Disorder Driven Lock-In Transitions of CDWs and Related Structures

Thomas Nattermann, Thorsten Emig and Simon Bogner
Institut für Theoretische Physik, Universität zu Köln, Zülpicherstr. 77, D-50937 Köln, Germany

Abstract. Thermal fluctuations are known to play an important role in low-dimensional systems which may undergo incommensurate-commensurate or (for an accidentally commensurate wavevector) lock-in transitions. In particular, an intermediate floating phase with algebraically decaying correlations exists only in $D = 2$ dimensions, whereas in higher dimensions most features of the phase diagram are mean-field like.

Here we will show, that the introduction of frozen-in disorder leads to strong fluctuation effects even in $D < 4$ dimensions. For commensurate wavevectors the lattice pinning potential dominates always over weak impurity pinning if $p \leq p_c = 6/\pi$ ($D = 3$), where $p$ denotes the degeneracy of the commensurate phase. For larger $p$ a disorder driven continuous transition between a long-range ordered locked-in phase and quasi-long-range ordered phase, dominated by impurity pinning, occurs. Critical exponents of this transition, which is characterized by a zero temperature fixed point, are calculated within an expansion in $4 - D$. The generalization to incommensurate wavevectors will be discussed. If the modulation in the quasi-long-range ordered phase has hexagonal symmetry, as e.g. for flux-line lattices, the algebraic decay is non-universal and depends on the Poisson ratio of the elastic constants. Weakly driven transport is dominated by thermally activated creep in both phases, but with different creep exponents.

Incommensurate (I) phases appear in a large variety of systems (for a review see e.g. [1]). Examples are:
(i) Charge density waves in quasi one and two dimensional conductors (e.g. in TTF–TCNQ, 2H–TaSe).
(ii) Spin density waves (e.g. in CuGeO$_3$).
(iii) Mass density waves in adsorbed monolayers (e.g. He, Kr on graphite or metal surfaces) or of reconstructed surfaces (e.g. of Mo).
(iv) Polarization density waves in ferroelectrics with an incommensurate phase (e.g. in K$_2$SeO$_4$).
(v) Flux density waves in type II superconductors or Josephson junctions in an external field.
Charge density waves are usually accompanied by a mass density wave like in superionic conductors or reconstructed metal surfaces. A common feature of the I phase is, that the wave vector $q_0$, which describes the spatial modulation of the
density wave in the absence of any coupling to the lattices, varies continuously with the parameter of the system (e.g. temperature $T$, pressure $p$, chemical potential $\mu$, magnetic field $H$ etc.). If $2\pi/q_0$ is close to a multiple of the spacing of the underlying crystal lattice, i.e. if $|g/p - q_0| = |\delta| < \delta_c$, commensurability effects may become important. Here $g$ denotes a reciprocal lattice vector of the crystal and $p$ is an integer. The modulation then may become commensurate (C) with the crystal lattice. The most striking effect of the C–phase is the existence of a gap in the excitation spectrum, in contrast to the I–phase, where the low–lying excitations are gapless.

The systematic mean–field theory of the IC–transition was worked out by Bruce, Cowley and Murray in 1978 [2]. These authors distinguish IC–transition of type–I and type–II, depending on the absence or existence, respectively, of an inversion symmetry around $g/p$ in the (disordered phase) soft mode dispersion. In the most simple case of type–I transition, condensation takes place only on wave vectors $\pm q_0$. For temperatures sufficiently below the mean–field transition temperature $T_c$, the system can be described, ignoring amplitude fluctuations, by the sinus–Gordon Hamiltonian.

$$\mathcal{H} = \gamma \int d^D x \left\{ \frac{1}{2} (\nabla \phi - \delta)^2 - g^2 v \cos p \phi \right\}, \quad (1)$$

where $\phi(x)$ describes the long–wavelength distortions of the charge (spin, mass, flux etc.) density

$$\rho(x) = \rho_0 + \rho_1 \text{Re} \left\{ e^{i \frac{4\pi}{p}(g x + \phi(x))} \right\}. \quad (2)$$

Minimization of (1) yields for $\delta < \delta_c \approx gv^{1/2}$ the solution of the C–phase $\phi = \frac{2\pi}{p} n \ (n = 0, 1, \ldots, p - 1)$. The solution for $\delta > \delta_c$ is a regular lattice of phase–solitons of distance $l \sim \ln \left( \frac{\delta - \delta_c}{\delta_c} \right)$ and internal widths $\xi_0 \approx 1/(pg v)^{1/2}$, which describe the I–phase close to the IC–transition. Far from the transition on has $\phi(x) \simeq \delta x$. Type–I transitions are therefore continuous. In general, a large number of C–phases is possible which may lead in certain lattice models to a devil’s staircase behaviour of the modulation vector as a function of the misfit $\delta$ [1].

Type–II transitions, on the contrary, are discontinuous and show in the I–phase an almost sinusoidal modulation of the order parameter. A recent example is the spin–Peierls system CuGeO$_3$ [3].

Thermal fluctuations have a strong effect on the IC–phase diagram in $D = 2$ dimensions. If we exclude topological defects (i.e. vortices), then

(i) the IC transition becomes an inverted Beresinskii–Kosterlitz–Thouless–transition with a reduced transition temperature $T_c(\delta = 0) \approx 8\pi\gamma/p^2$.

(ii) Inside the I–phase solitons interact now by entropic repulsion. Close to the IC–transition the soliton–distance $l$ increases as power law $l \sim (\delta - \delta_c)^{-\beta_s}$ where $\beta_s = \frac{\zeta}{2(1-\zeta)}$. Here $\zeta$ is the thermal roughness exponent of a single soliton (domain
(iii) The spatial variation of the density \( \delta \rho(x) = \rho(x) - \rho_0 \) shows in the I–phase only quasi long range order (LRO):

\[
K(x) = \langle e^{i(\phi(x) - \phi(0))} \rangle \sim |x|^{-\eta} \cos(2\pi z/pl),
\]

where \( \delta = \delta e_z \). \( \eta \) depends on \( l, T/\gamma \) and \( p \) and approaches \( 2/p^2 \) for \( l \to \infty \).

(iv) Topological defects diminish further the ordered (C and I) phases and even change the topology of the phase diagram for \( p \leq 4 \). In particular, for \( p \leq 2 \) there is no direct IC–transition, both phases are separated by a fluid phase [4]. Closely results are expected for 1–dimensional quantum systems. It is interesting to remark, that a qualitatively similar picture emerges also in lower dimensions \( 1 < D < 2 \), but with different singularities at the transitions [5].

In three (and higher) dimensions, thermal fluctuations have only minor effects on the phase diagram and are relevant essentially only in the critical region [6].

In the rest of the paper we investigate the influence of randomly distributed frozen impurities on the lock–in transition. Since impurities favour certain values of the phases, the impurity Hamiltonian can be written in the form

\[
\mathcal{H}_{imp} = \gamma \int d^D x V(x, \phi)
\]

\[
V(x, \phi) = \sqrt{\Delta} \cos(\phi(x) - \alpha(x)), \quad \Delta = \rho_0^2 V_0^2 n_{imp}
\]

\( \alpha(x) \) is a randomly frozen phase \( (0 \leq \alpha \leq 2\pi) \), \( \gamma V_0 \) and \( n_{imp} \) denote the strength and the concentration, respectively, of the impurities. The model defined by (1) and (4) describes also an XY–model in a crystalline (corresponding to a \( p \)–fold axis) and a random field.

We will first discuss the case of a vanishing lattice potential, \( v = 0 \), and exclude topological defects for most parts of the rest of the paper. Larkin and in the present context first Fukuyama and Lee [7] have shown, that the impurities destroy the translational LRO of the charge density wave on scales \( L \gg L_\xi \approx \Delta^{1/(4-D)} \) in all dimensions \( D \leq 4 \). Later studies [8] have shown, that for \( 2 < D < 4 \) \( K(x) \) decays as a power

\[
K(x) \sim e^{\delta} |x|^\bar{\eta},
\]

with a universal exponent \( \bar{\eta} = (\frac{\pi}{3})^2 \epsilon \) in lowest order in \( \epsilon = (4 - D) \). Thus, we regain now quasi–LRO in the I–phase in all dimensions \( 2 < D < 4 \).

In systems in which the modulation of the I–phase has hexagonal symmetry, like in flux line lattices, the situation is more complicated. If we describe the distortions of flux lines by the displacement field \( u(x) \), the relevant correlation function
to describe long range translational order is given by $K_G(x) = \langle e^{iG(u(x) - u(0))} \rangle$, where $G$ denotes the reciprocal lattice vector of the Abrikosov lattice. Recently, Emig at al. [9] found from a functional renormalization group (FRG) calculation

$$K_G(x) \sim \left[ L_\xi(x^2_z + \kappa z^2) \right]^{\eta_G/2},$$

where $x = (x^2_z, z)$, $z_l = (c_{11}/c_{44})^{1/2}z$ and $\kappa = c_{66}/c_{11}$. $c_{11}, c_{44}$ and $c_{66}$ are the effective elastic constants of the flux line lattice (renormalized by thermal and disorder effects). In the marginal cases $\kappa = 0$ and $\kappa = 1$ one finds from (6) for the structure factor

$$S(G + q) = \int d^3x \, e^{i\mathbf{q}\cdot \mathbf{x}} K_G(x) \sim \left( q^2 + \frac{c_{44}}{c_{66}} q^2 \right)^{-3/2},$$

i.e. the structure factor exhibits Bragg-peaks. The exponent $\bar{\eta}_G$ is non-universal and depends on the value of $\kappa$ ($1.143 \leq \bar{\eta}_G \leq 1.159$ for $1 \geq \kappa \geq 0$). In a large range of external fields $\kappa \approx \phi_0/16\pi \lambda^2 B$ such that one could in principle test these predictions by measuring the field-dependence of width of the Bragg peaks.

Next we come back to our original model (1), (4) keeping the lattice potential $v$ finite. Neglecting the non-Gaussian character of $\phi(x)$, which is justified for $\epsilon \ll 1$, lowest order perturbation theory in $v$ yields an effective Hamiltonian with a mass

$$g^2 p^2 v < \cos p\phi > \sim e^{-p^2 <\phi^2>/2} \sim \left( \frac{L}{L_\xi} \right)^{-p^2 \bar{\eta}/2}.$$ 

Comparing this power of $L$ with the $L^{-2}$ behaviour of elastic term, we conclude, that the periodic perturbation is always relevant if $p < p_c = \frac{6}{\pi^2 \epsilon}$. In this case, even an arbitrarily weak periodic potential will be relevant and we regain true translational LRO of the C-phase.

For $p > p_c$, on the other hand, weak periodic pinning is irrelevant, but for $p$ close to $p_c$ we expect a transition to a commensurate phase for sufficiently strong $v$. A simple estimate for the threshold value $v_c$ follows from a comparison of the forces resulting from impurity and lattice pinning. With $f_{\text{imp}} \approx \gamma L_\xi^{-2}$ and $f_v \approx g^2 pv$ we get for the transition line $v_c = v_c(\Delta) \approx 1/(g^2 pL_\xi^2)$ (or, inversely, $\Delta_c(v) \approx (g^2 pv)^{(4-D)/2}$).

A more accurate description of the transition can be obtained from a functional renormalization group treatment [10], which confirms this estimate. The transition turns out to be second order with a divergent correlation length $\xi \sim (v - v_c)^{-\nu}$ in the C-phase, here $\nu^{-1} = 4 \left( \frac{p^2}{p_c^2} - 1 \right)$. Moreover, the order parameter for translational LRO

$$\langle \psi \rangle = \langle e^{-i\theta} \rangle \sim (v - v_c)^\beta, \quad \beta = \frac{\nu \pi^2}{18}$$

is finite in this phase. On the contrary, in the I-phase the quasi-long range order of (3) is regained. The fixed point, which describes this transition is at zero
temperature. The temperature eigenvalue $-\theta = -2 + \epsilon$ appears in the modified hyperscaling relation $\nu(D - \theta) = 2 - \alpha$ typical for zero-temperature fixed points.

Figure 1: (a) Schematic RG-flow for $\delta = 0$ and $p > p_c$ in the $v - \Delta$ plane. $I, C$ and $D$ denote the I-, C- and the disordered phase. (b)Possible phase diagram for finite $\delta$ at fixed $v$ for $p > p_c$ and (c) for $p < p_c$.

As a site remark we note, that these exponents describe for $p = 2$ also the transition between the low temperature phase of the random field Ising model and the quasi–long range ordered phase of the random field XY–model.

Apart from the change in the correlation functions at the transition there is also a change in the response on a small external drive $f_{ex} \ll f_{imp}, f_v$. The creep velocity $u_{\text{creep}}$ can be written in the form

$$u_{\text{creep}}(f_{ex}) \sim e^{-\frac{E_c}{T}(\frac{f_{ex}}{f_{\text{imp}}})^\mu}.$$ \hspace{1cm} (10)

Here $E_c \approx \gamma \xi^{-2}$, $f_c \approx \max (f_{\text{imp}}, \gamma \xi^{-2})$ and $\mu = (D - 2)/2$ and $\mu = D - 1$ for the I– and the C–phase, respectively. Because of the pronounced difference in the creep exponent $\mu$ in both phases measurement of the creep should give a clear indication about which phase is present.

Recently measured I-V curves of the conductor o-TaS$_3$ at temperatures below 1K can be fitted by (10) with $\kappa = 1.5 - 2$ [11]. The experimentally observed tendency to larger $\kappa$ for purer crystals confirms the above interpretation. In several materials, such as K$_{0.3}$MoO$_3$, the periods are near $p = 4$ commensurability at low temperatures. For this material one obtains $\xi_0 \approx 10^{-6}$cm [10]. The typical parameters $\gamma V_0 \approx 10^{-2}$eV, $\rho_1 = 10^{-2}$ and $v_F = 10^7$cm/sec yield, after proper rescaling of anisotropy, the estimate $L_\xi \approx 10^{-4}$cm for an impurity density of 100ppm. Thus it should in principle be possible to see commensurability effects if the misfit $\delta$ becomes small enough, i.e. at low temperatures.

So far, we have excluded topological defects. These can be considered if we treat $\phi(x)$ as a multivalued field which may jump by multiples of $2\pi$ along certain
surfaces. These surfaces are bounded by vortex lines. For \( \delta = 0 = v \) it has been shown recently that for weak enough disorder strength \( \Delta < \Delta_D \), the system is stable with respect to the formation of vortices [12]. However, vortex lines will proliferate for \( \Delta > \Delta_D \). At present it is not clear whether the corresponding transition is continuous or first order. For \( \delta = 0 \) but \( v > 0 \) we expect that this transition extends to a line \( \Delta_D(v) \) until \( v \) reaches a critical value \( v_D \) with \( \Delta_D(v_D) = \Delta_c(v_D) \) (see Figure 1). For larger \( v \) the transition is probably in the universality class of the \( p \)-state clock model in a random field, which has an upper critical dimension \( D_c = 6 \). A non-zero value of \( \delta \) will in general increase the size of the incommensurate phase, as schematically sketched in Figure 1.

Our results can also be applied to the pinning of flux line lattices in type-II superconductors. In layered superconductors, the \( \text{CuO}_2 \) planes provide a strong pinning potential favoring, for flux lines oriented parallel to the layers, a smectic phase with translational order present only along the layering axis [13]. The influence of disorder on this phase is described by the CDW model studied in this paper, if the CDW phase \( \phi(x) \) is identified with the deviations of the smectic layers from their locked-in state. Also a FLL oriented perpendicular to the layers in general feels a weak periodic potential of the underlying crystal, but now the flux line displacements are described by a vector field. Since also in this case weak disorder leads only to logarithmically growing transverse displacement of the flux lines [9], a disorder driven roughening transition of the CDW type studied above can be expected for the flux line lattice.
References

1. G. Grüner, *Density waves in solids*, (Addison–Wesley, Reading, 1994),
   P. Bak, *Rep. Prog. Phys.* **45**, 587 (1982),
   V. L. Pokrovsky and A. L. Talapov, *Theory of Incommensurate Crystals*,
   Harwood Academic Publishers. 1984.
   P.M. Chaikin and T.C. Lubensky,*Principles of Condensed Matter Physics*, Cambridge UP 1995
2. A.D. Bruce, R.A. Cowley and A.F. Murray, *J. Phys. C* **11**, 351 (1978),
3. S.M. Battarcharjee, T. Nattermann and C. Ronnewinkel, *Phys.Rev.B* **58**, 2658 (1998).
4. S.N. Coppersmith et al.,*Phys. Rev. Lett.* **46**, 549 (1981).
5. J.M. Kosterlitz, *J. Phys. C* **10**, 3753 (1977).
6. A. Aharony and P. Bak,*Phys. Rev. B* **23**, 4770 (1981).
7. A.I. Larkin,*Sov. Phys. JETP*, **31**, 784 (1970),
   H. Fukuyama and P.A. Lee, *Phys. Rev. B* **17**, 535 (1978).
8. S. E. Korshunov, *Phys. Rev. B* **48**, 3969 (1993),
   T. Giamarchi and P. Le Doussal,*Phys. Rev. Lett.* **72**, 1530 (1994).
9. T. Emig, S. Bogner and T. Nattermann,*Phys. Rev. Lett.* **83** (1999), in press.
10. T. Emig, and T. Nattermann,*Phys. Rev. Lett.* **79**, 5090 (1997).
11. S. V. Zaitsev-Zotov, G. Remenyi and P. Monceau, *Phys. Rev. Lett.* **78**, 1098 (1997).
12. M. Gingras and D. A. Huse, *Phys. Rev. B* **53**, 15193 (1996)
   J. Kierfeld, T. Nattermann and T. Hwa, *Phys. Rev. B* **55**, 626 (1997),
   D. S. Fisher, *Phys. Rev. Lett.* **78**, 1964 (1997).
13. L. Balents and D.R. Nelson, *Phys. Rev. B* **52**, 12951 (1995).