

Physics in One Dimension

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Abstract

Due to progress in nanotechnology high-quality quantum wires can nowadays be fabricated. The behavior of particles in one dimension differs significantly from that in three-dimensional (3D) systems, yet the physics of such low-dimensional systems is generally not very well represented in standard undergraduate or graduate curricula. For instance, the Fermi liquid paradigm, working well for electrons in 3D systems, breaks down in 1D and has to be replaced by the Tomonaga-Luttinger liquid (TLL) description. However, most of the introductory papers on the TLL restrict themselves to a summary of results to be compared with experiments, while review papers are often fraught with technical details only accessible to the theorist. The present paper provides an elementary discussion of some phenomena distinguishing quantum wires and quasi-one-dimensional systems from their 3D counterparts targeting experimentalists and graduate students. It aims to convey the basic ideas of TLL theory and to relate it to alternative phases, such as charge and spin density waves. The important role of fluctuations in quasi-1D systems is pointed out and the connection is made to the problem of high- T_c superconductivity. The discussion is kept on a level, which should be accessible with a basic knowledge of quantum mechanics.

Keywords: Luttinger liquids, density waves, spin-charge separation, high- T_c superconductivity.

Preamble: Use in Classroom

With the rapid development of nano-science and technology in recent years dimensionally constrained materials are becoming commonplace in both, basic science and also industrial application. It is therefore desirable to convey the essentials of the theory of low-dimensional systems not only to the students of theoretical physics – for which excellent reviews and books are available – but also to experimentalists, graduate students of physics and of materials science.

The present text specifically addresses one-dimensional systems and is intended for students who have already a basic education in quantum mechanics. It is assumed that they have been confronted with creation and annihilation operators for instance in the discussion of the harmonic oscillator. Furthermore, they should have a basic knowledge of the Fourier transform formalism. Armed with these tools they should be able to follow the discussion in the introduction and the basic theory of Luttinger liquids up to section III. The one major omission in this discussion is the proper introduction of the fields $\Phi(x)$ and $\Theta(x)$. This is associated with some technicalities, which at least for a first reading can be omitted. As always in this context, the technical details can be found in Giamarchi (2004). Here they are avoided as much as possible in order not to obscure the view onto the general concept.

The subsequent two sections address the spin dynamics in Luttinger liquids. These chapters are predominantly intended for experimentalists. They are of particular interest for angle-resolved photoemission spectroscopy (ARPES) on (quasi)-one-dimensional systems. To make optimal use of these chapters it is advisable to study e.g. chapter 33 in Ashcroft & Mermin (1987) or chapter 16 in Kittel (2005) in advance. The aim of the discussion of spin dynamics in the present paper is to provide an intuitive understanding of the many-body interactions shaping the spectral function of Luttinger liquids.

The next chapter (“Interactions”) is a phenomenological description of effects occurring if electron-electron and electron-phonon interactions are turned on. As such, it can be used in an advanced solid-state course, which introduces correlated systems. Particular emphasis is given to a qualitative description of the $2k_F$ interaction giving rise to charge and spin density instabilities. Finally, a special chapter is devoted to fluctuations, since fluctuations are prominent in low-dimensional systems. As antiferromagnetic, charge density wave and orbital order fluctuations are nowadays central to the discussion of the unconventional superconductivity, they should be briefly discussed in every advanced solid state course.

Introduction

Life in one dimension can be rather annoying, as most of us have experienced on a Friday afternoon while being stuck in a traffic jam on a highway. With no chance of evading sideways or, as some might wish, by taking off into the third dimension, everybody in the file is affected by a single event clogging the lane. So what could provide the motivation to deliberately abandon the degrees of freedom offered by higher-dimensional space and engage in the physics of one-dimensional (1D) systems?

Quite often this question is answered by reference to Moore’s law. Extrapolating the present trend towards ever smaller structures in semiconductor industry one can estimate that even within the present decade the cross section of interconnects in integrated circuits should shrink to below 1 nm, i.e. almost atomic dimensions. However, this vision is not likely to come true for precisely the reason mentioned above: There is no fault tolerance in 1D systems in the sense that any single point defect radically changes the properties and the performance. Thus, reducing the critical dimension of interconnects to the extent of creating 1D or quasi-1D systems would presumably increase the rejection rate to economically unacceptable levels.

Let’s set aside for the moment questions of large-scale production and economic feasibility. What is intriguing in 1D systems is the absence of efficient screening which results in long-range interactions, strong correlation and the break-down of the independent particle approximation in favor of a strong collective response to external perturbations. As a consequence, the phase diagram of quasi-1D systems is very rich and the competing order parameters in synergy with the low-dimensionality give rise to an abundance of exotic properties (see Fig. 1). The term phase diagram in the present context has to be used with caution, since, due to competing interactions; spatio-temporal fluctuations are common in these systems. In fact, it is widely believed that unconventional superconductivity is intimately correlated to anti-ferromagnetic fluctuations. One should not be surprised to encounter high- T_c superconductivity in a discussion of quasi-1D systems, although the most prominent representatives, namely the cuprates and the Fe pnictides, are layered compounds, hence seemingly 2D materials. At this stage we restrict ourselves to mentioning the enigmatic striped phase of the cuprates (Zaanen, 2006) and, similarly, the recent observation of nematicity in the Fe pnictides (Chu et al., 2010; Dusza et al., 2011) in order to justify the inclusion of these materials into the present discussion. Let’s return now to the question of technological relevance. High- T_c superconductivity has been mentioned, but various magnetically ordered phases - and the option to switch between them - are no less attractive features of quasi-1D systems. As outlined above, nearly degenerate phases promote quasi-critical fluctuations in a wide range of parameter space. Quasi-critical fluctuations in turn are associated with maxima in the response function or susceptibility. Since the susceptibility governs the materials response to external perturbations, quasi-1D systems can be tuned to exhibit technologically interesting switching properties. Presumably, applications within the near future will be predominantly related to superconductivity, to spintronics and to chemical-switching devices. They will very likely incorporate self-assembled quasi-1D materials rather than single, isolated 1D chains. This ensures a certain tolerance to statistically occurring defects, although their influence is definitely more important here than in higher-dimensional materials.

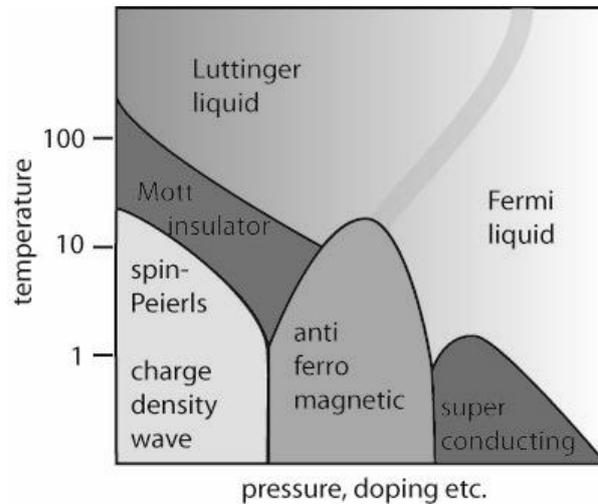


Fig. 1: Schematic phase diagram of quasi-1D organic conductors. Adapted from Bourbonnais (2000).

In the following we shall briefly consider the properties of 1D or quasi-1D systems with particular emphasis on the phase diagram. The discussion aims on an intuitive understanding of the most salient features. Thus the present article is intended as an introduction for pedestrians to the physics in one dimension.

In section II we introduce the concept of a Tomonaga-Luttinger liquid (TLL) as opposed to the more familiar Fermi liquid paradigm. The formal analogy to the Hamiltonian of a vibrating string is made to emphasize the collective character of the low-energy excitations. In section III the ground state of the 1D spin system is discussed by mapping the spin chain onto a spinless Fermion system. In section IV the results of section III are used to provide an intuitive interpretation of angle-resolved photoemission spectra from 1D systems (quantum wires). Section V addresses electronic interactions in 1D systems and the resulting phase diagram. The Luttinger liquid regime is put into the broader context of various density wave and superconducting phases. In section VI follows a brief introduction into the concept of charge density waves. Section VII deals with fluctuations that is a very prominent topic not only for 1D systems but also in the physics of high- T_c superconductivity. The paper concludes with a short outlook concerning the role of the dimensionality and a few remarks for the use of the present material in physics, physical chemistry and materials science classes.

Tomonaga-Luttinger Liquid

Intuitively, it is clear that the quasi-particle concept of Fermi liquid theory cannot hold in 1D systems. As shown in Fig. 2, one cannot excite, remove, or add a particle without perturbing the whole chain of particles in a fundamental way. The mathematical treatment of low-energy excitations in the 1D system is based on the introduction of a linearized dispersion extending to infinite negative energies as indicated in Fig. 3. (Giamarchi, 2004; Schönhammer, 2002) This seemingly unphysical model is justified, if one is interested only in the physics of low-energy excitations with the ground state as reference. Adding high-binding-energy states to the system, which remain unaffected in the low-energy excitations under consideration, does not change the physics.

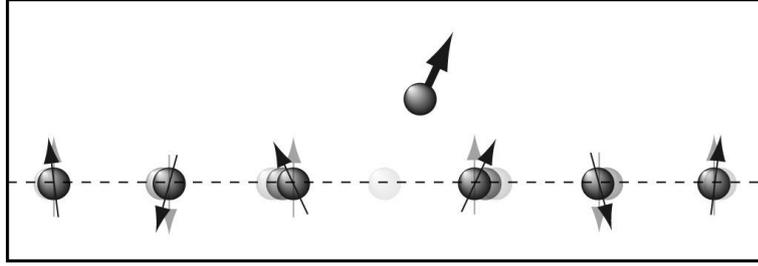


Fig. 2: Excitations of the charge and spin degree of freedom in a linear chain upon removal of a particle.

The linear dispersion implies a constant density of states (DOS). For the low-energy excitations only the DOS around the Fermi level is relevant, hence the somewhat brutal assumptions about the DOS far below E_F will not affect the low-energy physics, but simplify the mathematics considerably. The dispersion relation is written with respect to Fermi energy and Fermi wave vector as reference levels for energy and momentum, respectively:

$$e_{R,L} = \hbar v_F (\pm k - k_F) \quad (1)$$

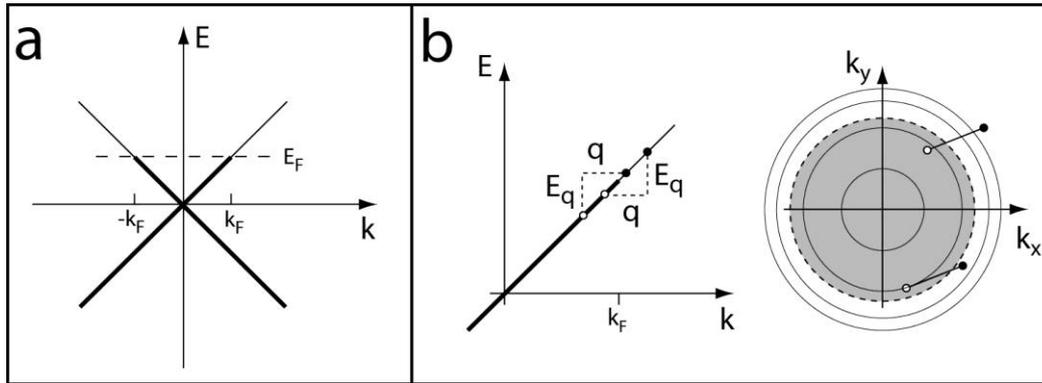


Fig. 3: (a) Linear approximation of the dispersion underlying the Luttinger-Liquid description of 1D systems. The model dispersion is chosen so as to approximate the real dispersion in the vicinity of E_F , while it becomes totally unrealistic at higher binding energies. This, however, is irrelevant, as long as only low-energy excitations are considered. (b) Due to the linear dispersion, all excitations in a 1D system with wave vector q belong to the same energy E_q . This is not the case in a 2D system, where the wave vector q can connect points on either side of the Fermi surface with different energy separation. The shaded area symbolizes the filled part of a (parabolic) 2D band. Circles are iso-energetic contour lines, the dashed circle corresponds to the Fermi energy.

Here R and L refer to right moving ($k > 0$) and left moving ($k < 0$) particles. $v_F = \frac{1}{\hbar} \frac{dE}{dk}$ is the Fermi velocity. Below, we will set $\hbar = 1$, as customary. Next, density fluctuation operators $\rho_R(x), \rho_L(x)$ and $\rho_R(q), \rho_L(q)$ are introduced, which characterize the density of right and left moving Fermions relative to the ground state. For instance,

$$\rho(x) = c_x^\dagger c_x \quad (2)$$

with $c_x^\dagger c_x$ being the particle number operator at position x . Taking the Fourier transform of the creation and annihilation operators one obtains

$$\rho(x) = \sum_{k,k'} \frac{1}{\Omega} e^{i(k-k')x} c_{k'}^\dagger c_k \quad (3)$$

with Ω the normalization volume. Defining $k' - k = q$ one arrives at

$$\rho(x) = \sum_{k,q} \frac{1}{\Omega} e^{-iqx} c_{k+q}^\dagger c_k \quad (4)$$

Therefore the density operators in reciprocal space can be written for instance as:

$$\rho_R(q) = \sum_{k>0} c_k^\dagger c_{k-q} \quad (5)$$

with c_k^\dagger creating a particle in state k and c_{k-q} annihilating a particle in state $k-q$ which increases the total momentum of the system by q . $\rho_{R,L}(q)$ are density fluctuations with momentum vector q and, since they contain two Fermion operators, are bosonic (they create pairs of Fermions – particle and hole – with opposite spins). In a one-dimensional system with linear dispersion all particle-hole excitations with the same wave-vector q have the same energy (see Fig. 3b). Therefore, the density fluctuations as defined in eqn. (5) are Eigenstates of the Hamiltonian

$$H\rho(q)|0\rangle = E_q\rho(q)|0\rangle \quad (6)$$

where $|0\rangle$ is the many-particle ground state. These states obviously involve collective oscillations in the chain with wave-vector q . Actually, these are the only low-energy excitations existing in the 1D system. The Coulomb interaction in the system can be written as

$$V = \frac{1}{2} \int V(x-x') \rho(x) \rho(x') dx dx' \quad (7)$$

or in terms of the Fourier transform (see appendix A in Giamarchi (2004)):

$$V = \frac{1}{2L} \sum_{k,k',q} V(q) c_{k+q}^\dagger c_{k'-q}^\dagger c_k c_k \quad (8)$$

This is true up to an additive term, which contains the total particle number and can be interpreted as the chemical potential. Thus the particle interactions, while being quartic in terms of the Fermion operators, can be expressed as a bilinear function of the density operators. The same applies to the kinetic energy. Defining appropriately normalized Bosonic operators and exploiting the commutator relationships one arrives at a Hamiltonian

$$H = \frac{1}{2\pi} \int \left[(uK \nabla \theta(x))^2 + \frac{u}{K} (\nabla \Phi(x))^2 \right] dx \quad (9)$$

Here

$$\nabla \Phi(x) = -\pi [\rho_R(x) + \rho_L(x)] \quad (10)$$

i.e. the sum of left and right moving particles at point x or, equivalently, the $q \approx 0$ part of the density fluctuations at point x .

$$\nabla\theta(x) = \pi[\rho_R(x) - \rho_L(x)] \tag{11}$$

is the difference between left and right moving particles at point x and hence proportional to the current operator. For a more detailed discussion of the field $\Phi(x)$ see Giamarchi (2004). u and K can be interpreted by analogy to a vibrating string. Invoking the continuity equation

$$\nabla j + \frac{\partial \rho}{\partial t} = 0 \tag{12}$$

one obtains

$$\nabla j = \frac{1}{\pi} \frac{\partial \nabla \Phi}{\partial t} \tag{13}$$

which in 1D can be straightforwardly integrated to yield

$$j = \frac{1}{\pi} \frac{\partial \Phi}{\partial t} \tag{14}$$

With the definition of the current operator

$$j = \frac{1}{\pi} u K \nabla \theta(x) \tag{15}$$

the Hamiltonian can be written as

$$H = \frac{1}{2\pi} \int \left[\left(\frac{\partial \Phi}{\partial t} \right)^2 + \frac{u}{K} \left(\frac{\partial \Phi}{\partial x} \right)^2 \right] dx \tag{16}$$

Thus the Hamiltonian (9) is analogous to the Hamiltonian of an elastic string

$$H = \frac{1}{2} \int \left(\mu \left(\frac{\partial y}{\partial t} \right)^2 + T \left(\frac{\partial y}{\partial x} \right)^2 \right) dx = \frac{\mu}{2} \int \left(\left(\frac{\partial y}{\partial t} \right)^2 + c^2 \left(\frac{\partial y}{\partial x} \right)^2 \right) dx \tag{17}$$

Here, y is the amplitude, T is the Elastic modulus of the string and $c = \sqrt{T/\mu}$ is the sound velocity in the string. Accordingly, $T = 1/\pi K$ is a measure of the “stiffness” and $\mu = 1/\pi u$ a measure of the effective mass. Actually, K is defined as a dimensionless constant specifying the interaction ($K > 1$: attraction, $K < 1$: repulsion; interactions will be discussed further below) and u has the dimension of a velocity (remember that the model is based on a linearized dispersion). The analogy with the string brings out the collective character of the low-energy excitations in the TLL model, i.e. collective Fermion density fluctuations. Intuitively it is clear that a single particle excitation cannot survive in the system, since the one-dimensionality forces immediate transfer of momentum to the neighbors and coherent spreading throughout the system. Another interesting property follows from the fact that $\Phi(x)$ and $1/\pi \nabla \theta(x)$ are canonically conjugate variables. The non-zero commutator implies quantum fluctuations in the field $\Phi(x)$ and therefore in the density.

Finally, we note an important difference between a solid in higher dimension and in 1D: For $D > 1$ a solid may be characterized by the presence of long-wavelength transverse modes, which are absent in a liquid. In 1D, however, transverse modes are forbidden, hence the difference between solid and liquid is gone.

So far we have neglected the spin degree of freedom. In principle one can carry out the above considerations for each spin species separately. However, interactions couple the excitations in separate spin channels. A diagonalized Hamiltonian can be obtained, if new variables are defined:

$$\begin{aligned} \rho(x) &= \frac{1}{\sqrt{2}}(\rho_{\uparrow}(x) + \rho_{\downarrow}(x)) \\ \sigma(x) &= \frac{1}{\sqrt{2}}(\rho_{\uparrow}(x) - \rho_{\downarrow}(x)) \end{aligned} \quad (18)$$

This leads to separate Φ_{ρ} and Φ_{σ} as well as θ_{ρ} and q_s fields. Accordingly, the Hamiltonian separates into a charge and a spin part

$$H = H_{\rho} + H_{\sigma} \quad (19)$$

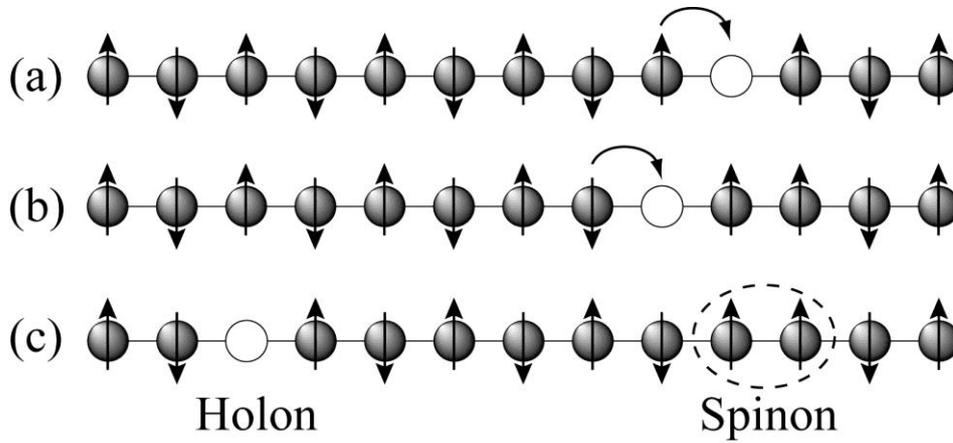


Fig. 4: Schematic illustration of spin-charge separation in a 1D chain. Removal of a particle causes excitations in both, the spin and the charge channel. The two excitations can travel along the chain with different velocities.

The charge part is the same as in eq. (9), except with modified u_{ρ} and K_{ρ} . The spin part contains the quadratic Hamiltonian (9) H_{σ}^0 with u_{σ} and K_{σ} plus an additional term

$$H_s = H_s^0 + \frac{2g_{\perp\wedge}}{(2\rho a)^2} \int \cos(2\sqrt{2}F_s) dx \quad (20)$$

$g_{\perp\wedge}$ is the matrix element for a scattering process involving two particles at $\pm k_F$ with opposite spin and a momentum transfer of $\sim 2k_F$ and will be discussed in more detail below. This second term favors a Φ_{σ} minimizing the cosine term, i.e. a static, ordered field. The term competes with the first, quadratic part of the Hamiltonian, which enforces a fluctuating field Φ_{σ} . Since the spin and the charge part of the Hamiltonian can be separated, one speaks of spin-charge separation in TLLs. For the interaction-free case, however, $u_{\rho} = u_{\sigma} = v_F$ (Fermi velocity) and $K_{\rho} = K_{\sigma} = 1$. In this case spin and charge excitations travel with the same velocity and no separation is observed. If interactions are switched on, the velocities are renormalized and spin and charge excitations can separate. This is illustrated in Fig. 4.

The Ground state of the Spin System

The alert reader may notice a certain discrepancy between Fig. 2, where removal of an electron is (correctly) depicted as a collective excitation in the charge and the spin channel, while Fig. 4 shows two localised excitations in order to clearly illustrate the concept of spin-charge separation. In the following we shall briefly outline the nature of the ground and excited state in the spin system in order to obtain a more realistic picture. To this end we consider a one-dimensional spin chain in the so-called xxz model:

$$\begin{aligned}
 H &= \mathbf{J} \sum_j \mathbf{S}_{j+1} \cdot \mathbf{S}_j = J_{xy} \sum_j (S_{j+1}^x S_j^x + S_{j+1}^y S_j^y) + J_z \sum_j S_{j+1}^z S_j^z = \\
 &= \frac{J_{xy}}{2} \sum_j (S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+) + J_z \sum_j S_{j+1}^z S_j^z
 \end{aligned}
 \tag{21}$$

S^x, S^y, S^z are the Pauli spin matrices, $S^\pm = S^x \pm iS^y$, j is the site index along the chain and J denotes the exchange interaction. It is assumed to be isotropic in xy, hence we can write $J_{xy} = J$ and $J_z = J\Delta$. Furthermore we assume a local antiferromagnetic interaction, i.e. $J > 0$ for nearest neighbor sites and $J = 0$ for all larger distances. S^+, S^- are creation and annihilation operators, respectively, in the sense that S^\pm applied to an eigenstate $|S\rangle$ of S^z increases (reduces) the spin component in z direction by one unit:

$$S^z S^\pm |S\rangle = (S \pm 1) S^\pm |S\rangle
 \tag{22}$$

Accordingly, the first part of the Hamiltonian describes the propagation of spin waves from site j to site $j+1$ and vice versa, i.e. the kinetic energy, while the second part contains the nearest neighbor interaction (see the discussion of magnons in solid state textbooks (Ashcroft & Mermin, 1987; Kittel, 2005)). For $J_z/J_{xy} > 1$ the second part enforces antiferromagnetic order and the system adopts an Ising antiferromagnetic phase. Similarly, for $J_z/J_{xy} < -1$, the system is in an Ising ferromagnetic phase. At $J_z/J_{xy} = \pm 1$ an isotropic Heisenberg (anti)Ferro magnet is obtained. $|J_z/J_{xy}| < 1$ corresponds to the TLL regime. The formal treatment of the spin chain is provided in Giamarchi (2004), chap. 6. A discussion and pictorial representation of spin waves is given by Keffer, Kaplan & Yafet (1953). Here we take a shortcut in order to obtain more information about the ground state and the lowest excitations. To this end we map the spin chain onto a spinless Fermion or hard-core Boson chain by interpreting the eigenvalue S of S_i^z as occupation number. Every lattice site i with $S = 1/2$ is considered to be occupied, while $S = -1/2$ corresponds to an empty lattice site. Furthermore, we note that every lattice site can carry only a spin $1/2$, so double occupancy is forbidden. With these conventions the spin-chain Hamiltonian can be translated into a spinless-Fermion Hamiltonian:

$$H = t \sum_j (c_{j+1}^\dagger c_j + h.c) + V \sum_j \left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2} \right) \left(c_j^\dagger c_j - \frac{1}{2} \right)
 \tag{23}$$

Here, $t = J_{xy}/2$ and $V = J_z$. The operator $c_{j+1}^\dagger c_j$ corresponds to a particle hopping from site j to site $j+1$, $c_j^\dagger c_j$ is the particle number operator as usual. This Hamiltonian is almost identical to a conventional spinless-Fermion Hamiltonian with nearest-neighbor interaction apart from the sign change in the kinetic energy term. The solution for the kinetic energy is thus

$$\varepsilon_{kin}(k) = J_{xy} \cos(ka)
 \tag{24}$$

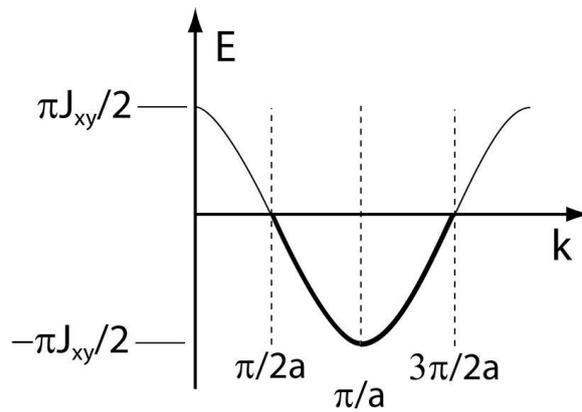


Fig. 5: Band structure of the spinon band (24) as obtained from mapping the spin Hamiltonian (21) onto a spinless-Fermion Hamiltonian (23). In the antiferromagnetic case the band is half-filled. Note that the actual bandwidth is not $2J_{xy}$ but πJ_{xy} .

The interaction part adds a constant, which for the present purpose is neglected in the TLL regime $|J_z/J_{xy}| < 1$. Since in the ground state we have $N/2$ particles (spin up sites) in our spin chain, the “spinon” band eq. (24) is half occupied (full occupation corresponds to the ferromagnetic case). Consequently we obtain for the ground state the situation shown in Fig. 5. It is characterized by a superposition of spin waves with k vectors ranging from $\pi/2 \leq k \leq 3\pi/2$. Accordingly, the spins are constantly fluctuating and the ground state is spin-isotropic (in contrast for instance to the antiferromagnetic Ising model). Armed with this result we can now at least qualitatively understand the spectral function of a TLL as measured by UV photoemission.

Qualitative Interpretation of Photoemission Spectra

Fig. 4 illustrates how a photo-hole can decay into two separate quasi-particles (or topological defects) travelling independently along an antiferromagnetic chain. This complicates the interpretation of PE spectra, since energy and momentum is now distributed among three entities: the outgoing photoelectron, the holon and the spin excitation. A qualitative interpretation of the photoemission spectrum has been proposed by Maekawa & Tohyama (2001). In order to understand the kinetics of the holon we consider the Hubbard model for a half-filled band. Here, antiferromagnetic ordering and a tight-binding type band structure are obtained as indicated in Fig. 6. The lower Hubbard band is completely occupied. The band structure of the holon corresponds to that of a hole placed into this otherwise filled band. It is the negative replica, i.e. the holon has the lowest energy at $k = \pi/a$ (where it costs the least energy to remove an electron) and the maximum energy at $k = 0; 2\pi/a$.

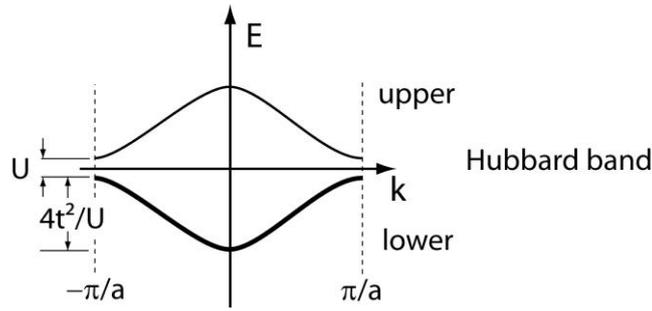


Fig. 6: Band structure obtained from a Hubbard model with half-filling and $U/t \gg 1$. The lower Hubbard band is completely occupied.

Next we address the spin excitation. The photoelectron carries away a spin from the system. This is equivalent with removing a spinless Fermion from our spinless-Fermion chain eqn. (23). In other words, a hole is created in the spinon band (24) (annihilation of a spinon). To create the lowest energy excitation we can annihilate a spinon at $k = 3\pi/2a$. The photo hole has therefore the momentum $k_{ph} = k_{holon} - k_{spinon} = \pi/a - 3\pi/2a = -\pi/2a$. If k_{holon} is kept constant and k_{spinon} is reduced to π/a , one obtains the spinon branch. The actual total bandwidth of the spinon band obtained in the exact calculation is πJ_{xy} in contrast to $2J_{xy}$ suggested by our qualitative reasoning above (Cloizeaux and Pearson, 1962). With $k_{spinon} = const.$ and k_{holon} being varied one obtains the holon branch in the photoemission spectrum. Here the total bandwidth is the tight binding result $4t$ obtained for $U/t \rightarrow 0$. Finally, noting that the photoelectron momentum $k_{e^-} = -k_{ph}$ one obtains the schematic dispersion plot shown in Fig. 7. A comparison between actual photoemission measurements and a calculated spectral distribution can be found for instance in Kim et al. (2006). In concluding this paragraph we note that the k integrated density of states for the spin isotropic case ($K_\sigma = 1$) can be written (Voit, 2001; Schönhammer, 2002) as

$$n(\varepsilon) = |\varepsilon - \varepsilon_F|^{-\frac{1}{2}} \sqrt{\frac{1}{4}(K_\rho - K_\rho^{-1}) - \frac{1}{2}} \quad (25)$$

For an experimental test see Blumenstein et al. (2011) and references cited therein. Next, we take a closer look at the possible interactions in the TLL model.

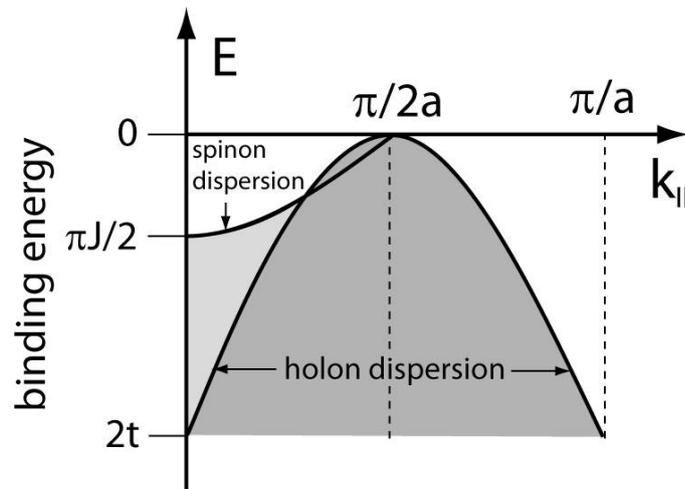


Fig. 7: Schematic illustration of a photoemission spectrum in case of spin-charge separation. The spinon and holon bandwidth scale with J and t , respectively. Spinon and holon dispersion delineate the photoemission intensity distribution. Within these limits the latter forms a continuum, since energy and momentum can be distributed between the two excitations. After Maekawa & Tohyama (2001).

Interactions

We start with expression (8) for the particle-particle (or, more appropriately, density-density) interactions in a one-dimensional chain. The interaction is written in terms of particle removal from states k, k' and particle creation in states $k+q, k'-q$. In other words it can be interpreted as a sum over scattering events with momentum exchange q . These scattering processes mix $k+q$ states into k states and vice versa. In calculating the amplitude of the states being mixed in, the energy difference between initial and final state appears in the denominator as a weighting factor. In the present case this means that those terms will dominate the interactions, for which the energy difference between $k, k+q$ and $k', k'-q$ or $k, k'-q$ and $k', k+q$ goes to zero. This is the case, if both states lie at the Fermi level, i.e. $k, k' \approx \pm k_F$. The corresponding processes are illustrated in Fig. 8. The interaction matrix elements resulting from these processes are denoted g_i for historical reasons. Consequently, the exploration of the ensuing phase diagrams has become known as “g-ology”. It is discussed in several books and reviews, e.g. Giamarchi (2004), Grüner (1994), Sólyom (1979), Jérôme & Schulz (2002). Here we briefly review a few aspects of particular interest for the experiment.

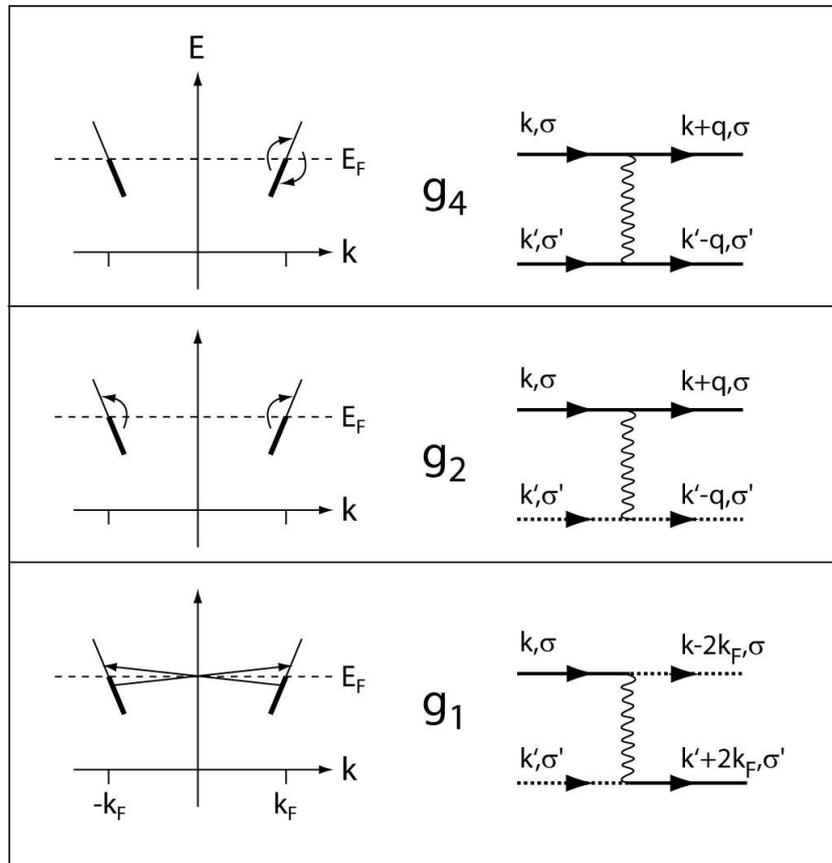


Fig. 8: Left: Low-energy scattering processes with momentum conservation in 1D. Right: Diagrammatic representation of the scattering processes. Solid lines signify right moving, dotted lines left moving particles. Adapted from Giamarchi (2004).

Interaction g_4 is a momentum exchange among particles moving in the same direction (forward scattering: both particles retain their direction), while g_2 describes forward scattering between particles moving in opposite direction. In both cases the momentum exchange is close to zero and the resulting Fourier coefficient $V(q)$ belongs to an inter-action potential with $\lambda \rightarrow \infty$. g_1 involves a momentum exchange close to $2k_F$, which implies that the scattered particles reverse their direction (backward scattering). For spinless particles g_1 and g_2 are identical, since in this case the particles cannot be distinguished. If particles with spin are considered, $g_{1\perp}$ appears as an extra term in the spin part of the interacting Hamiltonian (20) since here the spin is exchanged between left and right moving particles and there is no analogous interaction in the charge Hamiltonian. We omit here process g_3 , which appears for exact half filling, involves a reciprocal lattice vector exchange and results in a $4k_F$ interaction.

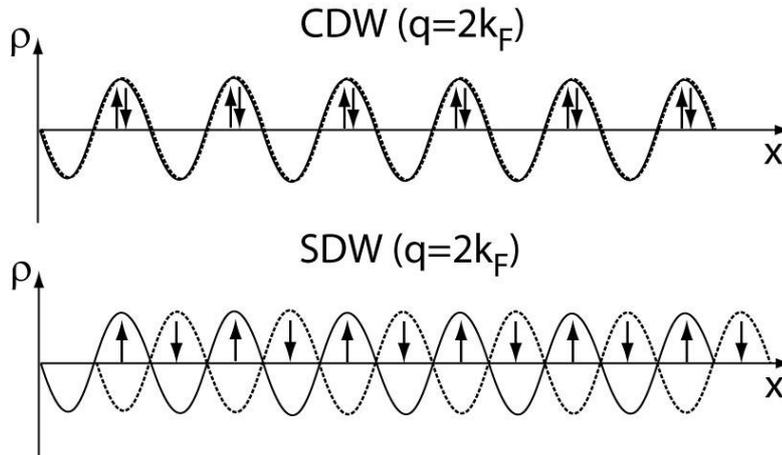


Fig. 9: In a CDW spin-up and spin-down charge densities are in phase. The charge density is modulated, the spin density is not. In contrast, if spin-up and spin-down charge densities are offset by 180° , the charge density is constant and the spin density is modulated which results in a SDW.

If Coulomb repulsion dominates, g_2 and g_4 are positive. g_4 renormalizes the velocities u_ρ, u_σ while g_2 shifts the weights between the terms $\nabla\Phi$ and $\nabla\theta$ in the Hamiltonian (9). For $g_2 > 0$, $K_\rho < 1$ and charge or spin density fluctuations prevail.

The TLL is a paramagnetic metal. For $g_2 < 0$, i.e. attractive interaction between particles from opposite parts of the Fermi surface, one obtains $K_\rho > 1$ and the system exhibits an instability towards the superconducting phase. If $|g_1|$ increases in eqn. (20), this term will eventually force Φ_σ into the minima (or maxima) of $\cos(2\sqrt{2}\Phi_\sigma)$, depending on the sign of g_1 . Accordingly one may have two types of excitation, i.e. magnon-like oscillations of the spin density around the minima of the cos term or soliton-type jumps within the chain from one minimum to the other. Both types of excitations are gapped, hence in this case the Luttinger-liquid is no longer a paramagnetic metal. Such systems are referred to as Luther-Emery liquids.

For $g_{1\perp} < 0$ one has spin density wave and charge density wave correlations. In a spin density wave (SDW) the charge density modulation for ρ_\uparrow and ρ_\downarrow exhibits a phase difference of π , so that the total charge density remains uniform, while the spin density oscillates as shown in Fig. 9. In fact, the field Φ_σ determines the offset between the modulations:

$$\begin{aligned} \rho_\uparrow(x) &\propto \cos(2k_F x - \sqrt{2}\Phi_\rho - \sqrt{2}\Phi_\sigma) \\ \rho_\downarrow(x) &\propto \cos(2k_F x - \sqrt{2}\Phi_\rho + \sqrt{2}\Phi_\sigma) \end{aligned} \quad (26)$$

Since in a TLL the fields fluctuate, the spin and charge correlations decay rapidly in space and time. For sufficiently large $|g_1|$, in contrast, static modulations arise. In a charge density wave (CDW) the modulation for both species is in phase, so that the charge density oscillates, while there is zero spin modulation. Intuitively, one should expect the SDW to be more stable, because Coulomb correlation tends to oppose a CDW. The strength of all the interactions discussed here depends, however, on additional effects, most prominently on electron-phonon interaction. It is due

to these effects that CDW phases can be stabilized and are in fact quite common in low-D compounds.

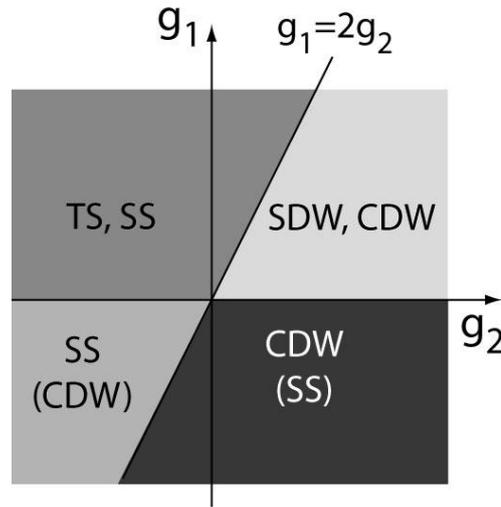


Fig. 10: “Phase diagram” for 1D chains showing how the dominant correlations depend on g_1 and g_2 assuming spin-independent interactions.

Fig. 10 shows a “phase diagram” of 1D systems for spin independent interactions. Since in 1D pure phases are not stable (see below) the diagram essentially shows the strongest correlations, i.e. those for which the correlation functions decay most slowly. Phases shown in brackets are subdominant correlations.

Charge Density Waves

As stated above, CDW phases are stabilized by electron-phonon interaction. For a 1-D system the mechanism can be illustrated as in Fig. 11: In 1D there is a forbidden range in the particle-hole excitation spectrum at finite energies between $q = 0$ and $q = 2k_F$ (Tosatti, 1975; Bertel & Menzel, 2010). This is easily seen from a consideration of possible single particle excitations in a 1D parabolic band.

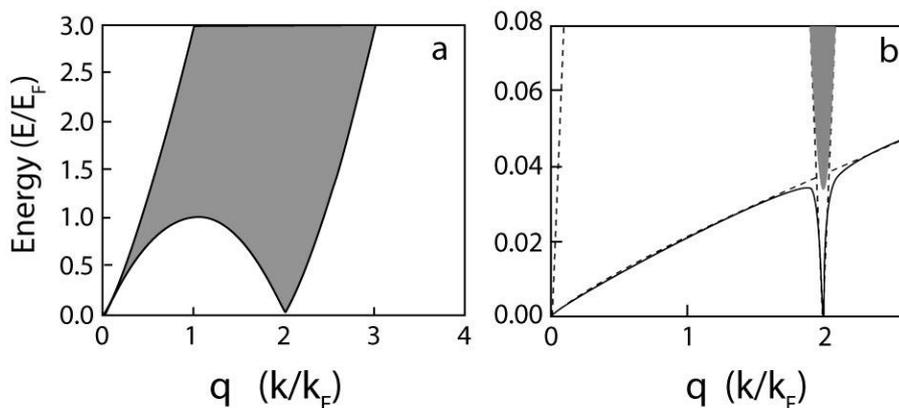


Fig. 11: (a) In 1D, the low-energy particle-hole excitation continuum exhibits a forbidden low-energy range for $0 < q < 2k_F$. (b) At $2k_F$ an acoustic phonon branch can hybridize with the particle-hole excitations thus opening a gap in the excitation spectrum and simultaneously generating a frozen phonon, i.e. a static periodic lattice distortion (PLD).

At $q = 2k_F$, energy and momentum conservation allows hybridization of particle-hole excitations with acoustic phonons (see Fig. 11). As a consequence, the phonon softens, i.e. is depressed in energy. One may envision this process as being caused by the $2k_F$ charge density modulation resulting from the $k' \rightarrow k' - q$ and $k \rightarrow k + q$ excitations. The induced charge density screens the restoring force for the oscillating ions. Accordingly, the response function $\chi(q)$ determines the stability of a CDW phase. The response function is defined by the charge response to a local perturbing potential

$$\langle \rho(q, \omega) \rangle = \chi(q, \omega) V_{loc}(q, \omega) \quad (27)$$

For global stability considerations we may neglect fluctuations and replace the dynamic susceptibility $\chi(q, \omega)$ by its static counterpart

$$\chi_0(q) = \frac{1}{\Omega} \sum_k \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k} \quad (28)$$

with f_k being the Fermi function. The local potential is the combined effect of the “external” potential V_{ext} , and the potential caused by the induced charge $\rho(q)$

$$V_{ind}(q) = g\rho(q) \quad (29)$$

With eq. (27) we arrive at

$$\rho(q) = \chi_0(q)(V_{ext}(q) + g\rho(q)) \quad (30)$$

Defining an effective response function we finally obtain

$$\rho(q) = \chi_{eff}(q)V_{ext}(q) = \frac{\chi_0(q)}{1 - g\chi_0(q)} V_{ext}(q) \quad (31)$$

Eqs. (27)-(31) can be interpreted as resulting from an iterative process: (i) calculate the charge density ρ_{ind} induced purely by V_{ext} , (ii) use this charge density to calculate V_{ind} , (iii) combine V_{ext} and V_{ind} to V_{loc} and re-calculate ρ_{ind} , (iv) start the cycle again from (ii) (note that the coefficient of χ_0 in (31) $(1 - g\chi_0)^{-1}$ has the form of the sum of a geometric series). Thus the charge response function χ_{eff} contains contributions from both interactions, the g_1 and g_2 type mentioned above up to infinite order. In the present context of CDW instabilities we are interested in perturbations with wavelength $\lambda = 2\pi/q = \pi/k_F$. Consequently, the strength of the $2k_F$ (i.e. g_1) interaction dominates the behavior of χ_{eff} . If only the charge density fluctuations are considered and the potential set up by the ion cores is omitted, Coulomb interaction dominates and $g = e^2/\varepsilon_0 q^2$ (see Bertel & Menzel, 2010). Since the charge response function $\chi(q)$ is < 0 , it is clear that the Coulomb interaction tends to suppress a CDW phase. On the other hand, if the ion cores are included into the balance, g may switch sign and a singularity can appear in eq. (31). Such a singularity indicates a phase instability, in the present case the transition into a CDW phase. Simultaneously, the $2k_F$ phonon energy drops to zero, which is equivalent to the appearance of a static periodic lattice distortion (PLD). Eq. (31) indicates that a singularity in the “bare” response function $\chi_0(2k_F)$ is not sufficient to cause a

phase transition. In contrast, the Fermi-surface nesting criterion often used in discussing CDW instabilities, is based on precisely this argument. Letting $\varepsilon_{k+q} = \varepsilon_k \rightarrow \varepsilon_F$ one obtains a divergent $\chi_0(2k_F)$, if the summation in eq. (28) extends over a finite interval, i.e. if finite sections of the opposite Fermi surfaces can be connected by the same $q = 2k_F$. Since in one dimension the Fermi surface is composed of two infinite parallel sheets at $\pm k_F$, the criterion of Fermi surface nesting is always fulfilled. However, applying this criterion is equivalent to using eq. (27) instead of eq. (31). Following the discussion presented by Johannes and Mazin (2008) we can identify several effects opposing a transition into a CDW phase: (i) In 1D, long-range order is always destroyed by fluctuations at any finite temperature; (ii) no real material is purely one-dimensional. Coupling to adjacent chains or to a substrate will always cause some deformation (warping) of the Fermi surface and thus reduce the nesting; (iii) at finite temperatures the divergence of χ_0 is rapidly attenuated due to the Fermi function broadening; (iv) using χ_{eff} instead of χ_0 , thus including the interactions contained in the coupling constant g , will in general destroy the divergence as well. Nevertheless, CDW phases are observed in a number of bulk (J erome & Schulz, 2002; Johannes & Mazin, 2008; Whangbo, Canadell, Foury & Pouget, 1991) and surface systems (Bertel & Menzel, 2010; Hasegawa, 2010; Oncel, 2008). A key point is the inclusion of electron-phonon coupling as pointed out above. As evident from (31), a divergence in χ_{eff} may occur if $g\chi_0(q) \rightarrow 1$. Another point is that the actual energy gain upon formation of a CDW/PLD is not restricted to the Fermi surface. While we have argued above that the 0 and $2k_F$ contributions from Fermi-surface to Fermi-surface excitations are strongest due to the energy denominator, other contributions are non-negligible, if integrated over the (surface) Brillouin zone. Consequently, the interaction is not well localized in k-space. In fact, there is a smooth transition between the long-range CDW interaction (sometimes called weak-coupling CDW) and the local bond distortion regime (strong-coupling CDW) where the interaction is localized in real space and is almost completely smeared out in k-space (Aruga, 2006).

The preceding discussion can be summarized as follows: (i) A CDW phase is hardly ever restrained to the electronic system. Coulomb interaction would rather favor a SDW in such a case. Instead, a CDW requires an enhanced electron-phonon coupling and is generally associated with a PLD. (ii) The occurrence of a CDW instability is governed by χ_{eff} rather than the bare charge susceptibility χ_0 . Accordingly, Fermi surface nesting is not a reliable criterion to identify possible CDW systems, although a certain extent of phase space for low-energy $k \rightarrow k+q$ excitations is certainly required. This can be provided by nesting, but also by the presence of saddle points at E_F (Rice & Scott, 1975).

Phase Transitions and Fluctuations

The question of phase transitions in 1D is often discussed with reference to the Ising model. This is a special case, because it doesn't have a continuous symmetry. If the interaction has a finite range, the correlation length diverges only as $T \rightarrow 0$. A simple argument based on assuming a nearest neighbor interaction J only is the following: Reversal of a single spin in an otherwise perfectly ordered chain costs a magnetic exchange energy of $2J$. The associated entropy gain, however, is $k \ln \omega$. Here ω is the number of configurations with a flipped spin, i.e. N , the chain length. The Free Energy change is consequently $\Delta F = 2J - kT \ln N$, which is always negative if $N \rightarrow \infty$ and $T > 0$. A more precise statement is: The correlation length decays exponentially for all finite temperatures.

In contrast, phase transitions at finite T exist, if the system exhibits long-range interactions J_{kl} which decay as $1/|r_k - r_l|^\alpha$ and $1 < \alpha \leq 2$. Furthermore, the Wagner-Mermin-Theorem asserts that there is no spontaneous symmetry breaking of *continuous* symmetries in $D \leq 2$. This still allows the evolution of algebraically decaying correlation functions in a Kosterlitz-Thouless transition under certain circumstances, for instance for a Heisenberg chain with spin $\frac{1}{2}$ particles. Algebraically decaying correlation functions establish quasi-long-range order. In practice, the observation area is always limited, for instance by a finite coherence length in a diffraction experiment or by the terrace size in a surface experiment, so experimentally the difference between quasi-long-range and true long-range order would be washed out.

In any case, fluctuations are a hallmark of low-dimensional systems. While fluctuations in a 3D system with a continuous phase transition are limited to a narrow temperature range around T_c , the prominence of fluctuations is considerably enhanced in low dimensions with respect to both, temperature range and intensity. The role of the dimensionality can be most easily appreciated by examining the Ginzburg-Levanyuk criterion. It has been developed to establish the validity range of the Landau theory of continuous phase transitions. On the one hand, Landau theory is based on the truncated expansion of the free energy in powers of the order parameter around T_c . This works only close to T_c . On the other hand, it is a mean-field theory that is expected to fail, if fluctuations become important, as they do around T_c . The mean-field theory stays meaningful as long as the fluctuations are small in comparison to the expectation value of the order parameter. The latter criterion can be cast into the following form (Stolze, 2007)

$$1 \gg \frac{\lambda k_B T_c}{\kappa^D} (\alpha_0 |T - T_c|)^{\frac{D-4}{2}} \quad (32)$$

Here, λ and α_0 are parameters in the Landau expansion and κ is a measure of the domain wall formation energy. Thus fluctuations become negligible for $D > 4$ as $T \rightarrow T_c$, $D = 4$ is the marginal dimension and for $D < 4$ fluctuations become increasingly important around T_c . As D is lowered to 1, they extend over an ever-wider temperature range.

The presence of fluctuations has very interesting consequences for the behavior of a material. The dissipation-fluctuation theorem relates a material's response to an external perturbation with the internal fluctuations. Specifically, the static response function can be expressed in terms of the order parameter fluctuation:

$$\chi(\omega = 0, T) = \frac{1}{k_B T} (\langle m^2 \rangle - \langle m \rangle^2) \quad (33)$$

where m is the order parameter. Thus a strongly fluctuating material (in thermodynamic equilibrium!) exhibits a "giant" response to external fields and should therefore be technically relevant for sensor and switching applications. By virtue of the Clausius-Mosotti equation a large response function is associated with a large macroscopic polarizability. A particularly interesting situation arises, if the critical temperature for the continuous phase transition associated with the fluctuations approaches zero. In that case one has a quantum phase transition. At sufficiently low temperature quantum fluctuations take over from thermally driven fluctuations and an entirely different regime of scaling laws applies (Sachdev, 1999; Sachdev, 2000; Vojta, 2003). A glance at phase diagrams of cuprate superconductors reveals their likely connection to quantum phase transitions as illustrated in Fig. 12. The phase boundary between the pseudo gap and the strange metal phase drops with increasing doping and is believed to head towards a quantum critical point. It is, however, not reached, because the quantum critical point is preempted by the superconducting

phase. The strange metal phase is, among other things, characterized by an anomalous temperature dependence of the resistivity, while the pseudo gap phase is either associated with phase fluctuations of the superconducting order parameter or with other fluctuating order parameters, such as SDW or CDW order parameters. In fact, the pairing interaction in the superconducting phase is very likely connected to such fluctuations. A semi-intuitive picture for d-wave symmetry interactions generated by antiferromagnetic fluctuations is shown in Monthoux, Pines & Lonzarich (2007) (see also Bertel & Menzel, 2010). Another manifestation of fluctuations, in this case fluctuations of the charge density, is the striped phase of cuprate superconductors (Zaanen, 2006). While there appears to be general consensus about quantum fluctuations driving high temperature superconductivity, it is not clear, which type of correlations (antiferromagnetic, charge density wave, orbital ordering,...) is the critical factor in raising T_c far beyond the limit of BCS theory (Norman, 2011). The recent discovery of the Iron based superconductors added another twist to the game. Although the symmetry of the order parameter is apparently different from that of the cuprates (Mazin, Singh, Johannes & Du, 2008) (s_{\pm} symmetry instead of d-wave symmetry), there are some conspicuous parallels (Basov & Chubukov, 2011).

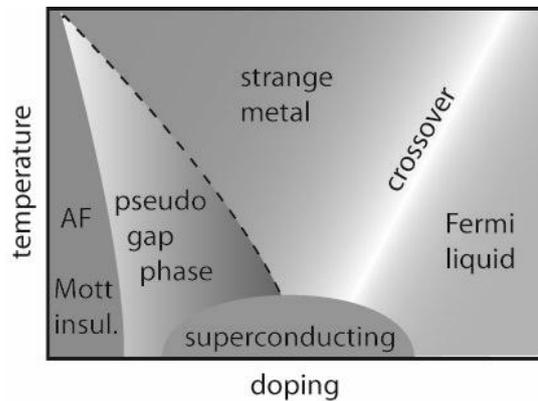


Fig. 12: Schematic phase diagram of a cuprate superconductor. Adapted from Canfield (2011).

The prevailing view is that the high T_c in the iron superconductors is caused by spin density wave fluctuations. Evidence for nematicity, i.e. broken rotational symmetry has been found in these compounds as well. This is reminiscent of the cuprate stripes and represents another hint that one-dimensional physics may hold a key to unconventional superconductivity. Perhaps “one-dimensional” should be interpreted a bit more loosely in this context, for instance as the presence of a $2k_F$ interaction, where the coupling vector q designates a preferred direction in which CDW or SDW correlations develop.

Outlook and Concluding Remarks

Towards the end of this short walk along 1D systems it should be mentioned that despite the impressive progress made in the theoretical modeling, the understanding of coupled 1D systems is still incomplete. However, from the brief discussion of fluctuations and unconventional superconductivity it appears fair to say that the most exciting physics arises at the transition from 1D to 2D, i.e. precisely as 1D systems start interacting, or at the transition from 2D to 1D, i.e. as 2D systems start to spontaneously develop 1D features. Quantum wires at surfaces (Blumenstein et al., 2011; Bertel & Menzel, 2010) offer a unique opportunity to tune the interactions and simultaneously to image the ensuing correlations in both, direct and reciprocal space. While this

might not help in avoiding Friday afternoon traffic jams, it is likely to promote a deeper understanding of physics in low dimension and – among other things - it may eventually even help to solve the problem of the still enigmatic high- T_c superconductivity.

The present paper has been written with the aim to foster an intuitive understanding of basic concepts used to describe 1D systems. It offers some complementary material for a physics undergraduate course of solid-state physics, where correlated materials are often underrepresented. Hopefully, experimentalists, chemists working in materials science and other interdisciplinary scientists from related fields, who lack the formal training to delve into the TLL theory proper may profit from the material presented here.

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