_z$ is necessary to obtain an error less than 1%. This constraint has been applied in all fits of the main text (Figs. 4 and 5).

The relative error $E_{\text{limit},N_y,N_z}$ for $N_y \neq N_z$ is shown in Figure F.2 where the blue region corresponds to relative errors less than 1%. As in Figure F.1, $E_{\text{limit},N_y,N_z} < 1\%$ when $N_y$ and $N_z$ are both larger than 63 (region in the lower right part of Fig. F.2).

After studying the worst convergence case ($k_1, k_2 \ll 1$), the convergence of the sum in the general case for any $k_1, k_2$ values has been computed.

$$S_{N_y,N_z}(k_1,k_2) = \sum_{0 \leq n_y \leq N_y \atop 0 \leq n_z \leq N_z} \frac{(-1)^{n_y+n_z}\tanh \left( \frac{\pi}{2} a_{n_y,n_z} \right)}{(2n_y+1)(2n_z+1)a_{n_y,n_z}}$$

(F.6)

Since no analytical form exists for the relative error in the general case (similar to Eq. (F.5)), the relative error is computed with the approximation $S_{\infty,\infty}(k_1,k_2) \approx S_{2000,2000}(k_1,k_2)$:

$$E_{N_1,N_2}(k_1,k_2) \equiv \left| \frac{S_{2000,2000}(k_1,k_2) - S_{N_1,N_2}(k_1,k_2)}{S_{2000,2000}(k_1,k_2)} \right| .$$

(F.7)
The results are shown in Figure F.3 for several \( \{k_1, k_2\} \) values. As expected, the least convergent case occurs when \( k_1, k_2 \ll 1 \) (see Fig. F.3d).

In conclusion, a sum up to \( N_y, N_z = 63 \) is necessary to get a less than 1% relative error. We went further and took into account \( N_y, N_z = 100 \) for all the fits displayed in the main text (Figs. 4 and 5).

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