TECHNISCHE UNIVERSITÄT MÜNCHEN

Prof. Roland Netz
Lehrstuhl Weiche Materie T37
netz@ph.tum.de

Solid State Theory
Problem Set 10 — Defects

hand-out Fri 24.06., return Fri 01.07.

1) Interacting dislocations. In a two-dimensional crystal with the basis axes denoted by x and y, the displacement field of two dislocations with equal and opposite Burgers vectors separated by distance x_0 along the x axis is

$$u(x, y) = \frac{a}{2\pi} \Im \left[\ln (x + \mathrm{i}y) - \ln (x - x_0 + \mathrm{i}y) \right] . \quad (1)$$

a) Starting from the general expression for the potential energy cost U of introducing these two dislocations into an otherwise perfect crystal

$$U = \frac{a\mu}{2} \int \mathrm{d}^2\vec{r} \, (\nabla u)^2 , \quad (2)$$

show that for eqn. (1) it is legitimate to write

$$U = -\frac{a\mu}{2} \int \mathrm{d}^2\vec{r} u \nabla^2 u . \quad (3)$$

Here, a is the lattice spacing, $\vec{r} = (x, y)$, and μ is the shear modulus. Why would this equation be incorrect for a displacement field given by

$$u(x, y) = \frac{a}{2\pi} \Im \left[\ln (x + \mathrm{i}y) \right] \quad (4)$$

which describes the situation for a single dislocation?

b) Show that $\nabla^2 u$ is proportional to a delta function when applied to eqn. (4). What is the proportionality factor?

c) As a consequence, show that one obtains

$$U = \frac{a^3\mu}{2\pi} \ln \left(\frac{x_0}{a} \right) \quad (5)$$

from eqn. (1) for the case of two dislocations. Note that at short lengths, the integral must be cut off at the scale of the lattice spacing a, because the continuum mechanics breaks down. In order to still have a well-behaved solution, one usually adds an additional term of $2w$ to eqn. (5) in order to account for the energy needed to form the core of the two dislocations.[1]

[1] For 1) & 2) see also Marder, *Condensed Matter Physics*. Excerpt copies can be obtained from A. Serr.

2) Stresses at end of an elliptical hole.

a) The curvature κ of a general plane curve is defined by

$$\kappa = \frac{1}{R} = \frac{\partial \theta}{\partial s}, \tag{6}$$

where θ is the angle of a tangent vector, and s is the arc length along the curve. R is the radius of curvature. Show that for a general parameterization of the curve via t one obtains

$$\kappa = \frac{\frac{\partial x}{\partial t}\frac{\partial^2 y}{\partial t^2} - \frac{\partial y}{\partial t}\frac{\partial^2 x}{\partial t^2}}{\left[\left(\frac{\partial x}{\partial t}\right)^2 + \left(\frac{\partial y}{\partial t}\right)^2\right]^{3/2}}. \tag{7}$$

b) Consider an elliptical hole defined by the contour

$$\zeta = x + \mathrm{i}y = \omega + \frac{p}{\omega}, \tag{8}$$

where $\omega = \exp(\mathrm{i}\gamma)$ lies on the unit circle (γ being real) and $0 \leq p \leq 1$. Show that the radius of curvature at the tip of the ellipse is described by

$$R = \frac{(p-1)^2}{p+1}. \tag{9}$$

c) Show that the maximum stress at the tip of the ellipse is given by

$$\sigma_{max,tip} = \frac{2\Sigma\mu}{1-p}. \tag{10}$$

Here, $\Sigma\mu$ is the value for the stress applied far away from the hole. For that, use the results derived in the lecture, i.e.

$$\sigma_{xz|yz} = \mu\frac{\partial u}{\partial x|y}, \tag{11}$$

$$u(\zeta) = \frac{\phi(\zeta) + \overline{\phi(\zeta)}}{2}, \text{ and} \tag{12}$$

$$\phi(\zeta) = -\mathrm{i}\frac{\Sigma\zeta}{2}\left(1 + \sqrt{1 - \frac{4p}{\zeta^2}}\right) + \mathrm{i}\frac{\Sigma\zeta}{2p}\left(1 - \sqrt{1 - \frac{4p}{\zeta^2}}\right). \tag{13}$$

In these equations, u is the displacement and $\bar{\phi}$ is the complex conjugate of ϕ. All other variables have already been defined above.

d) Verify that

$$\frac{\sigma_{max,tip}}{\Sigma\mu} \propto \sqrt{\frac{l}{R}} \tag{14}$$

holds for small radii of curvature R at the tip where l is the length of the hole.

3) Domain walls in mean-field theory; sine-Gordon equation; solitons.

a) Using Euler-Lagrange variational minimization $\delta(F/A)/\delta\phi = 0$, derive from the time-independent Landau total mean-field free energy per unit area relative to the energy of the ground state,

$$\frac{F}{A} = \int_{-\infty}^{+\infty} \mathrm{d}z \left\{ \tilde{f}(\phi) + \frac{1}{2} c \left(\frac{\mathrm{d}\phi}{\mathrm{d}z} \right)^2 \right\} , \tag{15}$$

the general differential equation

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}z} \right)^2 = \frac{2}{c} \tilde{f} + B . \tag{16}$$

Here, ϕ is a general order parameter, changing over the spatial coordinate z from one equilibrium value (at $z = -\infty$) to another (at $z = +\infty$), c is a phenomenological coefficient, $\tilde{f}(\phi) = f(\phi) - f_0$ is the free energy density in terms of the (locally averaged) order parameter, $f(\phi)$, relative to that of the ground state f_0. B is an integration constant.[2]

b) With that, show that the stationary kink solution $\phi(z)$ to the sine-Gordon potential

$$f(\phi) = -V_0 \cos\phi \tag{17}$$

is given by

$$\phi_{\pm}(z) = \pm 4 \arctan \left\{ \exp(z\sqrt{V_0/c}) \right\} , \tag{18}$$

where V_0 is half the potential depth. The different signs stem from the quadratic form of eqn. (16) and correspond to the kink and the anti-kink solution. Consider here the simple kink, i.e. the transition from the ground state at $\phi = 0$ to that at $\phi = 2\pi$. Therefore the boundary conditions are $(\mathrm{d}\phi)/(\mathrm{d}z)_{z=\pm\infty} = 0$, $\phi(z = -\infty) = 0$, and $\phi(z = +\infty) = 2\pi$. What do these conditions imply for B?

c) Show that

$$\phi_{SA} = 4 \arctan \frac{\sinh\left(\frac{\beta \bar{t}}{\sqrt{1-\beta^2}} \right)}{\beta \cosh\left(\frac{\bar{z}}{\sqrt{1-\beta^2}} \right)} \tag{19}$$

is a solution of the sine-Gordon eqn. (17) to the time-dependent (wave) equation of motion

$$\frac{1}{v_0^2} \frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial z^2} + \frac{1}{c} \frac{\mathrm{d}\tilde{f}}{\mathrm{d}\phi} = 0 . \tag{20}$$

where $\bar{t} = v_0 (V_0/c)^{1/2} t$, $\bar{z} = (V_0/c)^{1/2} z$, and $\beta = v/v_0$. ϕ_{SA} is indeed a soliton-anti-soliton pair moving towards each other with $\pm v$ – in contrast to simple kink-anti-kink pairs; i.e. at times way before the collision, it has the shape of a linear combination of a soliton and

[2] For more details, see also the recitation notes June 24^{th}, or Chaikin, Lubensky, *Principles of Condensed Matter Physics*. Copies can be obtained from A. Serr.

an anti-soliton, and at times long after the collision these shapes are recovered. Prove this by showing that

$$\phi_{SA} \to \phi_+\left(\frac{z+z_0+vt}{\sqrt{1-\beta^2}}\right) + \phi_-\left(\frac{z-z_0-vt}{\sqrt{1-\beta^2}}\right)\,, \text{ for both } t\to\pm\infty\,, \tag{21}$$

where $\phi_\pm$ are the (Lorentz-transformed) soliton and anti-soliton solutions eqn. (18). This shows that a soliton and an anti-soliton that are well separated at $t=-\infty$ pass through each other and emerge as a soliton-anti-soliton pair at $t=+\infty$. In the same fashion show that

$$\phi_{SS} = 4\arctan\frac{\beta\sinh\left(\frac{\bar{z}}{\sqrt{1-\beta^2}}\right)}{\cosh\left(\frac{\beta\bar{t}}{\sqrt{1-\beta^2}}\right)} \tag{22}$$

is a solution to the sine-Gordon equation that reduces to two solitons at $t=\pm\infty$.