# Pinning of charge density waves by strong impurities

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## Abstract

Starting with the energy functional of the charge density wave, the distribution of phase distortions due to impurities coupling strongly to the charge density wave phase is calculated. The inclusion of interference effects of different impurities allows an estimation of the phase coherence length. The results are found to be consistent with those obtained by the phenomenological ansatz of individual pinning.

## 1. Introduction

The phase pinning due to impurities is a fundamental problem in charge density wave (CDW) systems because it influences both thermodynamic and dynamic properties [1]. Based on the direct coupling of the CDW phase to impurities [2], Fukuyama and Lee developed a microscopic phase theory [3], from which Lee and Rice derived an energy functional of Ginsburg–Landau type [4]. Most analytic investigations followed the suggestions of Fukuyama, Lee and Rice and assumed the pinning to be either strong or weak.

Recently, Bâldea used a phenomenological ansatz generalizing strong (weak) to individual (collective) pining [5]. Starting from the strong pinning limit, the CDW phase $\theta(r)$ is – instead of being fixed to the value $\varphi_i$ at the impurity site $r_i$ – allowed to vary within the range $\varphi_0$ around $\varphi_i$. Similarly, the phase $\theta_\delta$ in the weak pinning domain $\delta$ is allowed to vary within $[\psi_\delta - \psi_0, \psi_\delta + \psi_0]$, where $\exp(i\psi_\delta) \equiv N_0^{-1/2} \langle \exp(-i\theta_i) \rangle_\delta$, i.e. the phase factor resulting from averaging over the $N_0$ impurities of the domain $\delta$.

This ansatz assumes a uniform distribution of $\theta - \varphi_i$ within $[-\varphi_0, \varphi_0]$ for individual pinning and $\theta_\delta - \psi_\delta$ within $[-\psi_0, \psi_0]$ for collective pinning. The energy functional is then expressed in terms of the phenomenological parameters $\varphi_0(\psi_0)$ and $\ell$, where the latter describes the extension of impurity induced phase deformations. The parameters are determined by minimizing the thermodynamic potential.

Starting with the complete energy functional $\Omega[\theta]$, the present work shows that impurities coupling strongly to the CDW phase indeed lead to a uniform distribution such as used in Ref. [5], as far as interference effects between different impurities are neglected. Inclusion of the latter enlarges $\varphi_0$ and smooths the edges of the distribution.

## 2. Energy functional and equation for the phase

If all variations over a distance of the order of the amplitude coherence length $\xi = \hbar v_{\rm F}/\Delta$ are small,

the energy functional of a system of chains parallel to the $x$-axes can be expressed [6] as

$$
\begin{aligned}
\Omega[\theta] = \sum_n \int dx \Bigg\{ & \frac{\hbar v_F}{4\pi} \left( \frac{\partial \theta_n}{\partial x} \right)^2 \\
& + \frac{1}{\pi} \sum_m J_{nm} [1 - \cos(\theta_n - \theta_m)] + \frac{e}{\pi} \frac{\partial \theta_n}{\partial x} \Phi_n \\
& - \sum_i V_i \delta_{nn_i}(x - x_i) \cos(\varphi_i - \theta_n) \Bigg\} \\
& - \int \frac{d^3 r}{8\pi} [\nabla \Phi(r)]^2,
\end{aligned} \tag{1}
$$

where $\Phi(r)$ is the electrostatic potential and $\Phi_n(x) = \Phi(x, r_n)$, $r_n$ being the transverse coordinate of chain $n$. The summation over $i$ runs over all impurities at positions $\{x_i, n_i\}$. The static CDW phase $\theta_n$ is then determined by the vanishing variation of Eq. (1) [7, 8]:

$$
\frac{\hbar v_F}{2} \frac{\partial^2 \theta_n}{\partial x^2} + \sum_m J_{nm} \sin(\theta_m - \theta_n)
$$

$$
+ \sum_i V_i \delta_{nn_i}(x - x_i) \sin(\varphi_i - \theta_n) = -e \frac{\partial \Phi_n}{\partial x}. \tag{2}
$$

For small temperatures no quasi-particles are present, and the phase gradient is connected to the charge density through

$$
\rho_n = \frac{1}{e} \frac{\kappa^2}{4\pi} \frac{\hbar v_F}{2} \frac{\partial \theta_n}{\partial x}, \tag{3}
$$

with $\kappa$ the inverse Thomas–Fermi screening length of the metallic state,

$$
\kappa^2 = \frac{8e^2}{\hbar v_F d_\perp^2}, \tag{4}
$$

and $d_\perp^2$ the cross-section of one chain. $J_{nm}$ describes interchain interaction. In the absence of an external electric field, $\Phi_n$ is created by the CDW charge and has to be found self-consistently with Eq. (3) and Poisson's equation.

To solve the problem analytically, some simplifications will be made [7]:

(i) The chains are assumed to form a square lattice, where each chain interacts only with its next neighbours, i.e. $J_{nm} = J$ for next neighbours and zero otherwise.

(ii) A discrete Laplacian in the transverse direction is used in the Poisson equation:

$$
- \frac{\partial^2 \Phi_n}{\partial x^2} - \frac{\Phi_{n+l_y} + \Phi_{n-l_y} - 2\Phi_n}{d_\perp^2}
$$

$$
- \frac{\Phi_{n+l_z} + \Phi_{n-l_z} - 2\Phi_n}{d_\perp^2} = 4\pi \rho_n. \tag{5}
$$

(iii) In the term describing coupling between chains, the sine is substituted by a sawtooth potential. Because distortions due to impurities are smaller than $\pi$ – at least in the absence of an external electric field – this procedure is equivalent to a linearization.

With these simplifications one obtains

$$
\frac{\kappa^2}{e} \frac{\hbar v_F}{2} \frac{\partial \theta_n}{\partial x} = \frac{\partial^2 \Phi_n}{\partial x^2} + \frac{\Phi_{n+l_y} + \Phi_{n-l_y} - 2\Phi_n}{d_\perp^2}
$$

$$
+ \frac{\Phi_{n+l_z} + \Phi_{n-l_z} - 2\Phi_n}{d_\perp^2}, \tag{6}
$$

$$
e \frac{\partial \Phi_n}{\partial x} = \sum_i V_i \delta_{nn_i}(x - x_i) \sin(\varphi_i - \theta_n) + \frac{\hbar v_F}{2} \frac{\partial^2 \theta_n}{\partial x^2}
$$

$$
+ J[\theta_{n+l_y} + \theta_{n-l_y} - 2\theta_n + \theta_{n+l_z} + \theta_{n-l_z} - 2\theta_n]. \tag{7}
$$

The phases will be measured from their values at infinity, i.e. $\tilde{\theta}_n \equiv \theta_n - \theta_\infty$, $\tilde{\varphi}_i \equiv \varphi_i - \theta_\infty$. Then, $\tilde{\theta}_n$ is the phase perturbation on chain $n$ at position $x$ due to impurities at positions $(x_i, n_i)$.

Eqs. (6) and (7) will be solved by Fourier transformation:

$$
f_n(x) = \int_{-\pi/d_\perp}^{\pi/d_\perp} \frac{dk_y}{2\pi} \int_{-\pi/d_\perp}^{\pi/d_\perp} \frac{dk_z}{2\pi}
$$

$$
\times \int_{-\infty}^{\infty} \frac{dq}{2\pi} f(q, k) e^{i(qx + knd_\perp)}, \tag{8}
$$

$$
f(q, k) = d_\perp^2 \sum_n \int_{-\infty}^{\infty} dx \, f_n(x) e^{-i(qx + knd_\perp)}. \tag{9}
$$

Denoting the electric potential due to internal phase deformations by $\tilde{\Phi}$, and assuming that no external field is present (the effect of which will be

discussed in Section 6), the coupled equations (6) and (7) transformed to Fourier space,

$$(q^2 + \hat{k}^2)e\tilde{\Phi}(q, k) = iq\kappa^2 \frac{\hbar v_F}{2} \tilde{\theta}(q, k), \tag{10}$$

$$(q^2 + \alpha\hat{k}^2)\frac{\hbar v_F}{2} \tilde{\theta}(q, k) - S(q, k) = iqe\tilde{\Phi}(q, k), \tag{11}$$

are then solved to yield

$$\tilde{\theta}(q, k) = \frac{2}{\hbar v_F} g(q, k) S(q, k), \tag{12}$$

$$g(q, k) = \frac{q^2 + \hat{k}^2}{q^2(q^2 + \kappa^2 + (1 + \alpha)\hat{k}^2) + \alpha\hat{k}^4}$$

$$\approx \frac{\hat{k}^2}{\kappa^2} \frac{1}{q^2 + \alpha\hat{k}^4/\kappa^2}, \tag{13}$$

with the anisotropy factor $\alpha = 2Jd_\perp^2/\hbar v_F$, $\hat{k}^2 = 4(\sin^2 d_\perp k_y/2 + \sin^2 d_\perp k_z/2)/d_\perp^2 \approx k_y^2 + k_z^2 \equiv k^2$ and the scattering matrix

$$S(q, k) \equiv d_\perp^2 \sum_i V_i \sin(\tilde{\varphi}_i - \tilde{\theta}_{n_i}(x_i)) e^{-i(qx_i + kn_i d_\perp)}. \tag{14}$$

The last step in Eq. (13) holds because $\kappa d_\perp \gg 1$ for relevant Fermi velocities, $v_F \approx 2 \times 10^5$ m/s.

## 3. Phase equation at impurity sites

To find the phase at the impurity position $(x_i, n_i)$, one has to transform Eq. (12) using Eq. (8):

$$\tilde{\theta}_{n_i}(x_i) = \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} \tilde{\theta}(q, k) e^{i(qx_i + kn_i d_\perp)}$$

$$= \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} \frac{2d_\perp^2}{\hbar v_F} \sum_j V_j \sin(\tilde{\varphi}_j - \tilde{\theta}_{n_j}(x_j)) g(q, k)$$

$$\times e^{i[q(x_i - x_j) + k(n_i - n_j)d_\perp]}. \tag{15}$$

In Eq. (15), the phase factors cancel for $i = j$. The corresponding term will therefore be extracted from the summation over impurities. Defining

furthermore

$$K_0 \equiv \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} g(q, k) \approx \frac{1}{2\kappa d_\perp^2 \sqrt{\alpha}}, \tag{16}$$

$$K_{ij} \equiv \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} g(q, k) e^{i[q(x_i - x_j) + k(n_i - n_j)d_\perp]} \tag{17}$$

and

$$\delta_i \equiv \varphi_i - \theta_{n_i}(x_i) \equiv \tilde{\varphi}_i - \tilde{\theta}_{n_i}(x_i), \tag{18}$$

one gets a system of implicit equations for $\delta_i$:

$$\tilde{\varphi}_i = \delta_i + \frac{1}{a}\left(\sin \delta_i + \sum_{j \neq i} \frac{V_j}{V_i} \frac{K_{ij}}{K_0} \sin \delta_j\right), \tag{19}$$

where $a \equiv \hbar v_F/2d_\perp^2 V_i K_0$ measures the strength of the coupling of impurities to the CDW phase. Strong coupling is equivalent to small $a$.

Using the approximation of Eq. (13), the $q$-integration in $K_{ij}$ (Eq. (17)) can be performed, yielding

$$K_{ij} = K_0 I_{ij}^{(y)} I_{ij}^{(z)}, \tag{20}$$

$$I_{ij}^{(y/z)} = \int_0^1 du \cos(n_{ij}^{(y/z)} \pi u) \exp(-u^2|x_i - x_j|/\ell_\parallel), \tag{21}$$

$$\ell_\parallel = \frac{\kappa d_\perp^2}{\pi^2 \sqrt{\alpha}}, \tag{22}$$

with $n_{ij}^{(y/z)}$ being the component of $\boldsymbol{n}_i - \boldsymbol{n}_j$ in the $y/z$-direction. $\ell_\parallel$ is the correlation length in the parallel direction, i.e. along the chain: impurities at sites $x_j$ with $|x_i - x_j| \gg \ell_\parallel$ do not interfere with phase distortions due to impurity $i$. Along one chain $(n_{ij} = 0)$, Eq. (21) can be expressed as $I_{ij} = \sqrt{\pi\ell_\parallel/4|x_i - x_j|} \, \text{erf}(\sqrt{|x_i - x_j|/\ell_\parallel})$. For $|x_i - x_{i+1}| \gg \ell_\parallel$, i.e. small impurity concentration $c_i \equiv d_\parallel/\langle|x_i - x_{i+1}|\rangle$ with longitudinal lattice constant $d_\parallel$, the error function becomes unity and $K_{ij}$ is therefore proportional to $c_i$. In the opposite limit, $|x_i - x_{i+1}| \ll \ell_\parallel$ (large impurity concentration), $I_{ij} \approx 1 - |x_i - x_{i+1}|/3\ell_\parallel$ and therefore $\tilde{K}_{ij} \equiv K_{ij}/K_0 < (1 - c_i d_\parallel/3\ell_\parallel)^2$.

In the transverse direction, $I_{ij}$ is vanishing for $x_i = x_j$. The maximum will be obtained when both the argument of the cosine and the exponential function are of the same order of magnitude, i.e. $|x_i - x_j|/\ell_\parallel \approx (n_{ij}\pi)^2$, yielding $(n_{ij}\pi)^{-1}$ as a rough estimation for $I_{ij}$. The decay of $K_{ij}$ is therefore

proportional to the squared inverse distance of the chains.

Note that $|I_{ij}| < 1$ and therefore $|\bar{K}_{ij}| < 1$. $\bar{K}_{ij}$ becomes very small if $|x_i - x_j|$ and/or $|\boldsymbol{n}_i - \boldsymbol{n}_j|$ become large, i.e. at small impurity concentration and high order of neighbourhood of impurities. To simplify further calculations, $V_i \equiv V \; \forall i$ will be assumed in the following considerations.

## 4. Distribution of $\delta_i$

Eq. (19) completely determines the phases at the impurity sites. However, in a real system the impurity positions are not known. Furthermore, most measured quantities only contain information about the average impurity distribution.

If the impurities are uniformly distributed in the sample, then also the $\tilde{\varphi}_i$ are uniformly distributed within the range $[-\pi, \pi]$, i.e.

$$P_\varphi(\tilde{\varphi}_i) = \begin{cases} (2\pi)^{-1}, & -\pi \leqslant \tilde{\varphi}_i \leqslant \pi, \\ 0, & \text{otherwise,} \end{cases} \tag{23}$$

is the corresponding distribution function. The $n$th moment of $\tilde{\varphi}_i$ is then given by

$$\langle \tilde{\varphi}_i^n \rangle = \frac{1 + (-1)^n}{2} \frac{\pi^n}{n+1}. \tag{24}$$

From the moments, the distribution function can be constructed by

$$P_\varphi(\tilde{\varphi}_i) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\sigma \sum_{v=0}^{\infty} \frac{\langle \tilde{\varphi}_i^v \rangle}{v!} (i\sigma)^v e^{-i\tilde{\varphi}_i\sigma}. \tag{25}$$

If one therefore succeeds to express all moments of $\delta_i$ by those of $\tilde{\varphi}_i$ via Eq. (19), the distribution of $\delta_i$ is completely determined. Although this cannot be done exactly, an approximation can be obtained for small values of the parameter $a$.

Because the $\tilde{\varphi}_i$ are not correlated, averages over products will factorize:

$$\langle \tilde{\varphi}_i^m \tilde{\varphi}_j^n \rangle |_{i \neq j} = \langle \tilde{\varphi}_i^m \rangle \langle \tilde{\varphi}_j^n \rangle$$

$$= \frac{1 + (-1)^m}{2} \frac{1 + (-1)^n}{2} \frac{\pi^m}{m+1} \frac{\pi^n}{n+1}. \tag{26}$$

Substituting $\tilde{\varphi}_i$ and $\tilde{\varphi}_j$ in the left-hand side of Eq. (26) by Eq. (19) gives a system of equations for the moments and correlations of $\delta_i$:

$$\langle \tilde{\varphi}_i^m \rangle \langle \tilde{\varphi}_j^n \rangle = \left\langle \left[ \delta_i + \frac{1}{a}\left( \sin \delta_i + \sum_{l \neq i} \tilde{K}_{il} \sin \delta_l \right) \right]^m \right.$$

$$\left. \times \left[ \delta_j + \frac{1}{a}\left( \sin \delta_j + \sum_{l \neq j} \tilde{K}_{jl} \sin \delta_l \right) \right]^n \right\rangle. \tag{27}$$

In the limit $a \to 0$, Eq. (27) is solved by $\delta_i = 0 \; \forall i$, resulting in $P_\delta(\delta_i) = \delta(\delta_i)$ as distribution function for $\delta_i$, whereas $a \to \infty$ leads to $\langle \tilde{\varphi}_i^m \rangle \langle \tilde{\varphi}_j^n \rangle = \langle \delta_i^m \delta_j^n \rangle$, i.e. $\delta_i$ has the same distribution as $\tilde{\varphi}_i$.

If $a \ll 1$ and therefore $\delta_i \ll 1$, the sines in Eq. (27) can be replaced by their arguments, leading to

$$\hat{a}^{m+n} \langle \tilde{\varphi}_i^m \rangle \langle \tilde{\varphi}_j^n \rangle$$

$$= \left\langle \left( \delta_i + \sum_{l \neq i} \hat{K}_{il} \delta_l \right)^m \left( \delta_j + \sum_{l \neq j} \hat{K}_{jl} \delta_l \right)^n \right\rangle, \tag{28}$$

with $\hat{a} \equiv a/(1 + a)$ and $\hat{K}_{ij} \equiv \tilde{K}_{ij}/(1 + a)$. Without interference effects between different impurities ($\hat{K}_{ij} = 0$) one gets

$$\langle \delta_i^m \delta_j^n \rangle = \frac{1 + (-1)^m}{2} \frac{1 + (-1)^n}{2} \frac{(\hat{a}\pi)^m}{m+1} \frac{(\hat{a}\pi)^n}{n+1}, \tag{29}$$

i.e. the parameter $\varphi_0 = \pi$ in the distribution $P_\varphi$ (Eq. (23)) is renormalized to $\varphi_0 = \hat{a}\pi$ and therefore

$$P_\delta(\delta_i) = \begin{cases} (2\hat{a}\pi)^{-1}, & -\hat{a}\pi \leqslant \delta_i \leqslant \hat{a}\pi, \\ 0, & \text{otherwise.} \end{cases} \tag{30}$$

To investigate the mutual influence of phase distortions at different impurity sites, the linearized version of Eq. (19),

$$\delta_i = \hat{a}\tilde{\varphi}_i - \sum_{j \neq i} \hat{K}_{ij}\delta_j, \tag{31}$$

will be used. It should be mentioned that, although $a \ll 1$ was assumed to justify the linearization of $\sin \delta_i$, Eq. (31) is not divergent even for $a \to \infty$, because $\hat{a} < 1$. Eq. (31) contains the coupling of $\delta_i$ to the phases at all other impurity sites $j$. The summation, however, can be restricted to impurities within $\ell_\parallel$ in longitudinal and $d_\perp$ in transverse direction, because the correlation between $\delta_i$ and $\delta_j$ is vanishing for impurities $j$ outside this region. Their contribution will therefore vanish in average, because the distribution of $\delta_i$ is symmetric.

If $|\sum_{j \neq i} \hat{K}_{ij}| < 1$, one can get corrections of the order of $\hat{K}_{ij}^{n}$ by iterating Eq. (31) $n$ times. In second order one then obtains

$$\delta_i = \hat{a}\left(1 + \sum_{j \neq i} \hat{K}_{ij}\hat{K}_{ji}\right)\tilde{\varphi}_i$$

$$+ \hat{a} \sum_{j \neq i}\left(\sum_{l \neq i, j} \hat{K}_{il}\hat{K}_{lj} - \hat{K}_{ij}\right)\tilde{\varphi}_j. \qquad (32)$$

Interference of phase distortions due to different impurities influences the distribution of $\delta_i$ in a twofold way:

(i) The first term, proportional to $\tilde{\varphi}_i$, broadens the distribution because it renormalizes $\hat{a}$ to $\hat{a}(1 + \sum_{j \neq i} \hat{K}_{ij}\hat{K}_{ji})$. However, it leaves the distribution uniformly.

(ii) The second term contains the contribution of impurities $j \neq i$. It leads to a smearing of the edges of the distribution.

Taking the $n$th power and averaging both sides of Eq. (31) and using Eq. (26) gives, up to second order in $\hat{K}$,

$$\langle \delta_i^n \rangle = \frac{1 + (-1)^n}{2}\left[\hat{a}\pi\left(1 + \sum_{j \neq i} \hat{K}_{ij}\hat{K}_{ji}\right)\right]^n$$

$$\times \left[\frac{1}{n+1} + \frac{n}{6}\sum_{j \neq i} \hat{K}_{ij}^2\right] + O(\hat{K}^3), \qquad (33)$$

which can be described by the distribution function

$$P_\delta(\delta) = \frac{1}{4\varphi_0}\begin{cases} 1 + \dfrac{1}{\varepsilon^2}\left(1 + \dfrac{\delta}{\varepsilon_0}\right)\left(2\varepsilon - \left|1 + \dfrac{\delta}{\varphi_0}\right|\right), \\ \qquad -(1 + \varepsilon) \leqslant \dfrac{\delta}{\varphi_0} < -(1 - \varepsilon), \\ 2, \qquad -(1 - \varepsilon) \leqslant \dfrac{\delta}{\varphi_0} < 1 - \varepsilon, \\ 1 + \dfrac{1}{\varepsilon^2}\left(1 - \dfrac{\delta}{\varphi_0}\right)\left(2\varepsilon - \left|1 - \dfrac{\delta}{\varphi_0}\right|\right), \\ \qquad 1 - \varepsilon \leqslant \dfrac{\delta}{\varphi_0} \leqslant 1 + \varepsilon. \end{cases} \qquad (34)$$

It contains two parameters, the pinning phase $\varphi_0$, describing the average amplitude of impurity induced phase distortions, and $\varepsilon$, measuring the interference of phase distortions due to different impurities. They are connected to the intrinsic parameters through

$$\varphi_0 = \hat{a}\pi\left(1 + \sum_{j \neq i} \hat{K}_{ij}\hat{K}_{ji}\right) = \hat{a}\pi\left(1 + \frac{\varepsilon^2}{2}\right), \qquad (35)$$

$$\varepsilon^2 = 2\sum_{j \neq i} \hat{K}_{ij}^2. \qquad (36)$$

Note that the distribution function is not unequivocal because all moments are only calculated up to the second order in $\hat{K}$. Therefore, calculating $P_\delta$ via Eq. (25) can lead to unphysical results. However, $P_\delta$ given in Eq. (34) agrees well with the expected behaviour described above.

## 5. Squared phase gradient

Now, all quantities depending on the distortion at the impurity sites $(x_i, \boldsymbol{n}_i)$ can be calculated. However, the energy functional also contains the elastic energy, which is – according to approximating the sine by a sawtooth potential in Eq. (2) – a function of the squared phase gradient, scaled in the transverse direction by $\alpha$.

At arbitrary position $(x, \boldsymbol{n})$, the phase distortion is given by

$$\tilde{\varphi}_n(x) = \frac{2d_\perp^2 V}{hv_F}\sum_i \sin \delta_i \int \frac{d^2k}{(2\pi)^2}\frac{dq}{2\pi} g(q, \boldsymbol{k})$$

$$\times \exp(i[q(x - x_i) + \boldsymbol{k}(\boldsymbol{n} - \boldsymbol{n}_i)d_\perp]). \qquad (37)$$

The scaled squared phase gradient is then obtained as

$$[\nabla\tilde{\theta}_n]^2 \equiv \left[\frac{\partial\tilde{\theta}_n}{\partial x}\right]^2 + \frac{\alpha}{d_\perp^2}[\tilde{\theta}_n - \tilde{\theta}_{n - l_y}]^2$$

$$+ \frac{\alpha}{d_\perp^2}[\tilde{\theta}_n - \tilde{\theta}_{n - l_z}]^2$$

$$= -\left[\frac{2d_\perp^2 V}{hv_F}\right]^2 \sum_{ij} \sin \delta_i \sin \delta_j \int \frac{d^2k\, d^2k'}{(2\pi)^4}\frac{dq\, dq'}{(2\pi)^2}$$

$$(qq' + \alpha\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}')g(q, \boldsymbol{k})g(q', \boldsymbol{k}')$$

$$\times \exp(i[q(x - x_i) + q'(x - x_j)$$

$$+ \boldsymbol{k}(\boldsymbol{n} - \boldsymbol{n}_i)d_\perp + \boldsymbol{k}'(\boldsymbol{n} - \boldsymbol{n}_j')d_\perp]). \qquad (38)$$

Integrating over $x$ and summing over $n$ results in

$$\sum_n \int dx \, [\nabla \tilde{\theta}_n]^2$$

$$= \left[\frac{2d_\perp^2 V}{\hbar v_F}\right]^2 \sum_i \left(L_0 \sin^2 \delta_i + \sum_{j \neq i} L_{ij} \sin \delta_i \sin \delta_j\right),$$

(39)

with

$$L_0 \equiv \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} (q^2 + \alpha \hat{k}^2) g^2(q, k)$$

$$\approx \frac{1}{2\kappa d_\perp^2 \sqrt{\alpha}} \left(\frac{1}{2} + \frac{\pi^2}{3\kappa^2 d_\perp^2}\right) \approx \frac{K_0}{2},$$

(40)

$$L_{ij} \equiv \int \frac{d^2k}{(2\pi)^2} \frac{dq}{2\pi} (q^2 + \alpha \hat{k}^2) g^2(q, k)$$

$$\times \exp(i[q(x_i - x_j) + k(n_i - n_j)d_\perp]).$$

(41)

The last step in Eq. (40) holds because $\kappa d_\perp \gg 1$, although this approximation is not essential for the further calculations.

Estimating $L_{ij}/K_{ij} = (1 + \beta)L_0/K_0$ with $\beta \ll 1$ and replacing the sines in Eq. (39) by their arguments one obtains

$$\left\langle \sum_j (\nabla \tilde{\theta}_n(x))^2 \right\rangle_{V_1}$$

$$= \frac{1}{2K_0 d_\perp^2 a^2} \left(\langle \delta_i^2 \rangle + (1 + \beta) \sum_{j \neq i} \bar{K}_{ij} \langle \delta_i \delta_j \rangle\right),$$

(42)

where $V_1$ is the volume per impurity.

Calculating the correlation function up to the first order in $\hat{K}$ in the same way as the moments,

$$\langle \delta_i \delta_j \rangle = -\tfrac{2}{3}(\hat{a}\pi)^2 \hat{K}_{ij},$$

(43)

and inserting the second moment gives

$$\left\langle \sum_j (\nabla \tilde{\theta}_n(x))^2 \right\rangle_{V_1} = \frac{\kappa^2 d_\perp^2}{3\ell_\parallel} \frac{\hat{a}^2}{a^2} \left(1 + \sum_{j \neq i} \hat{K}_{ij}^2\right)^2$$

$$\times \left[1 + \sum_{j \neq i} \hat{K}_{ij}^2 - 2(1 + \beta)(1 + a) \sum_{j \neq i} \hat{K}_{ij}^2\right]$$

$$= \frac{\kappa^2 d_\perp^2}{3\ell_\parallel} \left(1 - \frac{\varphi_0}{\pi}\right)^2 \left(1 + \frac{\varepsilon^2}{2}\right) - \beta \frac{\kappa^2 d_\perp^2}{3\ell_\parallel} \frac{\varepsilon^2}{1 + a}.$$

(44)

Besides $\varphi_0$ and $\varepsilon$, the length $\ell_\parallel$ (yet implicitly contained in $\varepsilon$) occurs as third parameter, characteristic for the extension of impurity induced phase deformations.

## 6. External electric field

Splitting the electric potential into two parts, the first containing an external electric field in the $x$-direction and the other effect of charges due to internal phase deformations, the Poisson equation (5) reads

$$-\nabla^2(\Phi_{ext}(x) + \tilde{\Phi}_n(x)) = \frac{\kappa^2 \hbar v_F}{2\varepsilon} \frac{\partial[\bar{\theta} + \theta_\infty + \tilde{\theta}_n(x)]}{\partial x}.$$

(45)

The constant part $\bar{\theta}$ has been split from $\theta_\infty$ because it is connected to the external field $E_{ext} = -\partial \Phi_{ext}(x)/\partial x$ by

$$\bar{\theta} = \frac{2e}{\kappa^2 \hbar v_F} E_{ext}.$$

(46)

Applying an external electric field can therefore be taken into account by a global shift of the phase $\theta$. However, the constant part of $\theta$ did not occur in the distribution function calculated above. The reason for this is that the system with randomly distributed impurities has many metastable states to each phase $\theta_\infty$ belonging to more or less the same energy. In configuration space, however, these states are separated by high potential barriers, so that no transition between these states is possible on short time scales, i.e. the system behaves glassy.

The calculations of the previous sections therefore belong to a situation where the system is in equilibrium with the external field, no matter whether the latter is vanishing or not. The polarization induced by an external field will therefore be "frozen" (in glassy sense) if the system has reached equilibrium. It will relax, following a stretched exponential law [9], when the external field is switched off.

The shift of $\theta_\infty$ by an external field can be taken into account by moving the center of the distribution $P_\varphi$ from 0 to $-\bar{\theta}$, keeping the average of $\theta$ at 0. Then, the impurities try to fix $\delta_i = \theta_{n_i}(x_i) - \varphi_i$. In fact, the distribution of $\delta_i$ will also be shifted by $\bar{\delta}$; calculating the first moment in the same way as in Eq. (33), but with shifted distribution $P_\varphi$, gives

$$\bar{\delta} = \varphi_0 \frac{\bar{\theta}}{\pi} \left[1 + \sum_{j \neq i} \hat{K}_{ij}\left(1 - \sum_{l \neq i,j} \hat{K}_{jl}\right)\right].$$

(47)

With $\bar{\delta}$, the fourth parameter is obtained, which is necessary to describe the behaviour of a pinned CDW in an external electric field.

## 7. Conclusions

Starting with the thermodynamic potential as functional of phase deformations $\theta_n(x)$ and the electrostatic potential (1), an implicit equation for $\theta$ in Fourier space was obtained, containing the phases of randomly distributed impurities. For the limit of impurities coupling strongly to the CDW phase, the distribution of $\theta$ at the impurity sites and the integral over the squared phase gradient, proportional to the elastic energy, have been calculated. They can both be expressed by the pinning phase $\varphi_0$, the longitudinal coherence length $\ell_\parallel$, and a parameter $\varepsilon$, describing the interference between phase deformations due to different impurities. Furthermore, the average phase displacement caused by an external electric field beyond the threshold field is given by $\bar{\delta}$. The slope of $\theta$ is therefore characterized by a distortion of $\varphi_0$ at the impurity sites, decaying on the length $\ell_\parallel$ in the longitudinal direction. Phase correlations in the transverse direction are restricted to neighbouring chains.

Let the equilibrium phase now be denoted by $\theta_{min}$. Because it has been found by minimizing the thermodynamic potential, any change in its slope must lead to higher energies. This especially holds for changing $\theta_{min}$ by varying the intrinsic parameters, but keeping its functional form constant. Using the correct functional form as input for $\Omega$ and looking for vanishing variation with respect to the parameters must therefore lead to the same result for the latter. In the same way, using a good approximation for $\theta_{min}$ will yield a good approximation for the parameters, as long as $\theta_{min}$ is a smooth function in parameter space.

This is the procedure performed in Ref. [5]: an ansatz for $\theta_{min}$, described by characteristic parameters, was used and the parameters determined by minimization. The occurrence of the same expressions for elastic energy and distribution function of $\delta_i$ as derived in the present approach, as far as interference effects between different impurities can be neglected, indicates that the ansatz for individual pinning was – with some restrictions – a good choice. The restrictions lie in the fact that – contrary to the energy functional used in this paper – the internal Coulomb interaction was neglected in Ref. [5], replacing the Thomas–Fermi screening length in $\ell_\parallel$ by the amplitude coherence length.

Besides the ansatz of individual pinning, supported also by the $+2k_F/-2k_F$ asymmetry (X-ray "white line" effect [10]) requiring a local phase distortion at the impurity sites, in Ref. [5] also weak pinning was generalized to *collective pinning*. Whether this approximation can be justified in the same way as *individual pinning* should be investigated in future work, solving Eq. (19) for large values of $a$, i.e. for small coupling of impurities to the CDW phase.

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