Zeitschrift: Helvetica Physica Acta

Band: 56 (1983)

Heft: 5

Artikel: Commensurate-incommensurate transitions in 2 dimensions

Autor: Puga, M.W. / Simanek, E. / Beck, H.

DOI: https://doi.org/10.5169/seals-115435

Helvetica Physica Acta, Vol. **56** (1983) 1070–1087 0018–0238/83/051070–18$1.50 + 0.20/0

Commensurate–incommensurate transitions in 2 dimensions

By M. W. Puga*), E. Simanek†) and H. Beck, Institut de Physique, Université de Neuchâtel, Rue A.-L. Breguet 1, CH-2000 Neuchâtel (Switzerland)

(25. II. 1983; rev. 1. VI. 1983)

Abstract. We study the commensurate–incommensurate transitions of a two-dimensional system via a renormalization group method which includes incommensurability as a renormalizable parameter. The phase boundary is found by numerical methods. The correlation length exponent ν is obtained and shown to depend continuously on the parameters of the model. For typical values of these parameters we find $\nu \approx 0.35$, in good agreement with experimental work on adsorbed monolayers.

1. Introduction

Structural transitions in two-dimensional (2D) systems of various kinds have been studied extensively in recent years, both experimentally and theoretically. Prominent examples of 2D lattices which undergo transitions from a state which is commensurate with respect to some external periodic structure to an incommensurate state (CI-transition) are mono-layers adsorbed on a substrate like graphite, 2D charge density waves and vortex lattices in thin type II superconductors [1].

The mathematical model which we analyse in this paper contains all the important features of a system undergoing a CI-transition. Its details, however, are specifically chosen such as to describe the physics of a vortex lattice in a superconducting layer. Such a lattice is created by applying a magnetic field perpendicular to an extremely thin superconductor [2]. The field is able to penetrate the film forming vortices of normal material in the superconducting background. They form a triangular lattice with the lattice constant depending on the magnetic field applied. Since those vortices have a self energy proportional to their actual length (thickness of the material), a modulation of the thickness has the effect of making it energetically more favorable for the vortices to sit in region of minimum thickness of the modulated substrate. Thus, a competition arises between the vortex–vortex interaction which tries to keep the vortices in their 'natural' lattice structure and the substrate which tries to make the lattice commensurate by forcing the vortices into its wells.

In the continuum approximation, the Hamiltonian of the system can be

---

*) Present address: Dépt de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland.

†) Permanent address: Physics Department, University of California, Riverside, CA 92502 (USA)

written as [3],

$$\mathcal{H} = \int d^2x \left\{ \frac{\lambda}{2} \left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right]^2 + \frac{\mu}{2} \left[\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right] + V_0 \cos\left(\frac{2\pi}{a} u + \delta x \right) \right\} \tag{1.1}$$

where λ and μ are the elastic constants of the system, u and v the components of the displacement vector along the x and y direction, respectively, V_0 the strength of the modulation that we assume to vary harmonically along the x direction, and δ the mismatch parameter which measures the incommensurability between the system and the substrate.

For $\delta = 0$, system and substrate are commensurate, such that for $T = 0$ we can have the vortices sitting in the potential wells *and* forming a triangular lattice as well ($u = 0$ everywhere). We have therefore a commensurate phase which can be unlocked by thermal fluctuations as the temperature rises. However, if the value of δ is strong enough, we might have already an incommensurate situation at zero temperature. We expect therefore a phase boundary in the δ, T plane with a locked commensurate phase for small values of δ and T, and an unlocked phase otherwise. In this paper, we present a study of this phase boundary and the analytical properties of various quantities near the boundary. We base our work on a renormalization group (RG) calculation which has the new feature of introducing δ as a renormalizable parameter, allowing for the study of the critical boundary.

In Section II, we present in detail the application of the RG techniques to (1.1). Section III is devoted to an analytical study of the RG equations in the case $\delta = 0$, and to the new phenomena appearing for $\delta \neq 0$. A survey of the complete RG solutions based on our nuumerical work is given in Section IV. We discuss and summarize the results in the last section of this work.

2. Renormalization group equations

In this section, we present the RG techniques which allow us to obtain a system of differential equations for the parameters of the Hamiltonian (1.1). We start by introducing a cut-off Λ in momentum space essentially related to the inverse lattice constant $a (\Lambda = 2\pi/a)$. We then define a second cut-off Λ' (infinitesimally) close to Λ and eliminate the field fluctuations between Λ' and Λ. Splitting the field in the following way:

$$u(\vec{x}) = u_0(\vec{x}) + u_1(\vec{x}) \equiv \int_0^{\Lambda'} \frac{d^2k}{(2\pi)^2} e^{i\vec{k}\cdot\vec{x}} u(\vec{k}) + \int_{\Lambda'}^{\Lambda} \frac{d^2k}{(2\pi)^2} e^{i\vec{k}\cdot\vec{x}} u(\vec{k}) \tag{2.1}$$

(and the same for v), defining the parameter $dt = 1 - \Lambda'/\Lambda$ and the scaled variables and fields

$$\begin{aligned} \vec{k}' &= \vec{k}/(1-dt) & \vec{x}' &= \vec{x}(1-dt) \\ u'(\vec{k}') &= u(\vec{k})/\xi & v'(\vec{k}') &= v(\vec{k})/\xi \end{aligned} \tag{2.2}$$

we obtain the following relations:

$$u_0(\vec{x})=\xi(1-dt)^2u'(\vec{x}'),\qquad v_0(\vec{x})=\xi(1-dt)^2v'(\vec{x}').$$

The calculation of the partition function

$$z=\int\prod_{q,k} du_q\, dv_k e^{-\mathscr{L}}$$

where $\mathscr{L}=\mathscr{H}/T$, can be achieved in two steps. We first integrate over the fast changing Fourier components of the field with $\Lambda'\leq q, k\leq\Lambda$ and then over the rest. This intermediate step allows us to define a new quantity $\mathscr{L}'$ by the following relation:

$$\begin{aligned} Z&=\int\prod_{q<\Lambda'}\prod_{k<\Lambda'} du_q\, dv_k e^{-\mathscr{L}'}\\ \mathscr{L}'&=\ln\int\prod_{q>\Lambda'}\prod_{k>\Lambda'} e^{-\mathscr{L}}.\end{aligned}\tag{2.3}$$

We can split $\mathscr{L}$ into two parts:

$$\begin{aligned}\mathscr{L}&=\mathscr{L}_0+N\\ \mathscr{L}_0(u,v)&=\int d^2x\left\{\frac{\alpha}{2}\left[\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right]^2\right.\\ &\quad\left.+\frac{\beta}{2}\left[\left(\frac{\partial u}{\partial x}-\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2\right]\right\}\\ N(u)&=\int d^2x\left\{\gamma\cos\left(\frac{2\pi}{a}u+\delta x\right)\right\}\end{aligned}\tag{2.4}$$

where we have defined: $\alpha=\lambda/T$, $\beta=\mu/T$, $\gamma=V_0/T$.

Splitting the fields according to (2.1) we find that the cross terms do not contribute to the integral in (2.3) and we obtain:

$$\begin{aligned}\mathscr{L}'&=-\ln\int\mathscr{D}u_1\mathscr{D}v_1 e^{-\mathscr{L}_0(u_0,v_0)-\mathscr{L}_0(u_q,v_q)-N(u_0+u_1)}\\ &=\mathscr{L}_0(u_0,v_0)-\ln\langle\exp(-N(u_0+u_1))\rangle\end{aligned}\tag{2.5}$$

where we use the notations:

$$\begin{aligned}\langle F\rangle&=\int\mathscr{D}_{u1}\mathscr{D}v_1 e^{-\mathscr{L}_0(u_1,v_1)}F\\ \mathscr{D}u_1&\equiv\prod_{k>\Lambda'}du_k.\end{aligned}\tag{2.6}$$

Using the expansion

$$\ln\langle e^{-\gamma t}\rangle=\sum_{n=1}^{\infty}\frac{(-\gamma)^n}{n!}\langle t^n\rangle_c$$

we obtain

$$\begin{aligned}\mathscr{L}'&=\mathscr{L}_0(u_0,v_0)\\ &\quad-\sum_{n=1}^{\infty}\frac{(-\gamma)^n}{n!}\left\langle\int\prod_{i=1}^{n}d^2x_i\cos\left(\frac{2\pi}{a}u(\vec{x}_i)+\delta x_i\right)\right\rangle_c\end{aligned}\tag{2.7}$$

where $\langle A\rangle_c$ denotes the cumulant part of $\langle A\rangle$. $\mathscr{L}_0(u_0, v_0)$ can be expressed in terms of the primed fields

$$\mathscr{L}_0=\int d^2x'\left\{\frac{\alpha}{2}\left[\frac{\partial u'}{\partial x'}-\frac{\partial v'}{\partial y'}\right]^2 + \frac{\beta}{2}\left[\left(\frac{\partial u'}{\partial x'}-\frac{\partial v'}{\partial y'}\right)^2\left(\frac{\partial u'}{\partial y'}+\frac{\partial v'}{\partial x'}\right)^2\right]\right\} \tag{2.8}$$

where we have chosen ξ, by

$$\xi(1-dt)^2=1$$

such that the argument of the cosine is left invariant.

We restrict ourselves to the first two terms of the series (2.7), i.e. $n=1$ and 2.

$n=1$:

$$\mathscr{L}_1=\gamma\int d^2x\left\langle\cos\left(\frac{2\pi}{a}(u_0+u_1+\delta x)\right)\right\rangle \tag{2.9}$$

The average $\langle\sin(2\pi/a)u_1\rangle$ vanishes by symmetry while

$$\left\langle\cos\frac{2\pi}{a}u_1\right\rangle=e^{-\frac{1}{2}(2\pi/a)^2\langle u_1^2\rangle}, \tag{2.10}$$

since (2.6) is an average over a Gaussian field distribution. Using the fact that $\langle u_1^2\rangle$ is linear in dt and expanding to first order we obtain

$$\mathscr{L}_1'=\bar{\gamma}\int d^2x'\cos\left(\frac{2\pi}{a}u'+\frac{\delta x'}{1-dt}\right)$$

where

$$\bar{\gamma}=\gamma(1+2dt)\left(1-\frac{2\pi^2}{a^2}\langle u_1^2\rangle\right) \tag{2.11}$$

which introduces a renormalization of γ.

For $n=2$, we have to evaluate

$$\mathscr{L}_2=-\frac{\gamma^2}{2}\int d^2x\int d^2\hat{x}\left\langle\cos\left(\frac{2\pi}{a}(u_0+u_1)+\delta x\right)\cos\left(\frac{2\pi}{a}(\hat{u}_0+\hat{u}_1)+\delta\hat{x}\right)\right\rangle_c.$$

We use the trigonometric identity

$$\begin{aligned}\cos(A_0+A_1)\cos(\hat{A}_0+\hat{A}_1)=\tfrac{1}{2}\{&\cos(A-\hat{A}_0)\cos(A_1-\hat{A}_1)\\ &-\sin(A-\hat{A}_0)\sin(A_1-\hat{A}_1)\\ &+\cos(A_0+\hat{A}_0)\cos(A_1+\hat{A}_1)\\ &-\sin(A_0+\hat{A}_0)\sin(A_1+\hat{A}_1)\}\end{aligned}$$

with

$$A_0=\frac{2\pi}{a}u_0+\delta x;\qquad A_1=\frac{2\pi u_1}{a}.$$

Since averages involve only u_1, $\hat{u}_1$, the averages $\sin(A_1\pm\hat{A}_1)$ vanish. The term $\cos(A_0+\hat{A}_0)$ generates a higher harmonic of the type $\cos(2u)$. We can see from an argument already given by Pokrovsky and Talapov [3] and Wiegmann [4] that an harmonic of the type $\cos(nu)$ contributes via the renormalization group to an equation similar to (2.11), but with the factor $(1-2\pi^2/a^2\langle u_1^2\rangle)$ replaced by $(1-(2\pi^2/a^2)n^2\langle u_1^2\rangle)$. For temperatures close to the transition temperature these contributions decrease more rapidly than the one generated by the first harmonic and can therefore be neglected. We therefore obtain:

$$\mathcal{L}_2=-\frac{\gamma^2}{4}\int d^2r\int d^2\rho \cos\left(\frac{2\pi}{a}\vec{\rho}\cdot\vec{\nabla}u+\delta\rho\cos\phi\right)\langle\cos(A_1-\hat{A}_1)\rangle_c$$

where we have defined $\vec{\rho}=\vec{r}-\hat{\vec{r}}$ and we have expanded the (slow) fluctuations of $\vec{u}$, keeping only terms in $\vec{\nabla}u$.

We now separate the sum inside the argument of the cosine and expand the terms in $\vec{\nabla}u$, keeping however the full expression for the terms in δ. We obtain:

$$\mathcal{L}_2=-\frac{\gamma^2}{4}\int d^2r\int d^2\rho\left[-\frac{2\pi^2}{a^2}(\vec{\rho}\cdot\vec{\nabla}u)^2\cos(\delta\rho\cos\phi)\right.$$
$$\left.-\frac{2\pi}{a}(\vec{\rho}\cdot\vec{\nabla}u)\sin(\delta\rho\cos\phi)\right]\cdot\langle\cos(A_1-\hat{A}_1)\rangle_c.$$

The function $\langle\cos(A_1-\hat{A}_1)\rangle_c$ is of first order in dt, it drops to zero very slowly $(\sim 1/\rho)$ for large ρ and needs to be approximated to make the previous integral converge.

We neglect its angular dependence and, following Wiegmann [4] approximate the ρ integrals by a constant of order unity. Introducing the primed variables and performing the angular integral, to first order in dt, we obtain,

$$\mathcal{L}_2=\frac{\gamma^2}{4}\int d^2x'\left[\frac{2\pi^2}{a^2}I\left(\left(\frac{\partial u'}{\partial x'}\right)^2+\left(\frac{\partial u'}{\partial y'}\right)^2\right)+\frac{2\pi}{a}J\frac{\partial u'}{\partial x'}\right]dt \tag{2.12}$$

with

$$I=\frac{2\pi}{\Lambda^4}J_1'\left(\frac{\delta}{\Lambda}\right)$$
$$J=\frac{2\pi}{\Lambda^3}J_1\left(\frac{\delta}{\Lambda}\right),$$

J_1 being the first order Bessel function. Moreover, we have approximated the coefficient of $(\partial u/\partial y)^2$ by the one of $(\partial u/\partial x)^2$, ignoring thus the small anisotropic effect created by the presence of a non-zero δ. (These terms are equal if $\delta=0$).

The essential features of formula (2.12) are the renormalization of the parameters associated with deformations perpendicular to the potential wells $((\partial u/\partial x)^2, (\partial u/\partial y)^2)$, and the appearance of a term linear in $\partial u/\partial x$ which was not present in the original Hamiltonian. This new term is due to a non-zero δ and can be eliminated by a simple translation of the fields.

For the sake of full generality we should, however, start from a more general $\mathcal{L}_0$ singling out the coefficients of $(\partial u/\partial x)^2$ and $(\partial u/\partial y)^2$ which are the ones subject to renormalization according to (2.12). We write (introducing a new parameter H)

$$\mathcal{L}_0=\int d^2x\left\{\frac{1}{2}\left[(H+\alpha)\left(\frac{\partial u}{\partial x}\right)^2+H\left(\frac{\partial v}{\partial y}\right)^2\right]+\frac{\alpha+\beta}{2}\left(\frac{\partial v}{\partial y}\right)^2\right.$$
$$\left.+(\alpha-\beta)\frac{\partial u}{\partial x}\frac{\partial v}{\partial y}+\beta\left[\frac{1}{2}\left(\frac{\partial v}{\partial x}\right)^2+\frac{\partial u}{\partial y}\frac{\partial v}{\partial x}\right]\right\}. \tag{2.13}$$

In order to compare the 'new Hamiltonian', i.e. $\mathscr{L}_0'+\mathscr{L}_1'+\mathscr{L}_2'$, with (2.13) we introduce the shifted fields $(\hat{u}, \hat{v})$ by

$$u' = \hat{u} + x'\Delta\, dt$$
$$v' = \hat{v} + y'\Delta'\, dt \tag{2.14}$$

and determine Δ and Δ' by requiring that the linear term in (2.12) be eliminated. This yields

$$\Delta = -\frac{\pi\gamma^2}{2a} J\bigg/\left(H-\beta+\frac{4\alpha\beta}{\alpha+\beta}\right)$$
$$\Delta' = -\frac{\alpha-\beta}{\alpha+\beta}\Delta. \tag{2.15}$$

The cosine term in L_1 gets now changed into

$$\cos\left(\frac{2\pi}{a}u' + \frac{\delta x'}{1-dt}\right) = \cos\left(\frac{2\pi}{a}\hat{u} + \left[\frac{\delta}{1-dt} + \Delta\, dt\right]x'\right).$$

The quantity in the square bracket gives the renormalized value of δ. To first order in dt we obtain:

$$\bar{\delta} = \delta + (\delta+\Delta)\, dt \tag{2.16}$$

and comparing (2.12) and (2.13)

$$\bar{H} = H + \frac{\gamma^2\pi^2}{a^2} I\, dt. \tag{2.17}$$

Formulae (2.11, 2.16 and 2.17) give now the renormalized parameters as a function of the old ones. From them, differential equations for $\bar{\alpha}$, $\bar{\beta}$, $\bar{\delta}$, $\bar{\gamma}$, $\bar{H}$ are readily obtained. We relate to Appendix A the calculation of $\langle u_1^2\rangle$, and introduce the variables

$$x \equiv \frac{\bar{H}}{\beta} \qquad y \equiv \frac{a\bar{\gamma}}{4\sqrt{\pi\beta}} \qquad z \equiv \frac{\bar{\delta}}{\Lambda}$$

and dimensionless constants

$$\theta = \frac{V_0}{\mu} \qquad \tau = \frac{\pi T}{\mu a^2} \qquad A = \frac{\lambda}{\mu}$$

to obtain

$$\dot{x} = 2y^2 J_1'(z) \qquad x(0) = 1$$
$$\dot{y} = y\left[2 - \frac{\tau}{2}G'(x)\right], \qquad G'(x) = \frac{2}{x}\left[1 - \frac{A}{x+A+\sqrt{x(x+A)(1+A)}}\right], \tag{2.18}$$
$$y(0) = \frac{\theta}{4\sqrt{\tau}}$$
$$\dot{z} = z - 2y^2\frac{J_1(z)}{x-1+\dfrac{4A}{1+A}} \qquad z(0) = \frac{\delta}{\Lambda},$$
$$\dot{\alpha} = 0 \qquad \dot{\beta} = 0$$

where we choose the initial value $H = \beta$ such that (2.13) agrees with (2.4) and find that the right hand side of the equations depend on the initial values A and τ due to the fact that the coefficients $\bar{\alpha}$ and $\bar{\beta}$ do not renormalize. The dot means differentiation with respect to t which we will interpret as 'time' for the purpose of illustration. In the next section, we study in detail these equations.

3. Analytical solutions of the RG equations

The set of equations (2.18) can now be analyzed to study the critical properties of our system. We start by studying in detail the case $\delta = 0$. If the initial value of z is zero, z remains zero, and the effective RG equations reduce to the more simple ones:

$$\begin{aligned} \dot{x} &= y^2 \\ \dot{y} &= y\left[2 - \frac{\tau}{2} G'(x)\right]. \end{aligned} \tag{3.1}$$

Eliminating t between the two equations, one gets an analytic solution for the RG-trajectory in the x, y plane given by

$$\begin{aligned} y^2 &= y_0^2 + 4(x+1) - \tau G(x), \\ G(x) &= \int_1^x G'(x)\,dx = 4 \ln\left[\frac{\sqrt{x} + \sqrt{\dfrac{x+A}{1+A}}}{2}\right] \end{aligned} \tag{3.2}$$

where y_0 is given in (2.18).

We present these trajectories in Fig. 1. Keeping all initial parameters fixed and varying the temperature, we obtain different values of y_0 as the initial condition for renormalization. For temperatures close to the transition temperature we observe two distinct behaviours:

(a) In some temperature domain, the value of y initially decreases and then increases, renormalizing the potential to a huge effective value. This shows the dominance of the potential part over the thermal fluctuations and signals a situation where the lattice is looked to the substrate [5]: we are in the commensurate phase.

(b) For higher temperatures, a different behavior sets in and the curves flow into the x-axis, effectively reducing the potential to zero and indicating the existence of an unlocked or incommensurate phase which has been described in previous papers [3, 6]. The variable x (renormalization of μ) reaches a finite value which is higher than the initial value.

There is a separatrix which has its minimum on the x axis and separates both behaviours. This curve is calculated by setting $y = 0$ at the minimum:

$$\frac{4(x_c - 1)}{\tau_c} + \frac{\theta^2}{16\tau_c^2} = G(x_c) \tag{3.3}$$

and

$$\frac{4}{\tau_c} = G'(x_c),$$

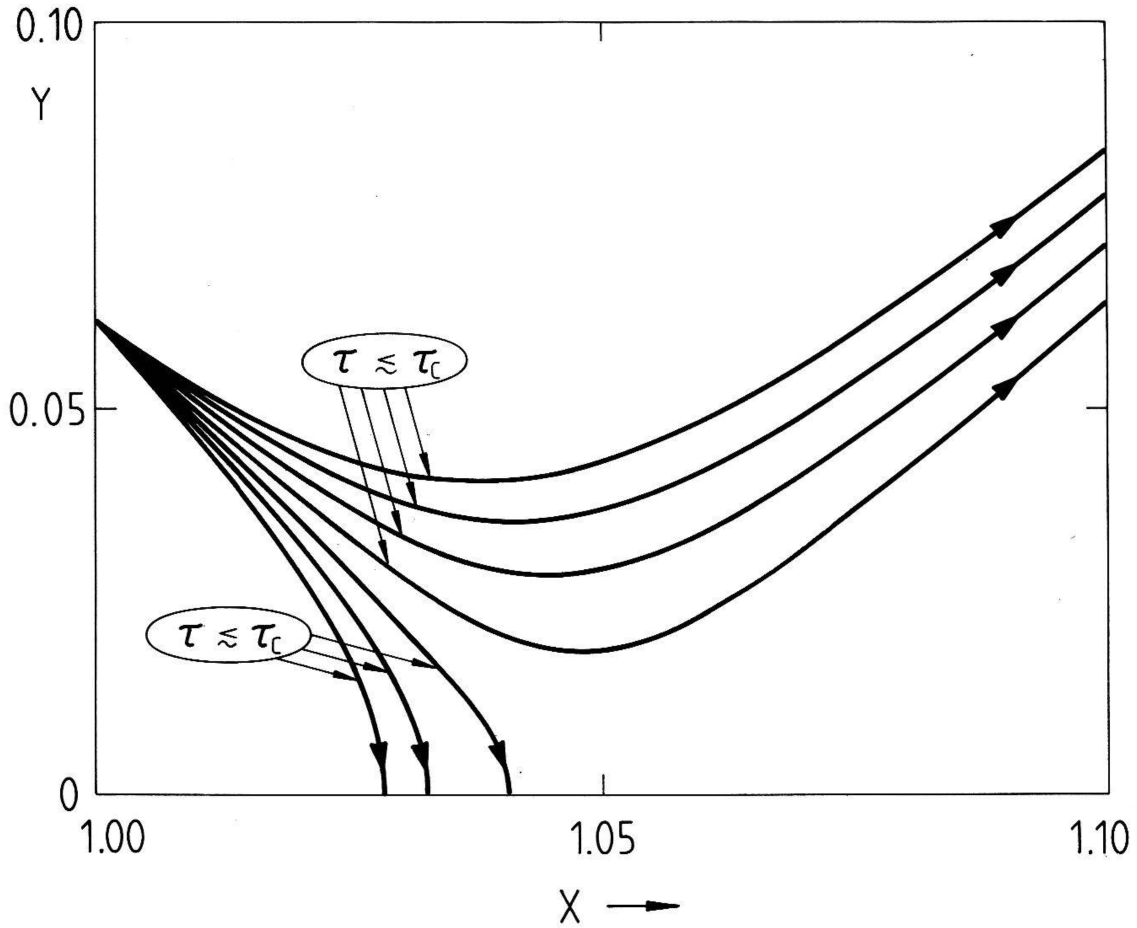

Figure 1
Renormalization group trajectories (solutions of (3.1) subject to the initial conditions given in (2.18)) in the (x, y)-plane for $\delta = 0$, $A = 1000$, $\theta = 0.5$. The various curves correspond to different initial values of y, i.e. to different (reduced) temperature values τ, close to the critical value (3.4).

where we have defined $\tau_c = \pi T_c/\mu a^2$, and $x_c = \bar{H}(\infty)/\beta$ is the final renormalized value of H at the critical temperature T_c. To calculate T_c one should eliminate x_c between both equations and solve for τ_c as a function of θ and A.

Solving (3.3) for small values of θ we find:

$$\tau_c = 4\frac{1+A}{2+A}[1+R\theta]+o(\theta^2) \tag{3.4}$$

with

$$R = \left[\frac{8(1+A)+3A^2}{2^9(1+A)^2}\right]^{1/2}. \tag{3.5}$$

Neglecting V_0 we find precisely the value given by Pokrovskii and Talapov [3]; to first order in V_0, some corrections appear in agreement with other previous work [5, 7].

In the high temperature phase, there is a sequence of stable fixed points (x_∞) on the x axis which give the renormalized values of the coupling constant H in (2.13) as a function of temperature. By putting $y = 0$ in (3.2) and expanding near x_∞, T_c we obtain the typical square root behaviour for μ near T_c:

$$\tilde{H}_\infty(T) = \tilde{H}_\infty(T_c) - D[T-T_c]^{1/2} \tag{3.6}$$

with D being a positive constant which depends on the initial parameters. We can also calculate the form of the correlation length below T_c. Following the method developed by Kosterlitz for a simpler problem [8], we first eliminate y between (3.1) and (3.2) to solve for x as a function of t:

$$t = \int_1^x dx' \left[4(x'-1) + \frac{\theta^2}{16\tau} - \tau G(x')\right]^{-1}. \tag{3.7}$$

For high values of x and y, the renormalization group equations become meaningless since they were based on a small y expansion. We therefore stop at a particular value of x (say x_R of order unity), and use (3.7) to solve for t as a function of temperature; clearly as T approaches T_c from below the integrand has a pole at $x = x_\infty(T_c)$ and t diverges; expanding the denominator for x' close to $x_\infty(T_c)$ and τ close to τ_c we obtain:

$$t = \int_1^{x_R} dx'[a(x' - x_\infty(T_c))^2 + b(\tau - \tau_c)]^{-2} \propto [\tau_c - \tau]^{-1/2}.$$

Since by definition $t = \ln \Lambda$, the divergence of t is associated with the divergence of the inverse correlation length, and we obtain:

$$\xi \propto e^{-t} \propto \exp[-\alpha/\sqrt{T_c - T}], \tag{3.8}$$

which is a typical 'Kosterlitz-Thouless behaviour' for T close to T_c^- and $\delta = 0$. This completes our study of the $\delta = 0$ case. All these conclusions have already been found in our previous analysis [4] of the more simple 2D Sine-Gordon Hamiltonian. The introduction of two field components (u, v) has changed the equations of the renormalization group. They keep, however, the same essential form close to the fixed point, which determines the critical behaviour of the system. For the case $\delta \neq 0$, the full equations given in (2.18) must be used. We first point out that besides the $\delta = 0$ fixed points discussed above (i.e. the points $(x_\infty, 0, 0)$), there is a new fixed point $P^* \equiv (x^*, y^*, z^*)$ with a non-zero value of z^*. It is given by the conditions:

$$\begin{aligned} &\frac{4}{\tau} = G'(x^*) \\ &y^* = \left[\frac{z^*(x^* - 1 + 4A/(A+1))}{2J_1(z^*)}\right]^{1/2} \end{aligned} \tag{3.9}$$

Due to the small y expansion on which our theory is based, we must use small values of y_0 as initial conditions. As we will see later, for such input values, only the smallest value of z^* satisfying (3.9) will be important to determine the transition. We therefore restrict ourselves to this first root. We should also notice that this is a plane of fixed points since P^* depends on the two initial parameters A and τ due to the fact that $\bar{\alpha}$ and $\bar{\beta}$ do not renormalize in (2.13).

To study the nature of such a new fixed point we linearize the equations near it; we easily obtain:

$$\begin{aligned} \dot{x} &= -a(z - z^*) \\ \dot{y} &= b(x - x^*) \\ \dot{z} &= z - c(y - y^*) + d(x - x^*), \end{aligned} \tag{3.10}$$

where we have defined the *positive* quantities:

$$a = 2y^{*2}\,|J_1''(z^*)| > 0, \qquad b = -\tau_c y^* G''(x^*)/2 > 0$$
$$c = 2z^*/y^* > 0, \qquad d = z^{*2}/(2y^{*2}J_1(z^*)) > 0.$$

Obviously (3.10), is solved by the usual exponential form $A - A^* \equiv \Delta A = \Delta A_0 e^{\omega t}$ for $A = x$, y or z, where ω is a root of the eigenvalue equation

$$\omega^3 - \omega^2 + ad\omega - abc = 0. \tag{3.11}$$

In Appendix A, we prove that for the usual range of experimental values of the parameters (i.e. $\zeta \geq \beta$) one finds a positive real root and two complex conjugate with a negative real part. In a neighbourhood of the new fixed point there is therefore a plane spanned by the two eigenvectors with complex eigenvalues. In this plane the trajectory will tend towards the fixed point in an oscillatory fashion. Slightly below (above) that plane the curve will move down (up) *away* from this point. Two limiting behaviours are then expected, which we first discuss qualitatively:

(a) If the initial temperature is such that we already were in the incommensurate phase for $\delta = 0$, a finite δ will only decrease the 'speed' at which x is growing ($J'(z) < 1$) and these smaller values of x will in turn reduce the rate of growth for y; we will therefore reach a point on the x axis ($x = x_\infty$, $y = 0$) which signals the incommensurate phase. This is as expected physically: a finite value of δ helps incommensurability. Notice that since $y \to 0$ and $J_1(z)$ is bounded we will approach a limiting behaviour for z of the exponential type:

$$\dot{z} = z.$$

This indicates that in the incommensurate phase the value of z (renormalization of δ) moves to higher and higher values physically suggesting a dominance of the δ terms (which favours incommensurability) over the V_0 terms (which favours commensurability).

(b) Suppose now that we start with a low value of temperature such that for $\delta = 0$ we would be in the commensurate phase. This means that the $\delta = 0$ curve moves towards a region of increasing x and decreasing y, until a value of $x \approx x_\infty(T_c)$ is reached. At this value $\dot{y}$ will change a sign and y will start increasing forcing x to keep increasing at a higher rate until very high values of x and y are reached signaling an effectively stong potential and the existence of the commensurate phase. If we now start with a non-zero δ, the term $J'(z) < 1$ will slow down the rate at which x is growing; but if δ is not very big the point $x_\infty(T_c)$ might be, nevertheless, approached and the previous analysis applies, indicating that the commensurate phase is still the most favorable. Such a value of δ, though non-zero, is not big enough to change the nature of the $\delta = 0$ phase.

Notice that in this case, in the z equation, the large values of y and small values of z cause the negative term to dominate over the positive one and we have z decreasing exponentially to zero. δ is being effectively renormalized to zero, a characteristic of the commensurate phase. If we now feed a bigger initial value of δ into our equations, x might be slowed down enough to prevent that

$x_\infty(T_c)$ is reached. This will cause y to decrease to zero, z to increase to infinity and the incommensurate phase will set in.

There are therefore two distinct behaviours. For small values of T and δ the system is renormalized to the asymptotic limit $(\infty, \infty, 0)$ which signals the commensurate phase. For large values of T or δ, the system tends towards $(x_\infty, 0, \infty)$ indicating the incommensurate phase. There is thus a curve in the T, δ plane which separates the two behaviours and that could in principle be calculated by choosing the initial conditions such that the renormalization curves will tend towards the new fixed point. We study this phase boundary by numerical methods in the next section.

4. Numerical studies

We numerically integrated the system of equation (2.18) for given values of the initial parameters V_0, μ, λ, T and δ. In Fig. 2, we present the results.

The plane x, y is a reproduction of Fig. 1, where we see the main behaviour of the solutions in the two phases. Starting now from the points B_1, B_2, B_3, where the system would be in the commensurate phase for $\delta = 0$, we observe the transition as it was pointed out before. For each value of temperature (below the critical point at $\delta = 0$) there is a critical value $\delta_c(T)$ of δ for which the system changes drastically its asymptotic behaviour. Close to the critical curve starting at B_2 and running into P^*, we observe the solutions to oscillate near P^* in accordance with the complex character of the eigenvalues mentioned in the previous section.

To study the shape of the phase boundary one has to integrate equations (2.18) keeping λ, μ and V_0 fixed, and varying δ for fixed T to search for the value

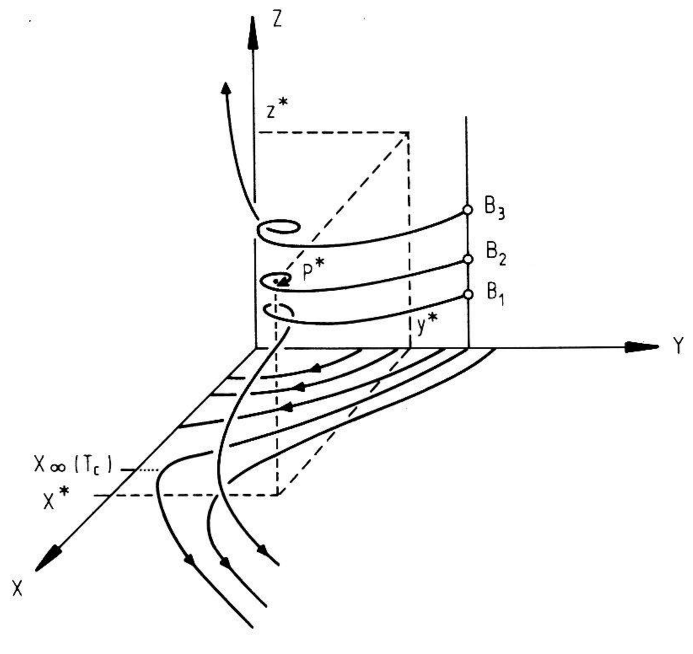

Figure 2
RG-trajectories (solutions of (2.18)) in (x, y, z)-space for various initial values of y and z, i.e. of temperature and δ (see text).

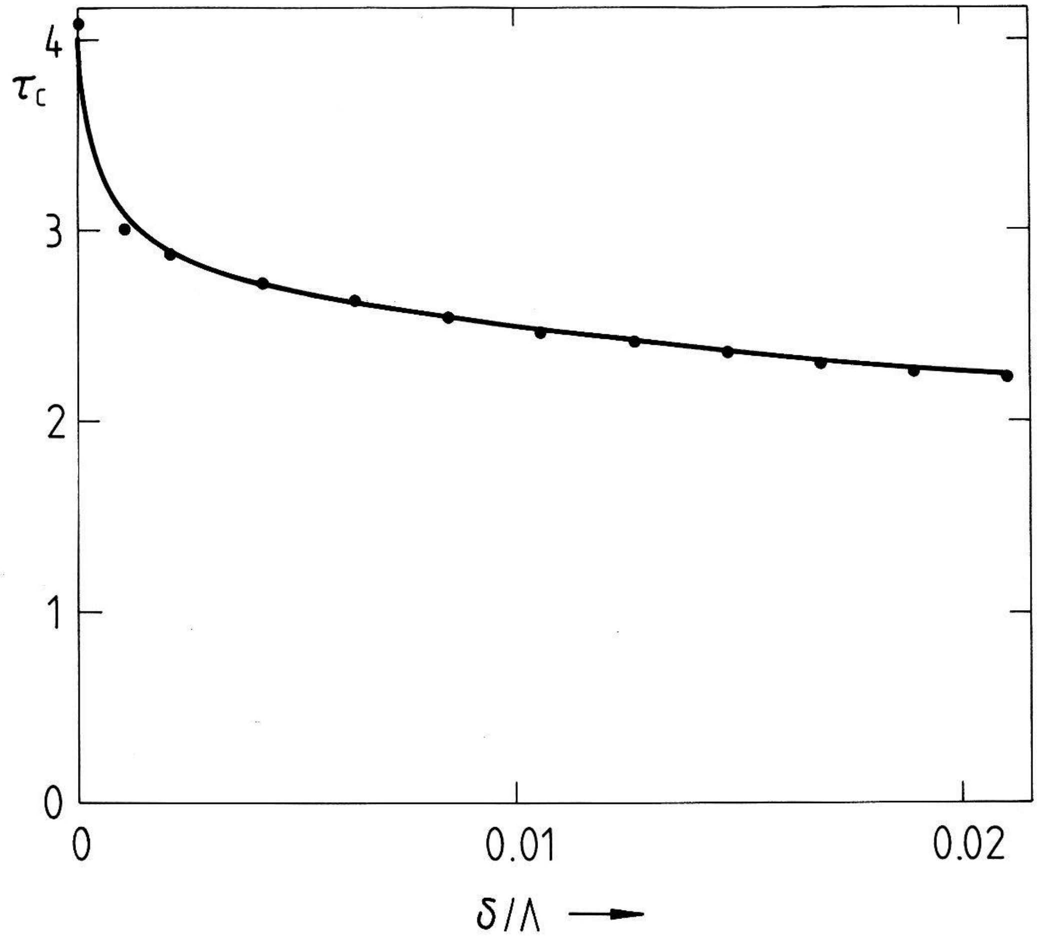

Figure 3
Phase boundary $\tau_c = \tau_c(\delta)$ between commensurate $(\tau < \tau_c)$ and incommensurate $(\tau < \tau_c)$ domains for $A = \infty$ (incompressible lattice), $\theta = 0.1$.

of δ (corresponding to B_2 in Fig. 2) at which the asymptotic behaviour changes. Repeating the procedure for different values of T, the shape of the phase boundary can be constructed numerically. This form will be more accurate for small values of δ since the renormalization equations are better for values of temperature close to the critical one for zero δ, i.e. for small y. The result of such a numerical search for the phase boundary is plotted in Fig. 3. We observe a linear relation in most of the range; for very small values of δ there is a cusp.

Information about the correlation length near T_c can be obtained from the system (2.18). As pointed out for the case $\delta = 0$, we integrate the equations below T_c up to the point where $z = z_{\hat{R}}$ is on the order of z^* and calculate the characteristic 'time' $\hat{t}$ for such value to be reached. The correlation length is then given by:

$$\xi \propto e^{\hat{t}}.$$

This $\hat{t}$ can be estimated from the fact that for z-values close to z^* we have an exponential growth:

$$z \approx z^* + \frac{\delta - \delta_c}{\Lambda} e^{\omega \hat{t}}$$

where ω is simply the real eigenvalue calculated in the linearization technique. Stopping at $z = z_R$ we have

$$(z_R - z^*)e^{-\omega \hat{t}} \propto \delta - \delta_c, \Rightarrow \xi = k(\delta - \delta_c)^{-1/\omega} \tag{4.1}$$

where k is an uninteresting constant, and the critical exponent ν is simply given by the inverse of the real root of equation (3.11). We notice that the coefficient ad in (3.11) is a numerical factor $\simeq 2.386$. However, the product (abc) depends on the parameters of the problem through τ_c, x^*, y^*, yielding the remarkable fact that the exponent is parameter dependent [9]. This is a direct consequence of the existing plane of fixed points generated as the values of A and τ change. In Appendix B we study in detail this exponent and find that the dependence on θ is small for the range of validity of our theory ($0 \leq \theta \lesssim 1$, since we have truncated a series in V_0 after the second order). The dependence on μ/λ is plotted in Fig. 4, for $\delta = 0$. We obtain a smooth curve between the limits 0.32 for $\lambda \to \infty$, and 0.44 for $\lambda = \mu$. The lowest value (0.32) is the one applicable for the vortex lattice, which is virtually incompressible. For an elastic lattice in general we would expect $\lambda > \mu$. Therefore ν should be around 0.35, which is in good agreement with experimental data for adsorbed monolayers [10, 11, 12]. There the misfit m, behaving like [9]

$$m \propto (\delta - \delta_c)^{\beta} \propto \xi^{-1}$$

is measured.

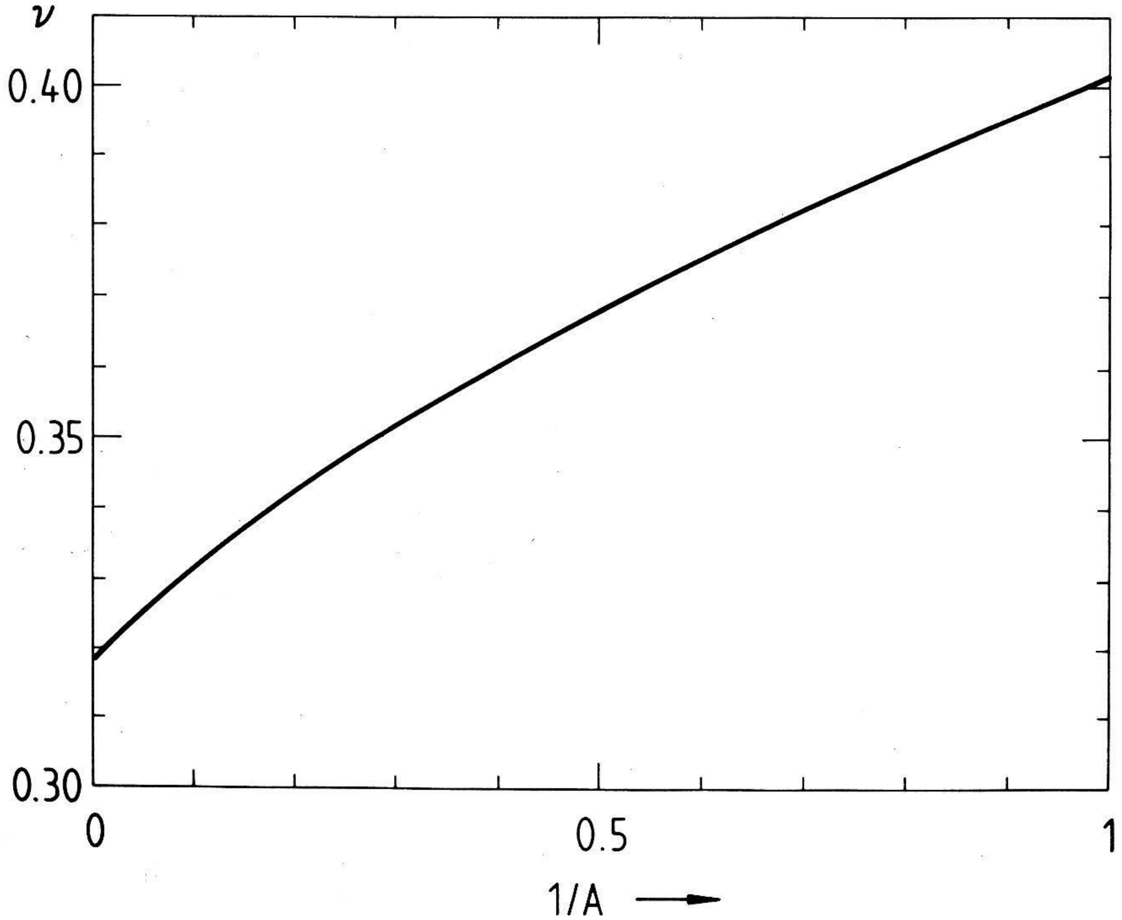

Figure 4.
Values of the critical exponent ν as a function of $A^{-1} = \mu/\lambda$ and small $\theta = V_0/\mu$ and δ_c.

When δ becomes non-zero, the τ_c-dependence of ω, through the coefficient abc in (3.11), becomes also apparent. In Appendix B we present some values of ν (for $A=\infty$), following the phase boundary $\tau_c(\delta)$. The general tendency is that ν decreases with decreasing T_c. It is interesting to note that this is precisely what Stephens et al. [10] found for Kr-monolayers on graphite: $\beta=\nu=0.32$ at $T_c=89$ K and $\nu=0.26$ for $T_c=80$ K. Although our theory is only reliable for small δ, it predicts an exponent $\nu=0$ in the limit $T_c\to 0$ (at the critical δ-value for the zero temperature CI transition, discussed by many authors [3, 6]). This is compatible with the logarithmic law ($\xi \propto \ln|\delta-\delta_c|$) put forward by Talapov [3]. As previously discussed in a recent publication [5], these numerical values of the critical exponents should not be regarded as exact due to the different approximations made. Discrepancies can appear due to the truncation after second order of our expansion on powers of y and the approximations made on the function $\langle\cos(A_1-A_1)\rangle_c$. Moreover, another approximation is related to the fact that the renormalization group transformation (2.2) is a linear transformation corresponding to a value of the usual critical exponent η describing the decay of the correlation at T_c, $\eta=0$.

5. Discussion of results

The Hamiltonian of a two dimensional elastic system under the action of a sinusoidal potential has been studied using the renormalization group techniques. Care has been taken to introduce a term which favours incommensurability between the substrate potential and the natural lattice of the 2D system and this term has been properly included in the renormalization procedure. Thus a renormalization of the elastic constants, potential and misfit parameter δ has been achieved. For the case of $\delta=0$, an extension of previous work [5] has been done which allows for the determination of the critical temperature (as a function of V_0) namely:

$$T_c=\frac{4a^2\mu(\mu+\lambda)}{\pi(\lambda+2\mu)}+AV_0+o(V_0^2); \qquad A>0.$$

Due to the substrate and the thermal fluctuations, the elastic behaviour of the system is anisotropic. The temperature dependence of those elastic constants which are associated with a deformation u, near T_c, in the incommensurate phase is calculated to be:

$$\mu\simeq\mu_c-D\sqrt{T-T_c}; \qquad T\geq T_c; \qquad D>0.$$

Below T_c the form of the correlation length presents the following behaviour

$$\xi\propto e^{-(B/\sqrt{(T_c-T)})}, \qquad B>0.$$

These results are very similar to the ones we found in the Sine-Gordon Hamiltonian:

$$\mathcal{H}=\int d^2x\left\{\frac{\mu}{2}\left[\left(\frac{\partial u}{\partial x}\right)^2+\left(\frac{\partial u}{\partial y}\right)^2\right]+V_0\cos\left(\frac{2\pi}{a}u+\delta x\right)\right\}$$

which has been analysed in a previous publication [5].

In the case $\delta \neq 0$ a new fixed point appears, describing a CI-transition. There are two types of asymptotic behaviour of the RG trajectories, depending on the initial value of δ: there is a phase boundary in the (T, δ)-plane which separates the low T (commensurate) and high T (incommensurate) phases. This phase boundary, evaluated numerically, is shown in Fig. 3. The most surprising result, however, is the fact that the correlation length exponent ν along the CI phase boundary depends on the parameters of the system in a continuous way. More precisely it depends explicitely on the ratio $A \equiv \lambda/\mu$ and on T_c, which is itself a function of λ, μ, V_0 and δ. Thus our calculation predicts a temperature variation of ν, when one follow the CI phase boundary of a system with given λ, μ, V_0. For small δ-values and highly incompressible lattices (such as the vortex lattice) ν lies in the vicinity of 1/3. A temperature variation of ν has also been reported for Kr-layers on graphite [10] with numerical values close to our theoretical predictions. Our results, however, should not be directly compared with experiments on monolayers, because there the substrate modulation is two-dimensional, whereas our Hamiltonian describes a 1D modulation. We hope that our results can be checked by future experimental work on the vortex lattice in a superconducting film whose modulation is of this type. Finally, we remark that in the limit $T_c \to 0$ we find $\nu = 0$, which is compatible with the logarithmic divergence of the correlation length predicted by variational ground state calculations [3].

We thank Prof. P. Martinoli for interesting discussions about the vortex lattice.

This work was supported by the Swiss National Science foundation.

Appendix A

The calculation of $\langle u_1^2 \rangle$ according to the definition given in (2.6) requires the Fourier transformation of the anisotropic Hamiltonian given in (2.13). To this effect we introduce:

$$u_{\vec{k}} = \int d^2x u(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$$

$$v_{\vec{k}} = \int d^2x v(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$$

in 2.13 to obtain

$$\mathcal{L}_0 = \tfrac{1}{2} \sum_k \{(Gk_x^2 + Kk_y^2) u_{\vec{k}}^* u_{\vec{k}} + (\beta k_x^2 + (\alpha+\beta) k_y^2) v_{\vec{k}}^* v_{\vec{k}} + \alpha k_x k_y (u_{\vec{k}}^* v_{\vec{k}} + v_{\vec{k}}^* u_{\vec{k}})\}.$$

In momentum space, the quantity $\langle u_1^2 \rangle$ becomes:

$$\langle u_1^2 \rangle = \int_{\Lambda'}^{\Lambda} \frac{k\, dk}{(2\pi)^2} \int_0^{2\pi} d\phi \langle u_{\vec{k}}^* u_{\vec{k}} \rangle$$

$$\langle u_{\vec{k}}^* u_{\vec{k}} \rangle = \frac{\int \prod_q du_q\, dv_q u_{\vec{k}}^* u_{\vec{k}} e^{-\mathcal{L}_0}}{\int \prod_q du_q\, dv_q e^{-\mathcal{L}_0}}$$

The evaluation of the Gaussian integrals is straightforward and yields:

$$\langle u_{\vec{k}}^{*} u_{\vec{k}} \rangle = \frac{\alpha k_y^2 + \beta k^2}{(\alpha k_y^2 + \beta k^2)(\alpha k_x^2 + H k^2) - \alpha^2 k_x^2 k_y^2}$$

where we have written $G = \alpha + H$ following (2.17). Performing the integrals in momentum space easily obtain:

$$\langle u_1^2 \rangle = (2\pi)^{-1} \frac{d\Lambda}{\Lambda} \frac{1}{H} \left[1 - \frac{\alpha\beta}{\alpha\beta + H\beta + \sqrt{\beta(\alpha + H)H(\alpha + \beta)}} \right].$$

Appendix B

In this appendix, we study the nature of the roots of equation (3.11)

$$\omega^3 - \omega^2 + ad \cdot \omega - abc = 0 \tag{B.1}$$

and calculate the real root whose inverse gives the critical exponent of the correlation length as shown in (4.1). The constants *a*, *b*, *c* and *d* are given after (3.10) in terms of the fixed point coordinates x^*, y^*, z^* given in (3.9).

We first notice that the product *ad* depends only on z^* which is a numerical constant : $ad \simeq 2.386$. The product *abc* however depends on the parameters of the problem. Using (3.9) we find

$$abc = -ad \left[x^* - 1 + \frac{4A}{1+A} \right] \tau G''(x^*). \tag{B.2}$$

The discriminant of equation (B.1) is given by:

$$\begin{aligned} \Delta &= \frac{(ad)^2}{108}(4ad - 1) + \frac{abc}{2}\left(\frac{abc}{2} + \frac{2}{27} - \frac{ad}{3}\right) \\ &\approx 0.4504 + \frac{abc}{2}\left(\frac{abc}{2} - 0.7213\right). \end{aligned}$$

Δ as a function of (abc) is then a parabola, with a *minimum* at about 0.32. We therefore conclude that $\Delta > 0$ for any value of the constant *abc* and we will have one real root and two complex conjugate. Denoting ω the real root and $R \pm Ii$ the complex ones we obtain from (B.1) the relations:

$$\begin{aligned} \omega \propto R &= 1 \\ 2R\omega + R^2 + I^2 &= ad \\ \omega(R^2 + I^2) &= abc. \end{aligned} \tag{B.3}$$

As noted after (3.10) the four constants *a*, *b*, *c*, *d* are positive, we therefore obtain from the last equation in (B.3)

$$\omega \geq 0.$$

The real root is always positive. We now proceed to find a lower bound for *abc*.

Using (8.2) together with (3.9) we obtain

$$\frac{abc}{ad}=2x^*\left[1+\frac{A}{x^*+\sqrt{x^*(x^*+A)(1+A)}}\right] \times\left(x^*-1+\frac{4A}{1+A}\right)|G''(x^*)|. \tag{B.4}$$

Experimentally we always expect $\lambda \geq \mu$ (for the vortex lattice $\lambda \to \infty$), we therefore can safely assume that $A \geq 1$. The right hand of (B.4) is a decreasing function of x^* with a limiting value of 4 at $x^* \to \infty$, therefore

$$abc \geq 4ad > ad, \tag{B.5}$$

and using(B.3)

$$ad\omega > 2R\omega^2 + ad \Rightarrow R < 0. \tag{B.6}$$

We thus have one positive real root and two complex conjugate with a negative real part.

The value of the real root, as explained in the main text, is the inverse of the correlation length exponent. It can be easily obtained to be

$$\omega = \tfrac{1}{3} + g_+ + g_-$$

with

$$g_\pm = [g - 0.3606 \pm \sqrt{0.4504 + g(g-0.7213)}]^{1/3} \tag{B.7}$$

where

$$g = \frac{abc}{2} = 2.386\,\frac{\tau_c}{2}\left(x^*-1+\frac{4A}{1+A}\right)|G''(x^*)|$$

and x^* and τ_c are related by the equation

$$\frac{4}{\tau_c} = G'(x^*). \tag{B.8}$$

We obtain a critical exponent $\nu = \nu(\theta, A, \delta)$ which depends on the parameters of the system ($\theta = V_0/\mu$, $A = \lambda/\mu$ and δ). We now proceed to a systematic study of this function.

Consider first the case $\delta = 0$. In this case, the second relation between τ_c and x^* has been calculated analytically in (3.3) to be:

$$\frac{4(x^*-1)}{\tau_c} + \frac{\theta^2}{16\tau_c^2} = G(x^*). \tag{B.9}$$

Using (B.8) and (B.9) we can solve for τ_c and x^* as a function of θ and A. For $\theta = 0$, we obtain

$$x^* = 1, \qquad \tau_c = 4\,\frac{1+A}{2+A}$$

which, substituted in (B.7), yields the limiting values:

$$\nu(0, 1, 0) = 0.402, \qquad \nu(0, \infty, 0) = 0.318.$$

Our theory is based in an expansion on power of V_0/μ and will not be reliable for large values of θ. Taking $\theta = 1$ as the highest admissible value and calculating τ_c and x^* numerically for $A = 1, \infty$ we obtain

$$\nu(1,1,0) = 0.408, \qquad \nu(1,\infty,0) = 0.325.$$

This shows that the change of ν with θ is negligible. Taking $\theta = 0$ corresponds to a picture in which the critical temperature is replaced by the value given by the self-consistent harmonic approximation [5, 7]. In this case, $x^* = 1$ independent of the value of A and we obtain the following simplifications:

$$g = 4.77 \frac{A}{A+2} \left[\frac{3A^2+8A+8}{(1+A)^2}\right].$$

From (B.7) we can now obtain the dependence of ν on A. In Fig. 4, we plot ν as a function of A^{-1}; it varies smoothly between the two limits of 0.32 at $A = \infty$ and 0.40 at $A = 1$. Further remarks are given in the main text.

For $\delta \neq 0$, the critical temperature (and therefore τ_c) is reduced. The value of ν decreases, the effect being more drastic for small values of θ, as we can see from the following data:

$$A = \infty,\ \theta = 0.5 \begin{cases} \delta = 0 & \tau_c = 4.158 & \nu = 0.322 \\ \delta = 0.01 & \tau_c = 3.1347 & \nu = 0.293 \\ \delta = 0.02 & \tau_c = 2.9536 & \nu = 0.287 \end{cases}$$

$$A = \infty,\ \theta = 0.1 \begin{cases} \delta = 0 & \tau_c = 4.033 & \nu = 0.319 \\ \delta = 0.01 & \tau_c = 2.4219 & \nu = 0.268 \\ \delta = 0.02 & \tau_c = 2.1727 & \nu = 0.257 \end{cases}$$

For $A = \infty$, the value of g is given by

$$g = \frac{2.386}{\tau_c^2}\left[2\tau_c^2 + 13\tau_c + 6 + (6-\tau_c)\sqrt{1+2\tau_c}\right].$$

REFERENCES

[1] For a recent review see *Ordering in Two Dimensions*, ed. S. K. Sinha (North-Holland, N.Y., 1980).
[2] P. Martinoli, Phys. Rev. B *17*, 1175 (1978).
[3] V. L. Pokrovskii and A. L. Talopov, Phys. Rev. Lett. *42*, 65 (1979); V. L. Pokrovskii and A. L. Talapov, Soviet Phys. JETP *51*, 134 (1980). A. L. Talapov, Phys. Rev. B *24*, 6703 (1981).
[4] P. B. Wiegmann, J. Phys. C *11*, 1583 (1978).
[5] M. W. Puga, E. Simanek and H. Beck, Phys. Rev. B *26*, 2673 (1982).
[6] T. Nattermann, J. Phys. C *13*, L265 (1980); T. Nattermann, Journal de Physique *41*, 1251 (1980).
[7] H. Yamamoto, Progr. Theor. Phys. *61*, 363 (1979).
[8] J. M. Kosterlitz, J. Phys. C *7*, 1046 (1974).
[9] M. W. Puga, H. Beck and E. Simanek, J. Phys. C *16*, L137 (1983).
[10] W. Stephens, P. Heiney, R. J. Birgeneau and P. M. Horn, Phys. Rev. Lett. *43*, 47 (1979).
[11] H. Shiba, J. Phys. Soc. Japan *48*, 211 (1980).
[12] C. Fain Jr., M. D. Chinn and R. D. Diehl, Phys. Rev. B *21*, 4170 (1980).