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**Displacement Correlation of Classical
Ions in the Incommensurate Fröhlich
Model of a Onedimensional Metal**

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E. Eisenriegler

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Displacement Correlation of Classical Ions in the Incommensurate Fröhlich Model of a Onedimensional Metal

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E. Eisenriegler

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A b s t r a c t

The one-dimensional Fröhlich model is investigated for $k_B T \ll \delta_0 \ll E_F$ with δ_0 the mean field Peierls gap at $T = 0$. Treating the ions classically and neglecting bandstructure and Umklapp effects the electronic energy for a given ion distortion is determined by Bogolyubov-type equations with a complex order parameter.

For $|p| \gg \delta_0/v_F$ (p is the wavevector deviation from $2k_F$) the (electron-renormalized) phonons are shown to be harmonic with a universal dispersion curve, i.e. independent of T and the possible presence of long wavelength ($|p| < \delta_0/v_F$) phonon excitations.

For an infinitely long ranged Peierls distortion the harmonic phonon excitations are calculated for arbitrary wavevector and temperature. If $|p| < \delta_0/v_F$, one obtains a mixing and energy splitting of the two phonons $2k_F + p$ and $-2k_F + p$ leading to the so-called harmonic phase and amplitude modes. This phonon coupling decreases rapidly for $|p| \gtrsim \delta_0/v_F$ and both dispersions merge into the universal dispersion.

The long wavelength ($|p| < \delta_0/v_F$) phonon excitations in general are described approximately by a Ginzburg-Landau (GL) energy functional where the important fluctuations occur in the phase of the order parameter. For wavelengths small compared to the GL phase-coherence length ($|p| \gg k_B T/v_F$), the harmonic phase (and amplitude) mode become well defined modes and determine the correlation function. Actually, the GL and harmonic results for the correlation function coincide for $k_B T/v_F \ll |p| \ll \delta_0/v_F$ in leading order in the small quantity $k_B T/\delta_0$.

The theory is compared with X-ray and neutron scattering experiments on KCP.

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Introduction

Recently the properties of highly anisotropic conductors consisting of well-separated parallel linear chains of metal ions have aroused considerable interest (for a review see Refs. (1)-(3)). For example, recent optical experiments⁽⁴⁾ have revealed a gap in the electronic excitation spectrum at the Fermi level of the substance KCP⁽⁵⁾, while X-ray⁽⁶⁾ and neutron diffraction measurements⁽⁷⁾⁻⁽¹⁰⁾ indicate (i) a (quasi) static distortion of the ions along the chains with wave-vector $2k_F$ and (ii) soft phonons with wave-vectors near $2k_F$ (k_F = Fermi wave-vector). KCP thus seems to display characteristic features of a "one dimensional" metal, i.e. a system long thought to be of only academic interest, where the conduction electrons are itinerant in one spatial direction only.

It was first noted by Peierls⁽¹¹⁾ and later demonstrated more quantitatively by Fröhlich⁽¹²⁾ and Kuper⁽¹³⁾ that at sufficiently low temperatures a one-dimensional metal is unstable against a periodic distortion of the lattice with wave-vector $2k_F$. This is because the conduction electron polarizability at this wave-vector becomes singular for $T \rightarrow 0$ owing to the existence of a large number of low-energy particle-hole excitations in one dimension. The force which under normal circumstances would restore a $2k_F$ -distortion to homogeneity is thus weakened ("giant Kohn effect") by an amount which increases as temperature decreases until at some finite temperature T_p ("Peierls" or "mean-field" transition temperature) it vanishes. In the molecular field approximation (i.e. neglecting thermal fluctuations of the lattice) the equilibrium state for $T < T_p$ thus corresponds to a lattice distortion

of wave-vector $2k_F$ ("Peierls" distortion) with an amplitude which increases with decreasing temperature. As a consequence of this distortion the electronic density of states exhibits a gap of width $2\delta_T$ at the Fermi energy which lowers the energy of the conduction electrons. At $T = 0$ the width of the gap $2\delta_0$ is of order $k_B T_P$.

In a real substance the Peierls distortion may or may not be commensurate with the basic lattice structure (i.e. $2\pi/2k_F$ may or may not be a simple fraction or multiple of the lattice constant). In the commensurate case the phase of the Peierls distortion will be fixed with respect to the lattice⁽¹⁴⁾. Commensurability is, however, not necessary for the existence of the Peierls transition as exemplified by our example KCP which is not commensurate. Thus it is of interest to supplement existing studies of commensurate Fröhlich models^{(15), (16)} of the Peierls phase with a detailed discussion of the original⁽¹²⁾ incommensurate version of the model where band-structure effects due to the undistorted lattice and Umklapp processes are ignored. This is equivalent to a continuum model for the lattice and leaves the phase of the Peierls distortion with respect to the lattice undetermined. As a consequence the energy of a long-wavelength phase fluctuation is very small.

It is well-known⁽¹⁷⁾ that in a one-dimensional system without long-range interactions the predictions of mean field theory concerning the existence of symmetry breaking long-range order are incorrect owing to the important role played by thermal fluctuations. Lee, Rice and Anderson⁽¹⁸⁾ pointed this out

specifically for the case of a completely phase-locked (commensurate) Peierls system (one-dimensional metal with fluctuating distortions). For the incommensurate case, one expects a qualitative enhancement of the effect of fluctuations owing to the existence of low energy phase fluctuations. In a real system the Peierls distortions in neighbouring chains are weakly coupled and one expects a true phase transition with three-dimensional long-range ordering at a temperature T_{3D} , much lower than $T_p^{(19)}$. In the present paper, we confine our attention to temperatures $T \gg T_{3D}$ where this interchain coupling can be neglected and the fluctuations are one-dimensional. The limit $T \rightarrow 0$ will be understood to mean $T_{3D} \ll T \ll T_p$.

The main aim of the present paper is to present a discussion of the equal-time displacement correlation function which primarily determines the scattering of X-rays by the system. We will be concerned with the influence of fluctuations within the incommensurate Fröhlich model in the limit $T \ll \delta_0 \ll E_F$.

Details of the model and a discussion of the free-electron polarizability are given in Section 1.

Owing to the special role played by the wave-vector $2k_F$, the potential exerted on the electrons by an arbitrary lattice distortion is expressed formally as an amplitude- and phase-modulated potential of the form $2|\Delta(x)|\cos[2k_F x + \arg\Delta(x)]$. The wave-vectors p contained in the corresponding complex modulation factor $\Delta(x)$ correspond to wave-vectors $|k| = 2k_F + p$

of the distortion field. For distortion potentials of main interest (weak compared to E_F , involving only wave-vectors with $|p| \ll k_F$) the Schrödinger equation of the electrons can be replaced by Bogolyubov-type equations (section 2) where only the modulation factor Δ appears as a "potential". The general formalism constitutes a generalization of the "nearly free electron approximation" for a weak periodic potential and is used in section 3 to rederive in a concise way the mean field results of Fröhlich and Kuper.

In our model the ions are treated as heavy, i.e. classical, particles. Therefore, the calculation of the displacement correlation for equal times separates into two subproblems: a) the evaluation of the (free) energy of the electrons moving in a time-independent potential due to a given lattice-distortion (called "distortion-fluctuation" or "fluctuation" in the following); b) performing a thermal average over all distortion-fluctuations by using essentially this free energy as a thermal weight.

In the next two sections (4 and 5), the electronic energy is calculated for distortion-fluctuations occurring at low temperature $k_B T \ll \delta_0$. Since the fluctuation states are expected to be in the "neighbourhood" of the low temperature mean field state, this will be considered as the "unperturbed problem" and its only inherent electronic length $\xi_0 \equiv \hbar v_F / \delta_0$ is expected to give a meaningful scale for the wave-vectors of the "perturbing" fluctuations. We therefore separate the modulation factor Δ into a long- and a short-wavelength part, Δ_0 and $d\Delta$, containing $|p| < \xi_0^{-1}$ and

$|p| > \xi_0^{-1}$ respectively.

In section 4 we show that for thermally probable Δ_0 's containing only $|p| < \xi_0^{-1}$ the electronic energy can be expanded in spatial derivatives of the modulation factor. The expansion has the usual Ginzburg-Landau form and shows that phase fluctuations are much more important than amplitude fluctuations.

The energy of thermally probable $d\Delta$ -modes with $|p| > \xi_0^{-1}$, on the other hand, is shown in section 5 to be a harmonic expression with universal dispersion, i.e. independent of $\Delta_0(x)$. This means that these $d\Delta$ modes are decoupled from Δ_0 .

This behaviour suggests the following approximate calculation (in section 6) of the thermal average needed for the displacement correlation with wave-vector $|k| = 2k_F + q$: For $|q| > \xi_0^{-1}$ all modes except the one for wave-vector $p = q$ cancel in the thermal average and one gets a harmonic result which is exact. For $|q| < \xi_0^{-1}$ the decoupled modes with $|p| > p_c > \xi_0^{-1}$ cancel and one approximately uses the Ginzburg-Landau expression up to second derivatives as thermal weight. This suppresses the non-contributing decoupled modes and represents the modes with $|p| < p_c$ quite well.

This last statement is checked by considering the harmonic expansion for arbitrary p starting from a constant Δ_0 (section 5). One obtains two modes which can be interpreted as (harmonic) phase and amplitude fluctuations[†] of Δ_0 . Their dispersion curves

[†] This calculation corrects and generalizes results in Ref. (14).

degenerate into the universal dispersion if p equals only a few ξ_0^{-1} 's where the Ginzburg-Landau behaviour is still qualitatively valid.

The thermal average with Ginzburg-Landau weight can be performed exactly (section 6) by standard techniques⁽²⁰⁾. The resulting displacement correlation for the long wavelength fluctuations is calculated and corresponds to a Peierls distortion with a finite correlation over a length $\xi = \hbar v_F / k_B T$. This decay of correlation is entirely due to thermal fluctuations in the phase of the Peierls distortion.

Consider this result for the correlation function for wavelengths short compared with the correlation length but still in the Ginzburg-Landau regime, i.e. $\xi^{-1} \ll |q| \ll \xi_0^{-1}$. In this case, it can be seen (section 6) to arise from harmonic fluctuations expanded around the equilibrium state of the infinitely long-ranged Peierls distortion with given phase, i.e. from the harmonic phase- (and amplitude-) fluctuations discussed above. If this harmonic expression is continued to large $|q|$ outside the Ginzburg-Landau regime, it essentially approaches the harmonic result for $|q| \gg \xi_0^{-1}$, which is determined by the universal dispersion. Thus a consistent expression is obtained for the displacement correlation for arbitrary wave-vectors.

In section 7 we compare the result with experimental data for KCP. The theory presented in this work is able to explain the gross features of the experimental diffraction pattern above the

temperature where interchain correlation becomes important. For a quantitative comparison an improvement of the experimental resolution is desirable. However, it is already clear that our discussion of the incommensurate Fröhlich model is only the necessary first step for a fully quantitative understanding. To achieve the latter one would have to perform a band-structure calculation (see Ref.(21)) to connect, at least in a one-particle picture, the effective electron-ion interaction with quantities related to the free planar complex $\text{Pt}(\text{CN})_4$. In addition one should discuss the related problem of the Coulomb interaction between the electrons of a single chain. This is complicated by the fact that mean field treatments such as Hartree or Hartree-Fock are extremely doubtful in one dimension⁽²²⁾. Finally an impurity problem due to the non-stoichiometric electron acceptors⁽²³⁾ must be considered. In this paper we have concentrated on the most fundamental aspect, the electron phonon interaction, and closer agreement between theory and experiment is not to be expected.

1. The model

We consider a linear chain of ions forming a bare Einstein lattice with potential energy

$$U = \frac{f_E}{2} \sum_{n=1}^N s_n^2 \quad . \quad (1.1)$$

Here s_n is the displacement (parallel to the chain) of the n 'th ion from its bare equilibrium position $n \cdot a$, with a the lattice constant. The Einstein springs establish long range order in the one-dimensional chain, which is achieved in reality by the surrounding three-dimensional crystal. The ions are considered to be heavy enough that a treatment within classical mechanics is appropriate. In addition we consider one-dimensional electrons without mutual interaction. Each ion interacts with the electrons via a potential

$$v(x) = \frac{1}{L} \sum_k e^{ikx} \tilde{v}_k \quad ; \quad k = \frac{2\pi}{L} \cdot (\text{integer}), \quad L = Na, \quad (1.2)$$

The total potential

$$V(x) = \sum_n v(x - na - s_n) \quad (1.3)$$

experienced by the electrons can be expanded to first order in s

$$V(x) \approx \frac{1}{a} \sum_{\tau} \tilde{v}_{\tau} e^{i\tau x} + \frac{1}{L} \sum_k e^{ikx} \tilde{v}_k ik \hat{s}_{k_r} \quad (1.4)$$

for displacements small compared to the range of v .

Here τ are integer multiples of $2\pi/a$, k_r is the representative of the set $\{k + \tau\}$ in the first Brillouin zone and

$$\hat{s}_{k_r} = \sum_n e^{-ik_r n a} s_n, \quad -\frac{\pi}{a} < k_r < \frac{\pi}{a} \quad . \quad (1.5)$$

In the following an important role is played by the wavevectors $k = \pm 2k_F$ which for simplicity are assumed to be in the first Brillouin zone. Moreover $\tilde{v}_k$ is assumed nonvanishing for k in the first Brillouin zone only. We call this the incommensurate situation since this assumption rules out band structure and Umklapp effects, i.e. the electrons do not feel the discrete lattice and possible electronic density waves have no reason to be commensurate with the lattice constant.

To be definite, $k\tilde{v}_k$ is assumed real and

$$k\tilde{v}_k \Theta(k) = : w_{k-2k_F} \quad (1.6)$$

with a function w_k which varies on the scale of k_F (compare Fig. 1). Then V can be written

$$\begin{aligned} V(x) &= \frac{1}{L} \sum_{k>0} e^{ikx} i w_{k-2k_F} \hat{s}_k + cc = \\ &= \Delta(x) e^{i2k_F x} + cc \end{aligned} \quad (1.7)$$

where

$$\tilde{\Delta}_p = i w_p \hat{s}_{2k_F+p}, \quad 0 < 2k_F + p < \frac{\pi}{a} \quad (1.8)$$

are $\frac{N}{2}$ independent complex variables, replacing the N real

variables s_n . In terms of the new variables, (1.1) becomes

$$U = \frac{f_E}{N} \sum_{0 < k < \frac{\pi}{a}} |\hat{s}_k|^2 = \frac{f_E}{N} \sum_{-2k_F < p < \frac{\pi}{a} - 2k_F} |\hat{\Delta}_p|^2 / w_p^2. \quad (1.9)$$

The quantities we are finally interested in are equilibrium properties of the form[†]

$$\frac{1}{Z} \int d^N s \, Q[s] \sum_{\mathcal{N}=1}^{\infty} \text{Tr}_{\mathcal{N}} \exp \frac{(-)}{T} \left\{ U + \sum_{i=1}^{\mathcal{N}} \left[\frac{p_i^2}{2m} + V(x_i) - E_F \right] \right\} \quad (1.10)$$

Here p_i , x_i are the momentum and position operators of electron i , we consider a grand canonical ensemble with chemical potential E_F , and Z is the integral with $Q = 1$. For $Q = s_n s_0$ Eq.(1.10) gives the equal time displacement entering in scattering experiments. We rewrite (1.10) as

$$\frac{\int d^N s \, Q[s] e^{-\mathcal{H}/T}}{\int d^N s \, e^{-\mathcal{H}/T}} = \frac{\int \mathcal{D}_{\Delta} Q e^{-\mathcal{H}/T}}{\int \mathcal{D}_{\Delta} e^{-\mathcal{H}/T}} \quad (1.11)$$

with (prime and double prime denote real and imaginary part)

$$\mathcal{H} = U + \Omega, \quad \mathcal{D}_{\Delta} = \prod_p d \hat{\Delta}_p' d \hat{\Delta}_p'' \quad (1.12)$$

and Ω is the free energy of electrons for given displacement of the ions (factor 2 for spin)

$$\begin{aligned} \Omega &= 2 \int dE \, N(E) (-)T \ln(1 + e^{-\hat{E}/T}) \\ &= \Omega_0 - 2 \int \frac{dz}{2\pi i} \frac{1}{e^{z/T} + 1} \text{Tr} \ln(1 - \frac{1}{z - H_0} V). \end{aligned} \quad (1.13)$$

†

We use units where $\hbar = k_B = v_F = 1$

Here $N(E)$ is the one-particle density of states per spin direction for electrons subjected to the external potential V , $\hat{E} = E - E_F$, and Ω_0 is Ω for $V = 0$. The integration path C encloses counterclockwise the real axis but not the Fermi poles, Tr denotes the trace over the one-particle Hilbert space and $H_0 = \frac{p^2}{2m} - E_F$. The second line in (1.13) is obtained by partial integration if the density of states is used in the form

$$N(E) = - \frac{1}{2\pi i} \text{Tr} \left(\frac{1}{\hat{E} + i\eta - H_0 - V} - hc \right), \quad (1.14)$$

To demonstrate the peculiarity of the one-dimensional electron gas, consider the free energy to second order in V if $\Delta(x) = \frac{\tilde{\Delta}p}{L} e^{ipx}$, i.e. for a distortion with wavevector $k = 2k_F + p$. Then (1.13) gives

$$\Omega^{(2)} = 2 \cdot \frac{|\tilde{\Delta}p|^2}{L^2} \sum_K \frac{f_K - f_{k+K}}{\frac{K^2}{2m} - \frac{(k+K)^2}{2m}} \quad (1.15)$$

For $T = 0$ and $k > 0$ one obtains

$$\Omega^{(2)} = \frac{|\tilde{\Delta}p|^2}{L^2} L \cdot \frac{1}{\pi} \frac{2m}{k} \ln \frac{|2k_F - k|}{2k_F + k}. \quad (1.16)$$

This quantity is sketched in Fig.2 and shows that the energy of one-dimensional electrons is extremely sensitive to perturbations with wavevectors k near $2k_F$. This is due to the large weight of particle-hole excitations with nearly vanishing excitation energy in one dimension. For $k \gg 2k_F$ the response tends to zero since the excitation energy for particle-hole

pairs with momentum difference k gets very large.

For $T \ll E_F$ and $k = 2k_F$ the expression (1.15) becomes

$$\Omega^{(2)} = - \frac{L}{\pi} |\Delta|^2 \int_0^{2E_F/T} \frac{dx}{x} \operatorname{Tgh} x = - L |\Delta|^2 \cdot \frac{1}{\pi} \ln \frac{cE_F}{T} \quad (1.17)$$

where $c = \frac{2}{\pi e^{\psi(1/2)}} \approx 4.54^{(24)}$ and ψ is the digamma function. The $2k_F$ response (1.17) diverges logarithmically for $T \rightarrow 0$. According to (1.9), (1.17) the harmonic restoring force for a $2k_F$ -distortion vanishes if T approaches the so called Peierls temperature T_p from above and the system becomes unstable against $2k_F$ -distortions for $T < T_p$. This temperature is given by rewriting the bare lattice energy (1.9) for the present case as

$$U = L |\Delta|^2 \cdot \frac{f_E a}{w_0^2} = L |\Delta|^2 \cdot \frac{1}{\pi} \ln \frac{cE_F}{T_p} \quad (1.18)$$

since we assume $f_E a/w_0^2$ such that

$$E_F/T_p \gg 1 \quad . \quad (1.19)$$

This is in agreement with experimental applications to be discussed later. According to (1.18) there is a large tendency towards the $2k_F$ instability, i.e. T_p large, if the bare lattice is soft and the electron phonon interaction is large. For a half filled tight binding band $U + \Omega^{(2)}$ has been calculated in Ref.(15)

2. Bogolyubov equations

The distortions of main interest are those with wavevectors k near $2k_F$ ($|k-2k_F| \ll k_F$), i.e. $\Delta(x)$ in (1.7) slowly varying on

the scale k_F^{-1} . These distortions determine physical properties like the X-ray scattering in the neighbourhood of the quasi-superstructure point with momentum transfer $2k_F$ or the optical absorption across the Peierls gap. Although distortions with wavevectors in the extreme neighbourhood of $2k_F$ will turn out to be thermally occupied in a macroscopic sense the resulting potential V turns out still much smaller than E_F if we assume (1.19). Starting from $V = 0$ the perturbation series for one-electron states ψ_α shows that only plane waves with momentum k in the neighbourhood of $\pm k_F$ will be perturbed appreciably by the potential V and there will be an admixture only of k 's near $\pm k_F$. Apart from corrections of $O(V/E_F)$ the one-electron states $\psi_\alpha(x)$ with $|E_\alpha - E_F| \ll E_F$ can therefore be written

$$\psi_\alpha(x) = \bar{u}_\alpha^+(x) e^{ik_F x} + \bar{u}_\alpha^-(x) e^{-ik_F x} \quad (2.1)$$

with $\bar{u}_\alpha^\pm$ slowly varying on the scale k_F^{-1} . Disregarding $u'' \ll k_F u'$ and disentangling slow and rapid variations in Schrödinger's equation for ψ_α one arrives at the pair of first order equations

$$\begin{pmatrix} \partial_x/i & , & \Delta(x) \\ \Delta^*(x) & , & -\partial_x/i \end{pmatrix} \begin{pmatrix} \bar{u}_\alpha^+(x) \\ \bar{u}_\alpha^-(x) \end{pmatrix} = \hat{E}_\alpha \begin{pmatrix} \bar{u}_\alpha^+(x) \\ \bar{u}_\alpha^-(x) \end{pmatrix} \quad (2.2)$$

where $\hat{E}_\alpha = E_\alpha - E_F$.

In the space of periodic vectors $(\bar{u}^+(x), \bar{u}^-(x))$ with $\bar{u}^+(L) = \bar{u}^+(0)$ the matrix operator in (2.2) is hermitean and its eigenvectors form a complete orthonormal set

$$\int_0^L dx (\bar{u}_\alpha^*(x), \bar{u}_\alpha^*(x)) \begin{pmatrix} \bar{u}_\beta^+(x) \\ \bar{u}_\beta^-(x) \end{pmatrix} = \delta_{\alpha\beta} \quad (2.3)$$

$$\sum_\alpha \begin{pmatrix} \bar{u}_\alpha^+(x) \\ \bar{u}_\alpha^-(x) \end{pmatrix} (\bar{u}_\alpha^*(y), \bar{u}_\alpha^*(y)) = 1 \cdot \delta(x-y)$$

with 1 the 2x2 unit matrix. Physical quantities of interest can be expressed most easily in terms of the Green's function

$$G(x, y; z) = \sum_{\alpha} \begin{pmatrix} \bar{u}_{\alpha}^{\dagger}(x) \\ \bar{u}_{\alpha}(x) \end{pmatrix} \frac{1}{z - \hat{E}_{\alpha}} \begin{pmatrix} u_{\alpha}^{\dagger}(y) \\ u_{\alpha}(y) \end{pmatrix} \quad (2.4)$$

determined by the equation

$$\left[1 \cdot z - \begin{pmatrix} \partial_x / i & \Delta(x) \\ \Delta^*(x) & -\partial_x / i \end{pmatrix} \right] G(x, y, z) = 1 \delta(x-y). \quad (2.5)$$

The density of states for $|\hat{E}| < E_F$ is given by (2.3), (2.4) as

$$N(E) = - \frac{1}{2\pi i} \int dx \left[\text{tr} G(x, x; \hat{E} + i\eta) - cc \right] \quad (2.6)$$

where tr denotes the trace in the 2x2 space.

The connection with the usual Green's function, $\langle x | (z - H_0 - V)^{-1} | y \rangle$, is given according to (2.1) by

$$\begin{aligned} \langle x | \frac{1}{\omega + i\eta - H_0 - V} - \frac{1}{\omega - i\eta - H_0 - V} | y \rangle &= \\ &= \begin{pmatrix} e^{ik_F x} & e^{-ik_F x} \end{pmatrix} \left[G(x, y; \omega + i\eta) - G(x, y; \omega - i\eta) \right] \begin{pmatrix} -ik_F \eta \\ e \\ ik_F \eta \\ e \end{pmatrix} \end{aligned} \quad (2.7)$$

for $|\omega| < E_F$.

3. Finite distortions with wavevector $2k_F$

According to (1.17), (1.18) the undistorted chain is unstable (no minimum of $\mathcal{H}$) for $T < T_p$. It is plausible (and will be shown in section 4) that the equilibrium configuration is a

$2k_F$ -distortion with a finite amplitude and undetermined phase. In this section the amplitude will be evaluated.

For the pure $2k_F$ distortion V is a periodic potential, the electron states ψ_α are Bloch functions and (2.2) is the corresponding "nearly free electron approximation". Since $\Delta(x) = \delta e^{i\phi}$ with δ, ϕ constant in space, Eq. (2.2) gives

$$\begin{pmatrix} u \\ \bar{u} \end{pmatrix}_{k, \pm} = \frac{e^{ikx}}{\sqrt{L}} \begin{pmatrix} e^{i\phi/2} (\pm) \sqrt{\frac{\epsilon_k \pm k}{2\epsilon_k}} \\ e^{-i\phi/2} \sqrt{\frac{\epsilon_k \mp k}{2\epsilon_k}} \end{pmatrix} \quad (3.1)$$

$$\hat{E}_{k, \pm} = \pm \epsilon_k, \quad \epsilon_k = \sqrt{|\Delta|^2 + k^2}$$

where the index α in (2.2) is now given by a Bloch vector k and a band-index $\pm$ for the upper and lower band (Fig. 3). For $|k| \gg |\Delta|$ the Bloch states according to (2.1), (3.1) reduce to single plane waves

$$\psi_{k>0, \pm} \rightarrow \frac{e^{ikx}}{\sqrt{L}} e^{\pm [ik_F x + i\phi/2]}, \quad \psi_{k<0, \pm} \rightarrow \pm \frac{e^{ikx}}{\sqrt{L}} e^{\mp [\quad]} \quad (3.2)$$

The orthonormality (2.3) is checked easily for our present eigenvector (3.1) and the Green's function (2.4), (2.5) becomes

$$G(x, y; z) = \frac{1}{L} \sum_k e^{ikr} \left[1 \cdot z - \begin{pmatrix} k, \Delta \\ \Delta^*, -k \end{pmatrix} \right]^{-1} =$$

$$= - \begin{pmatrix} z + \partial_r / i, \Delta \\ \Delta^*, z - \partial_r / i \end{pmatrix} \frac{e^{-|r| \sqrt{|\Delta|^2 - z^2}}}{2 \sqrt{|\Delta|^2 - z^2}} \quad (3.3)$$

Here $r = x-y$, the square root is positive for $-|\Delta| < z < |\Delta|$ and its branch cuts in z run from $|\Delta| \rightarrow \infty$ and $-|\Delta| \rightarrow -\infty$ on the real axis. The density of states (2.6) is

$$N(E) = \frac{L}{2\pi i} \left(\frac{\hat{E} + i\eta}{\sqrt{|\Delta|^2 - (\hat{E} + i\eta)^2}} - cc \right) = \frac{L}{\pi} \frac{|\hat{E}|}{\sqrt{\hat{E}^2 - |\Delta|^2}} \Theta(|\hat{E}| - |\Delta|), \quad (3.4)$$

To obtain Ω , insert the first expression (3.4) into the first line of (1.13) to get a contour integral. The contribution higher than second order in $|\Delta|$ is rewritten according to

$$\int_C \frac{dz}{2\pi i} f'(z) T \ln(1 + e^{-z/T}) = T \sum_{\alpha} f(i\omega_{\alpha}); \quad \omega_{\alpha} = \pi T \alpha, \quad \alpha \text{ odd} \quad (3.5)$$

for $f = \mathcal{O}(\frac{1}{z^2})$ for large $|z|$ and analytic apart from the real axis.

This gives

$$\begin{aligned} \Omega - \Omega_0 - \langle \Omega \rangle &= -2LT \sum_{\alpha} \left[W_{\alpha} - |\omega_{\alpha}| - \frac{|\Delta|^2}{2|\omega_{\alpha}|} \right] \rightarrow \\ &\rightarrow L|\Delta|^2 \cdot \frac{1}{\pi} \left[\ln \frac{c|\Delta|}{8T} - \frac{1}{2} \right], \end{aligned} \quad (3.6)$$

where $W_{\alpha} = \sqrt{\omega_{\alpha}^2 + |\Delta|^2}$ and the last expression holds for $T \ll |\Delta|$ as shown in appendix A. Therefore the total energy for a $2k_F$ distortion for $T \ll E_F$ is given by (1.17), (1.18), (3.6) as

$$\mathcal{H} - \Omega_0 = L \varepsilon_{\ell}(|\Delta|) \quad (3.7)$$

with the energy density

$$\varepsilon_{\ell}(|\Delta|) = \frac{|\Delta|^2}{\pi} \ln \frac{T}{T_p} - 2T \sum_{\alpha} \left[W_{\alpha} - |\omega_{\alpha}| - \frac{|\Delta|^2}{2|\omega_{\alpha}|} \right]. \quad (3.8)$$

For $T \ll |\Delta|$ the constant c drops out in the total electronic energy, (1.17)+(3.6), and with (1.18)

$$\begin{aligned} \epsilon_{\ell}(|\Delta|) &= \frac{|\Delta|^2}{\pi} \left[\frac{\pi f_E a}{w_0^2} + \ln \frac{|\Delta|}{8E_F} - \frac{1}{2} \right] \\ &\equiv \frac{|\Delta|^2}{\pi} \left[\ln \frac{|\Delta|}{\delta_0} - \frac{1}{2} \right] . \end{aligned} \quad (3.9)$$

The expression for the gap $|\Delta| = \delta_0$ of minimal energy ϵ_{ℓ} ,

$$\frac{1}{\pi} \ln \frac{8E_F}{\delta_0} = \frac{f_E a}{w_0^2} \quad (3.10)$$

has been derived in Ref.(12) (see appendix A). A comparison of (3.10) and (1.18) gives⁽¹³⁾

$$\delta_0 = \frac{8}{c} T_p \approx 1.76 T_p. \quad (3.11)$$

Eq.(3.10) together with (1.9), (1.16) provides a simple connection of δ_0 with the harmonic expansion around $s \equiv 0$ of the total energy for $T = 0$ and arbitrary wavevector

$$\frac{1}{L} \sum_{0 < k < \frac{\pi}{a}} |\hat{s}_k|^2 [f_E a + J_k] \quad (3.12)$$

$$[] \rightarrow w_0^2 \left(\frac{f_E a}{w_0^2} + \frac{1}{\pi} \ln \frac{|2k_F - k|}{8E_F} \right) \quad \text{for } |k - 2k_F| \ll k_F$$

With the assumption (1.19) the zeros of the dispersion are situated at $k = 2k_F \pm \delta_0$ as shown in Fig.4.

For later reference let us discuss the case of a linearly increasing phase $\Delta = \delta e^{i2qx}$ which means that the gap occurs at

$\pm (k_F + q)$. Then (2.5) gives

$$G(x, y; z) = \begin{pmatrix} e^{iqx}, 0 \\ 0, e^{-iqx} \end{pmatrix} \frac{1}{L} \sum_k e^{ikr} \begin{pmatrix} z - q - k, -\delta \\ -\delta, z - q + k \end{pmatrix}^{-1} \begin{pmatrix} e^{-iqy}, 0 \\ 0, e^{iqy} \end{pmatrix} \quad (3.13)$$

and the density of states (2.6) is given by (3.4) apart from a shift q in energy as expected. The corresponding energy change is given in terms of N in (3.4) as

$$2 \int_{-\infty}^{\infty} dE \left[N(E - q) - N(E) \right] (-T) \ln(1 + e^{-\hat{E}/T}) \rightarrow \frac{L}{\pi} q^2 \quad (3.14)$$

where the expression on the right hand side is valid for $T \ll \delta$ and $q \ll \delta$ (see appendix A).

4. Slowly varying $\Delta(x)$

The Green's function (3.3) for constant Δ varies spatially on the scale $(|\Delta|^2 + (\pi T)^2)^{-1/2} = W_1^{-1}$ for z on Fermi poles. If Δ is varying slowly on this scale a local approximation will be valid for the free energy. Starting from the local approximation one expects an expansion with $\left| \frac{\partial \Delta}{\partial x} \right| W_1^{-1}$ as the small parameter.

To obtain this expansion one introduces new variables in G (Eq. (2.5))

$$G(x, y) = \bar{G}(x, r) \quad , \quad r = x - y \quad (4.1)$$

Since

$$\partial_x G = (\partial_x + \partial_r) \bar{G} \quad , \quad (4.2)$$

Eq. (2.5) gives for the Fourier transform $\tilde{\bar{G}}_k(x)$ with respect to r

$$\left[1 \cdot z - \begin{pmatrix} k, \Delta(x) \\ \Delta^*(x), -k \end{pmatrix} \right] \tilde{\bar{G}}_k(x; z) = 1 + \begin{pmatrix} \frac{1}{i} \partial_x, 0 \\ 0, -\frac{1}{i} \partial_x \end{pmatrix} \tilde{\bar{G}}_k(x; z) \quad . \quad (4.3)$$

Neglecting the second term on the right hand side gives the local approximation, $\tilde{\bar{G}}_k = \tilde{\bar{G}}_k^l$,

$$\begin{aligned} G^l(x, y; z) &= \frac{1}{L} \sum_k e^{ikr} \left[z - \begin{pmatrix} k, \Delta(x) \\ \Delta^*(x), -k \end{pmatrix} \right]^{-1} = \\ &= \frac{1}{L} \sum_k e^{ikr} \begin{pmatrix} z+k & \Delta \\ \Delta & z-k \end{pmatrix} \frac{(-)}{k^2 + W_\alpha^2(x)} \end{aligned} \quad (4.4)$$

i.e. (3.3) with the local gap $\Delta(x)$. The local approximation for

the free energy is therefore given by (compare (3.7), (3.8), (3.9))

$$\mathcal{F}_\ell - \Omega_0 = \int dx \, \epsilon_\ell(|\Delta(x)|) \quad . \quad (4.5)$$

The expansion for slowly varying Δ is provided by rewriting (4.3) as

$$\tilde{G}_k(x, z) = \tilde{G}_k^\ell(x, z) + \tilde{G}_k^\ell(x, z) \begin{pmatrix} \frac{1}{i} \partial_x, 0 \\ 0, -\frac{1}{i} \partial_x \end{pmatrix} \tilde{G}_k(x, z) \quad . \quad (4.6)$$

According to (1.13), (2.6) and (4.1) the free energy correction to the local approximation is given by

$$\Omega - \Omega_\ell = 2 \int dx \int_C \frac{dz}{2\pi i} \frac{1}{L} \sum_k \text{tr} \left[\tilde{G}_k(x; z) - \tilde{G}_k^\ell(x, z) \right] \cdot (-)T \ln(1 + e^{-z/T}) \quad . \quad (4.7)$$

First order derivatives can be written as complete differentials and do not contribute to bulk properties. A straightforward calculation gives for the second order contribution (apart from a complete x -differential)

$$\frac{1}{L} \sum_k \text{tr} \left[\tilde{G}_k - G_k^\ell \right]_2 = - \partial_z \frac{1}{2} \int \frac{dk}{2\pi} \left\{ \frac{|\partial_x \Delta|^2}{(k^2 + |\Delta|^2 - z^2)^2} - \frac{1}{3} \frac{(\partial_x (|\Delta|^2))^2}{(k^2 + |\Delta|^2 - z^2)^3} \right\} \quad (4.8)$$

With (3.5) the free energy to second order in derivatives becomes

$$\Omega_2 = 2 \int dx \, T \sum_{\alpha > 0} \frac{1}{4} \left[\frac{|\partial_x \Delta(x)|^2}{W_\alpha^3(x)} - \frac{1}{4} \frac{(\partial_x (|\Delta(x)|^2))^2}{W_\alpha^5(x)} \right] \quad (4.9)$$

Apart from a factor $\frac{\pi}{3}$ this is identical with the corresponding 3-dimensional expression in the theory of superconductivity (compare e.g. Ref. (25)). From the form

$$\Omega_2 = \int dx \, T \sum_{\alpha > 0} \frac{1}{2} \frac{1}{W_\alpha^3} (\partial_{\mathbf{x}}^{\Delta'}, \partial_{\mathbf{x}}^{\Delta''}) \left[1 - \frac{|\Delta|^2}{W_\alpha^2} P^{\parallel}(\Delta) \right] \begin{pmatrix} \partial_{\mathbf{x}}^{\Delta'} \\ \partial_{\mathbf{x}}^{\Delta''} \end{pmatrix}$$

$$P^{\parallel}(\Delta) = \frac{1}{|\Delta|^2} \begin{pmatrix} \Delta' \\ \Delta'' \end{pmatrix} (\Delta' \Delta'') \quad (4.10)$$

it becomes apparent that Ω_2 is positive definite.

For $T \ll |\Delta|$ the sum in (4.10) can be approximated by an integral to give

$$\Omega_2 = \int dx \frac{1}{4\pi |\Delta(\mathbf{x})|^2} (\partial_{\mathbf{x}}^{\Delta'}, \partial_{\mathbf{x}}^{\Delta''}) \left[1 - \frac{2}{3} P^{\parallel}(\Delta) \right] \begin{pmatrix} \partial_{\mathbf{x}}^{\Delta'} \\ \partial_{\mathbf{x}}^{\Delta''} \end{pmatrix} \quad (4.11)$$

5. Small deviations with arbitrary wavelength from long wavelength fluctuations

The expansion of $\frac{\Omega}{|\partial_{\mathbf{x}} \Delta|^2}$ for slowly varying Δ given in the last section is valid only for $\frac{|\partial_{\mathbf{x}} \Delta|^2}{|\Delta|^2} \ll W_1^2(\mathbf{x})$. For $T \ll \delta_0$ where $\langle |\Delta|^2 \rangle \approx \delta_0^2$ the expansion holds only if $\tilde{\Delta}_p = 0$ for $|p| \gtrsim \delta_0$. In this section the influence of short wavelength fluctuations $|p| \gtrsim \delta_0$ will be discussed. It will turn out that for low temperature a harmonic expansion (up to 2nd order) in these fluctuations is sufficient and that fluctuations with $|p| \gg \delta_0$ (nevertheless $|p| \ll k_F$ may hold), i.e. the overwhelming number of fluctuations, do not influence the thermal probability of the long wavelength fluctuations ($|p| \lesssim \delta_0$).

To demonstrate these assertions we introduce a momentum cut-off p_c ($\sim \delta_0$ for $T \ll \delta_0$) and write

$$\Delta(x) = \frac{1}{L} \sum_{|p| < p_c} e^{ipx} \tilde{\Delta}_p + \frac{1}{L} \sum_{|p| > p_c} e^{ipx} \tilde{\Delta}_p = \Delta_0(x) + d\Delta(x) \quad (5.1)$$

According to (1.13), (2.5), (2.6) the correction to the free energy due to $d\Delta$ is given by

$$\Omega - \Omega[\Delta_0] \cong 2 \cdot \int_C \frac{dz}{2\pi i} \sum_{\mu=1}^{\infty} \text{Tr} \left\{ \left[G_0(z) \begin{pmatrix} 0 & d\Delta \\ d\Delta^* & 0 \end{pmatrix} \right]^\mu G_0(z) \right\} (-) \text{Tr} n(1 + e^{-z/T}) \quad (5.2)$$

where Tr denotes the trace in 2×2 space and multiple x -integration. The function $G_0(x, x'; z)$ satisfies (2.5) with the slowly varying $\Delta = \Delta_0$ and can be calculated with the methods of the preceding section. There are cutoff problems for the local G_0 -contribution in the $\mu = 2$ term (expressed by $\cong$) which however are resolved easily by comparison with (4.5) in the appropriate limit as we shall see below.

Using the spectral representation (2.4) for G_0 the trace in (5.2) can be written as a z -derivative

$$\text{Tr} = - \partial_z \frac{1}{\mu} \text{Tr} \left[G_0(z) \begin{pmatrix} 0 & d\Delta \\ d\Delta^* & 0 \end{pmatrix} \right]^\mu \quad (5.3)$$

and the free energy correction to μ 'th order in $d\Delta$, $\Omega^{(\mu)}$, can be written using (3.5)

$$\Omega^{(\mu)} \cong \frac{2}{\mu} T \sum_{\alpha} \text{Tr} \left[G_0(i\omega_{\alpha}) \begin{pmatrix} 0 & d\Delta \\ d\Delta^* & 0 \end{pmatrix} \right]^\mu. \quad (5.4)$$

a) Second order contribution $\Omega^{(2)}$ for constant Δ_0

Before discussing $\Omega^{(2)}$ for general $\Delta_0(x)$, we consider in some detail the important special situation $\Delta_0(x) \equiv \delta e^{i\phi}$ with δ, ϕ independent of x . In this case (B3) gives

$$\begin{aligned} \Omega^{(2)} \cong \frac{1}{2L} \sum_p \left\{ - |D_p^\perp|^2 T \sum_\alpha \frac{|\Delta_0|^2}{\tilde{W}_\alpha (\tilde{W}_\alpha^2 + \frac{p^2}{4})} + \right. \\ \left. + (|D_p^\parallel|^2 + |D_p^\perp|^2) T \sum_\alpha \frac{-\omega_\alpha^2}{\tilde{W}_\alpha (\tilde{W}_\alpha^2 + \frac{p^2}{4})} \right\}. \end{aligned} \quad (5.5)$$

Here

$$d\Delta_{\parallel, \perp}(x) = \frac{1}{L} \sum_p e^{ipx} \frac{D_p^{\parallel, \perp}}{\sqrt{2}} \quad (5.6)$$

are the real projections ($D_{-p} = D_p^*$) of the complex quantity

$$d\Delta(x) = \frac{\Delta_0}{|\Delta_0|} d\Delta_{\parallel}(x) + \frac{i\Delta_0}{|\Delta_0|} d\Delta_{\perp}(x) \quad (5.7)$$

parallel and perpendicular to Δ_0 . This implies

$$\begin{pmatrix} D_p^\parallel \\ D_p^\perp \end{pmatrix} = \frac{1}{\sqrt{2}|\Delta_0|} \begin{pmatrix} \Delta_0^*, \Delta_0 \\ \frac{1}{i}\Delta_0^*, -\frac{1}{i}\Delta_0 \end{pmatrix} \begin{pmatrix} \gamma_p \\ \gamma_{-p}^* \end{pmatrix}, \quad p > 0. \quad (5.8)$$

To get the proper expression for the second frequency sum in (5.5) one observes that for $d\Delta$ varying slowly on the scale $\tilde{W}_1^{-1}$, the local approximation (4.5) is valid for the free energy of $\Delta = \Delta_0 + d\Delta$ which to second order in $d\Delta$ gives

$$\mathcal{H}_\ell^{(2)} = \int dx \frac{1}{2} \left\{ d\Delta_{\parallel}^2 \frac{\partial^2 \epsilon_\ell}{\partial |\Delta_0|^2} + d\Delta_{\perp}^2 \frac{1}{|\Delta_0|} \frac{\partial \epsilon_\ell}{\partial |\Delta_0|} \right\} \quad (5.9)$$

since

$$|\Delta| = \sqrt{(|\Delta_0| + d\Delta_{\parallel})^2 + d\Delta_{\perp}^2} = |\Delta_0| + d\Delta_{\parallel} + \frac{1}{2} \frac{d\Delta_{\perp}^2}{|\Delta_0|} + \mathcal{O}(d\Delta^3),$$

From (3.8)

$$\frac{\partial^2 \varepsilon_{\ell}/2}{\partial |\Delta_0|^2} = \frac{1}{\pi} \ln \frac{T}{T_p} - T \sum_{\alpha} \left[\frac{\omega_{\alpha}^2}{W_{\alpha}^3} - \frac{1}{|\omega_{\alpha}|} \right] \quad (5.10)$$

$$\frac{1}{|\Delta_0|} \frac{\partial \varepsilon_{\ell}/2}{\partial |\Delta_0|} = \frac{1}{\pi} \ln \frac{T}{T_p} - T \sum_{\alpha} \left[\frac{1}{W_{\alpha}} - \frac{1}{|\omega_{\alpha}|} \right]$$

and a comparison of (5.9), (5.10) with the $p \rightarrow 0$ limit of (5.5) yields the proper expression

$$\begin{aligned} \mathcal{H}^{(2)} &= \frac{1}{L} \sum_{p > p_c} \left\{ |D_p^{\parallel}|^2 f_p^{\parallel} + |D_p^{\perp}|^2 f_p^{\perp} \right\} \\ f_p^{\parallel} &= \frac{\partial^2 \varepsilon_{\ell}/2}{\partial |\Delta_0|^2} + T \sum_{\alpha} \left[\frac{\omega_{\alpha}^2}{W_{\alpha}^3} - \frac{\omega_{\alpha}^2}{W_{\alpha} (\bar{W}_{\alpha}^2 + p^2/4)} \right] \\ f_p^{\perp} &= \frac{1}{|\Delta_0|} \frac{\partial \varepsilon_{\ell}/2}{\partial |\Delta_0|} + T \sum_{\alpha} \left[\frac{1}{W_{\alpha}} - \frac{\bar{W}_{\alpha}}{W_{\alpha}^2 + p^2/4} \right] \end{aligned} \quad (5.11)$$

The energy $\mathcal{H} \left[\Delta_0 + \frac{\gamma}{L} p e^{ipx} \right]$, to second order in $\hat{\Delta}_p$, and p not higher than second order, can be calculated either from (4.5), (4.10) or from (5.11), of course with the same result.

For $T \ll |\Delta_0|$ one obtains

$$\begin{aligned} \pi f_p^{\parallel} &= \ln \frac{\delta}{\delta_0} + \frac{\sqrt{1+\kappa^2}}{\kappa} \ln(\sqrt{1+\kappa^2} + \kappa) \\ \pi f_p^{\perp} &= \ln \frac{\delta}{\delta_0} + \frac{\kappa}{\sqrt{1+\kappa^2}} \ln(\sqrt{1+\kappa^2} + \kappa) \end{aligned}, \quad \kappa = p/2\delta \quad (5.12)$$

We are now in a position to demonstrate (for our constant Δ_0) that $\mathcal{H}^{(2)}$ is independent of Δ_0 and T for $\hat{\Delta}_p$'s with $k_F \gg |p| \gg \bar{w}_1$. In this limit (5.11), apart from corrections $\frac{\delta^2}{p^2} \ln \frac{p}{\delta}$ to the f 's, reduces to $\mathcal{H}^{(2)}$ for $\delta = 0$

$$\mathcal{H}_{\Delta_0=0}^{(2)} = \frac{1}{L} \sum_p |\hat{\chi}_p|^2 \cdot f_p \quad (5.13)$$

$$\pi f_p = \ln \frac{T}{T_p} - \psi\left(\frac{1}{2}\right) + \operatorname{Re} \psi\left(\frac{1}{2} + i \frac{p}{4\pi T}\right) .$$

This expression is the harmonic expansion around the minimum for $T > T_p$ and shows the giant Kohn anomaly. In our limit $k_F \gg |p| \gg T$ the second line of (5.13) becomes $\ln \frac{|p|}{\delta_0}$ by use of (1.17), (3.11). This is in agreement with our discussion of the Kohn effect for $T = \Delta_0 = 0$ in (3.12) which gives

$$\pi f_p = \frac{\pi}{w_p^2} [f_E^a + J_{2k_F+p}] \quad (5.14)$$

According to our previous discussion the dispersion (5.14) is valid also for nonvanishing $(\Delta_0, T) \ll E_F$ provided $|p| \gg \bar{w}_1$, $0 < 2k_F + p < \frac{\pi}{a}$.

Imagine for the moment that a long range ordered equilibrium state $\Delta_0 = \delta_T e^{i\phi}$ would exist, even at finite temperature, with a definite phase ϕ (broken symmetry) and δ_T the gap with minimal energy (3.7). Then (5.11) describes harmonic vibrations around the equilibrium state. Their frequency is determined by considering the kinetic energy of the ions

$$\frac{M}{2} \sum_n \dot{s}_n^2 = \frac{1}{L} \sum_{p>0} \frac{Ma}{w_p^2} (|\dot{D}_p^{\parallel}|^2 + |\dot{D}_p^{\perp}|^2) \quad (5.15)$$

with the result[†]

$$M \omega_p^2 = \frac{w_p^2}{a} f_p^{\parallel, \perp} \quad (5.16)$$

For our situation $\delta = \delta_T$ the dispersion $f_{p=0}^{\perp}$ vanishes as long as $\delta_T > 0$, i.e. $T < T_p$ ("Goldstone vibration") and $f_{p=0}^{\parallel}$ goes from $\frac{1}{\pi}$ at $T=0$ to zero for $T \nearrow T_p$ (soft phonon). At T_p the dispersions $f_p^{\parallel}$ and $f_p^{\perp}$ become identical and equal to f_p in (5.13). Above T_p , $f_{p=0}^{\parallel} = f_{p=0}^{\perp} = f_{p=0}$ rises as $\frac{1}{\pi} \ln \frac{T}{T_p}$ (soft phonon). These features are sketched in Fig.5.

As we shall see these harmonic vibrations do exist for $|p| > \delta_0$ and low temperatures where they are decoupled from the unavoidable phase fluctuations (for $p_c > \delta_0$ hidden in $\Delta_0(x)$) in our one-dimensional system. The harmonic vibrations probably exist also for $|p| \lesssim \delta_0$ for a system of coupled one-dimensional chains well below the 3-dimensional ordering temperature. The $\parallel$ and $\perp$ modes are also called amplitude and phase modes since in terms of amplitude and phase variables $d\delta$, $d\phi$

$$\Delta = \Delta_0 + d\Delta = (\delta_T + d\delta) e^{i(\phi + d\phi)} \quad (5.17)$$

the relations

$$d\Delta_{\parallel} = d\delta, \quad d\Delta_{\perp} = \delta_T d\phi \quad (5.18)$$

hold in linear approximation.

For the special case $|p| \ll \delta_0$ and $T=0$ the frequencies $\omega_p^{\parallel, \perp}$ have been calculated in Ref.(14). Unfortunately their expression for

[†] With (5.14), (3.12) one easily checks that $M\omega_p^2 = f_E$ for $2k_F + p \rightarrow \frac{\pi}{a}$ where $w_p \rightarrow 0$ in our incommensurate model.

$\omega_+^2 \equiv \omega^2$ contains a misprint, the prefactor 4/3 should correctly read 1/3 (see Fig.5a). Our adiabatic expression (5.16), (5.11) corresponds to the limit $\tilde{m}/m \nu(M/m) (\delta_0^2/w_0^2) k_F a \gg 1$ and is an extension of the calculation in (17) to arbitrary $|p| \ll k_F$ and $T \ll E_F$ for $\delta_0 \ll E_F$.

Let us discuss the result (5.11), (5.12) for $T=0$ qualitatively but in a more "physical" way. For constant Δ_0

$$V_0 = \Delta_0 e^{i2k_F x} + \text{cc} \quad (5.19)$$

is a periodic potential with Bloch states $|\alpha\rangle$ as eigenstates of the electrons. The electronic energy (compare (1.13))

$$\Omega^{(2)} = \sum_{\alpha\alpha'} |\langle \alpha | dV | \alpha' \rangle|^2 \frac{f_\alpha - f_{\alpha'}}{E_\alpha - E_{\alpha'}} \quad (5.20)$$

in second order $d\Delta$, or equivalently

$$dV = \frac{1}{L} \sum_k e^{ikx} i k \tilde{v}_k \hat{s}_k, \quad (5.21)$$

allows for mixed terms $\hat{s}_k \hat{s}_k^*$, with $k' = k + n \cdot 2k_F$.

Fig.6 shows the diagonal ($n=0$) and two types of nondiagonal ($|n|=2,1$) terms. The corresponding contributions to $\Omega^{(2)}$ are proportional to

$$\begin{aligned} (a) & \quad |\hat{s}_{2k_F+p}|^2 w_p^2 A_p \\ (b) & \quad \hat{s}_{2k_F+p} \hat{s}_{-2k_F+p}^* w_p w_{-p} B_p \\ (c) & \quad \hat{s}_{2k_F+p} \hat{s}_p^* w_p \cdot p \tilde{v}_p C_p \end{aligned} \quad (5.22)$$

where

$$\begin{aligned}
 A_p &\hat{=} \left(\int_{-\infty}^p + \int_0^{\infty} \right) dk \frac{\mu_k^2 \mu_{k+p}^2 + v_k^2 v_{k+p}^2}{\epsilon_{k+p} + \epsilon_k} + \int_{-p}^0 dk \frac{\mu_k^2 v_{k+p}^2 + v_k^2 \mu_{k+p}^2}{\epsilon_{k+p} + \epsilon_k} \\
 &= \frac{1}{2} \int_{-\infty}^{\infty} \frac{dk}{\epsilon_{k+p} + \epsilon_k} \left(1 + \frac{k(k+p)}{\epsilon_k \epsilon_{k+p}} \right) \\
 B_p &= \left(\int_{-\infty}^p + \int_0^{\infty} \right) dk \frac{2\mu_k v_k \mu_{k+p} v_{k+p}}{\epsilon_k + \epsilon_{k+p}} + \int_{-p}^0 dk \frac{2\mu_k v_k \mu_{k+p} v_{k+p}}{\epsilon_k + \epsilon_{k+p}} \\
 &= \frac{1}{2} \int_{-\infty}^{\infty} \frac{dk}{\epsilon_{k+p} + \epsilon_k} \frac{|\Delta|^2}{\epsilon_k \epsilon_{k+p}} \tag{5.23} \\
 C_p &= \left(\int_{-\infty}^p + \int_0^{\infty} + \int_{-p}^0 \right) dk \frac{\mu_k v_k (\mu_{k+p}^2 + v_{k+p}^2)}{\epsilon_{k+p} + \epsilon_k} = \frac{1}{2} \int_{-\infty}^{\infty} \frac{dk}{\epsilon_{k+p} + \epsilon_k} \frac{|\Delta|}{\epsilon_k}
 \end{aligned}$$

with the expressions (see (3.1))

$$\begin{aligned}
 \mu_k &= \sqrt{\frac{\epsilon_k + |k|}{2\epsilon_k}} \\
 v_k &= \sqrt{\frac{\epsilon_k - |k|}{2\epsilon_k}}
 \end{aligned}$$

Of course, expressions A_p , B_p could be obtained directly by integrating (B2) over α (for $T=0$) and are equivalent to (5.12) but we wanted to show their "physical" interpretation given by Fig.6: for $p \gg \delta$ the diagonal term $A_p \sim \ln p/k_F$ with negligible δ -dependence since the nonplanewave particle-hole excitations $|k| < \delta$ or $|k+p| < \delta$ enter with a large energy denominator. For $|p| \sim \delta$ the nondiagonal contribution (b) $\sim \ln \frac{p}{\delta}$ is comparable with (a) including the Einstein term. For $|p| \gg \delta$, (b) $\sim (\frac{\delta}{p})^2 \ln \frac{p}{\delta}$, and can be neglected. The nondiagonal elements of type (c) are negligible because of the small electron phonon interaction for

small wavevector

$$\frac{p}{k_F} c_p \sim \begin{cases} p/k_F & \text{for } 0 < p \ll \delta \\ \delta/k_F \ln p/\delta & \text{for } p \gg \delta \end{cases} \quad (5.24)$$

In this intuitively more appealing way we arrive at the same conclusions concerning the harmonic phonons as formally expressed by (5.11), (5.12): The modes D are linear combinations of $\hat{s}_{2k_F+p} \sim \lambda_p$ and $\hat{s}_{-2k_F+p} \sim \lambda_{-p}^*$ only, their degeneracy is removed only for $|p| \lesssim \delta$ and their δ -dependence is negligible for $|p| \gg \delta$. This behaviour of the mean field harmonic modes in our incommensurate Fröhlich model with $\delta_0 \ll E_F$ is quite different from the one suggested usually, e.g. Ref. (26) section 5 c.

b) Second order contribution $\overset{(2)}{\Omega}$ for arbitrary Δ_0

For $d\Delta$ varying rapidly on the scale $\overset{0}{W}_1^{-1}$, a Ginzburg-Landau expansion of $\mathcal{H}^{(2)}$ to arbitrary order in derivatives of Δ_0 is estimated in appendix B. The result is again (5.13) with the universal $\pi f_p = \ln \frac{|p|}{\delta_0}$.

For a linear phase variation, $\Delta_0(x) = \delta e^{i2qx}$ with $|q| < \delta$, the influence on Δ_0 of thermally excited short wavelength $d\Delta$'s (wavevectors $> p_c$) is calculated exactly in appendix B and is shown to be negligible for $p_c \gg \delta_0$.

c) Anharmonic contributions

To check whether the harmonic expansion $\overset{(2)}{\Omega}$ is sufficient for

the $d\Delta$ -modes, the contribution $\Omega^{(4)}$ will now be evaluated for the special case $\Delta_0 = 0$. From Eq. (5.4) one obtains ($|p_i| > p_c$)

$$\Omega^{(4)} = \frac{2}{L^3} \sum_{p_1, p_2, p_3} \frac{1}{4} T \sum_{\alpha} \int \frac{dk}{2\pi} \cdot \left[\frac{\tilde{\Delta}_{p_1} \tilde{\Delta}_{-p_2}^* \tilde{\Delta}_{p_3} \tilde{\Delta}_{p_1+p_2+p_3}^*}{(i\omega_{\alpha}-k)(i\omega_{\alpha}+k-p_1)(i\omega_{\alpha}-k+p_1+p_2)(i\omega_{\alpha}+k-p_1-p_2-p_3)} + cc \right] \quad (5.25)$$

In terms of an effective harmonic energy the contribution of $\Omega^{(4)}$ is given by replacing the four Δ 's by two, times the harmonic (Eq. (5.13)) mean value of the other two in all possible combinations. This gives

$$\Omega^{(4)} \rightarrow \frac{1}{L} \sum_{|p| > p_c} |\tilde{\Delta}_p|^2 f_p^c \quad (5.26)$$

where the correction f_p^c to the harmonic dispersion f_p

$$f_p^c \sim \frac{1}{L} \sum_{|p'| > p_c} \frac{T}{f_{p'}} T \sum_{\alpha} \int \frac{dk}{2\pi} \frac{1}{(k-i\omega_{\alpha})^2 (k-p'+i\omega_{\alpha}) (k-p+i\omega_{\alpha})} \quad (5.27)$$

for $T \ll \delta_0$ (then the sum can be replaced by an integral and $f_p \sim \ln|p|/\delta_0$) is given by

$$f_p^c \sim -\frac{1}{p} \int_{p_c}^{k_{BZ}} dp' \frac{T}{f_{p'}} \frac{1}{p'} \sim \frac{T}{p} \cdot \ln \frac{\ln p_c / \delta_0}{\ln k_{BZ} / \delta_0} \quad (5.28)$$

Despite the large number of $\tilde{\Delta}_{p'}$ -modes ($\delta_0 \sim p_c < p' < k_{BZ}$), these anharmonically influence a given mode $\tilde{\Delta}_p$ only negligibly for $T \ll \delta_0$ since the anharmonic coupling becomes very small for $|p'| \gg \delta_0$. The large value of f_p^c for $p_c \rightarrow \delta_0$ is due to the $\Delta_0 = 0$ dispersion and should turn out more favourably for $\Delta_0 = \delta_0$.

d) First order contribution $\Omega^{(1)}$

For $\Delta_0 = \delta e^{i2qx}$ with δ, q independent of x , i.e. a periodic potential, nonvanishing matrix elements of $\frac{1}{z-H_0}$ exist only for momentum differences $n \cdot 2(k_F + q)$ and therefore $\Omega^{(1)} = 0$ since $|2q| < p_c$.

Consider the general case with G_0 in local approximation. Then (5.4), (4.4) give

$$\Omega_\ell^{(1)} = -T \sum_\alpha \int dx \frac{d\Delta(x) \Delta_0^*(x) + d\Delta^*(x) \Delta_0(x)}{W_\alpha(x)} \quad (5.29)$$

Since Δ_0 and $d\Delta$ are composed of different wavevectors, the integral in (5.29) is $\sim |z_\alpha|^{-3}$ for large $|z_\alpha|$ and there are no cutoff problems.

With (5.10) we may write

$$\Omega_\ell^{(1)} = \frac{1}{L} \sum_{|p| > p_c} \lambda_p \int dx e^{ipx} \frac{\Delta_0^*(x)}{|\Delta_0(x)|} \frac{\partial \varepsilon_\ell / 2}{\partial |\Delta_0(x)|} + cc \quad (5.30)$$

It is remarkable that this coincides with the expansion to first order in $d\Delta$ of the totally local energy (4.5). For $T \ll \delta_0$ the order of magnitude of the integral in (5.30) is given by

$$\int dx e^{ipx} \frac{1}{\pi} \Delta_0^*(x) \ln \left[1 + \frac{|\Delta_0(x)| - \delta_0}{\delta_0} \right] \sim \lambda_{p_c} \left(\frac{T}{\delta_0} \right)^{p/2p_c} \quad (5.31)$$

since $\langle (|\Delta_0(x)| - \delta_0)^2 / \delta_0^2 \rangle \sim T / \delta_0$ as will be shown in the next section.

6. Approximate calculation of the functional integral for $T \ll \delta_0$

Consider the equal time correlation function (compare (1.8), (1.11))

$$\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle = \quad (6.1)$$

$$\frac{1}{Nw_p^2} \frac{\int_{|\bar{p}| < p_c}^{\Pi} \int_{-\infty}^{\infty} d\lambda_{\bar{p}}^I d\lambda_{\bar{p}}^{\Pi} e^{-\mathcal{H}/T} \int_{|\bar{p}| > p_c}^{\Pi} \int_{-\infty}^{\infty} d\lambda_{\bar{p}}^I d\lambda_{\bar{p}}^{\Pi} e^{-(\mathcal{H}-\mathring{\mathcal{H}})/T} \cdot |\Delta_p|^2}{\int_{|\bar{p}| < p_c}^{\Pi} \int_{-\infty}^{\infty} d\lambda_{\bar{p}}^I d\lambda_{\bar{p}}^{\Pi} e^{-\mathcal{H}/T} \int_{|\bar{p}| > p_c}^{\Pi} \int_{-\infty}^{\infty} d\lambda_{\bar{p}}^I d\lambda_{\bar{p}}^{\Pi} e^{-(\mathcal{H}-\mathring{\mathcal{H}})/T}}$$

with $\mathring{\mathcal{H}}[\Delta] \equiv \mathcal{H}[\Delta_0]$. This quantity essentially determines the X-ray scattering cross section for momentum transfer $2k_F+p$. For $|p| \gg \delta_0$ the λ_p -dependence of $\mathcal{H}-\mathring{\mathcal{H}}$ is given by the harmonic expression (5.13), (5.14), i.e. λ_p is decoupled from all other modes which cancel in (6.1) and

$$\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle = \frac{a}{w_p^2} \cdot \frac{T}{f_p} = \frac{\pi T a}{w_0^2 \ln 8 \frac{E_F}{\delta_0} - \frac{w_p^2}{1+p/2k_F} \ln \frac{4k_F+p}{|p|}} \quad (6.2)$$

which for $2k_F+p \rightarrow \frac{\pi}{a}$ decreases to the Einstein expression T/f_E , according to (3.10), since w_p vanishes.

Consider now $|p| < \delta_0$ where $w_p = w_0$. Then according to the discussion in the previous section we can find a p_c of the order of a few δ_0 's such that $\mathcal{H}-\mathring{\mathcal{H}}$ is harmonic and Δ_0 -independent and the integrals for $|\bar{p}| > p_c$ cancel in (6.1). We now make the first approximation of replacing $\mathring{\mathcal{H}}$ by $\mathring{\mathcal{H}}_0 + \mathring{\mathcal{H}}_2$, the first two terms (4.5), (4.11) of its Ginzburg-Landau expansion which are

expected to describe fluctuations with $|\bar{p}| < p_c = \mathcal{O}(\delta_0)$ quite well. This can be checked for special cases, e.g. for $\Delta(x) = \delta + \frac{1}{L} e^{i\bar{p}x} \tilde{\Delta}_{\bar{p}}$ in second order in $\tilde{\Delta}_{\bar{p}}$. Then $\overset{\circ}{\mathcal{H}}_0 + \overset{\circ}{\mathcal{H}}_2$ gives the exact expression (5.11) but with the dispersion curves (5.12) replaced by their parabolic expansions at $\bar{p} = 0$. As a second approximation we drop the cutoff p_c in our new Hamiltonian, $\overset{\circ}{\mathcal{H}}_0 + \overset{\circ}{\mathcal{H}}_2$, since it suppresses fluctuations with $|\bar{p}| \gg \delta_0$ anyway.

It will turn out that for temperatures ($T \ll \delta_0$) considered in this section, the fluctuation in $|\Delta_0(x)|$ around the equilibrium δ_0

$$\langle (|\Delta(x)| - \delta_0)^2 \rangle / \delta_0^2 \sim T / \delta_0 \quad (6.3)$$

is negligible and only phase fluctuations of $\Delta_0(x)$ are important. For convenience we therefore replace $|\Delta_0(x)|$ by δ_0 in (4.11). The approximation to (6.1) for $|\bar{p}| < \delta_0$ as discussed above is conveniently expressed as

$$\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle \approx \frac{a}{w_0^2} \int dx e^{ipx} \langle \Delta^*(x) \Delta(0) \rangle_{0,2} \quad (6.4)$$

where the thermal mean value on the right hand side is to be extended over all functions $\Delta(x')$ with $\Delta(0) = \Delta(L)$ and with the Hamiltonian $\overset{\circ}{\mathcal{H}}_0 + \overset{\circ}{\mathcal{H}}_2$. According to Ref.(27) one may divide the interval $(0, L)$ into L/η subintervals of width η , separated by the points $x = \ell\eta$; $\ell = 0, 1, \dots, \frac{L}{\eta} - 1$. By selecting for each $\ell\eta$ a special two dimensional vector $\vec{\Delta}(\ell\eta)$ and using in each subinterval $\ell\eta < x < (\ell+1)\eta$ a linear interpolation $\vec{\Delta}(x) = \vec{\Delta}(\ell\eta) + \frac{x}{\eta} [\vec{\Delta}((\ell+1)\eta) - \vec{\Delta}(\ell\eta)]$ (see Fig.7), one obtains a subset of functions $\Delta(x)$ for which the thermal mean value is given as a multiple integral over the $\vec{\Delta}(\ell\eta)$'s and which in the

limit $\eta \rightarrow 0$ can be considered representative for the functional integral over all functions $\Delta(x)$:

$$\langle \Delta^*(x) \Delta(0) \rangle_{0,2} = \lim_{\eta \rightarrow 0} \frac{\frac{L}{\eta} - 1 \int_{\ell=0}^{\frac{L}{\eta}} d^2 \Delta(\ell \eta) M(\vec{\Delta}(\ell \eta), \vec{\Delta}((\ell+1)\eta)) \Delta^*(x) \Delta(0)}{\frac{L}{\eta} - 1 \int_{\bar{\ell}=0}^{\frac{L}{\eta}} d^2 \Delta(\bar{\ell} \eta) M(\vec{\Delta}(\bar{\ell} \eta), \vec{\Delta}((\bar{\ell}+1)\eta))} \quad (6.5)$$

Here $\vec{\Delta}(L) = \vec{\Delta}(0)$, x is chosen to coincide with one of the discrete points $\ell \eta$ and M is a symmetric transfer operator which according to (4.5), (4.11) is given by

$$M(\vec{\Delta}, \vec{\Delta}') = \exp \frac{(-)}{T} \int_0^\eta dx \left\{ \varepsilon_\ell(|\vec{\lambda}(x)|) + (\partial_x \lambda_i)(\partial_x \lambda_j) \cdot \left[m_\perp \delta_{ij} + (m_\parallel - m_\perp) P_{ij}^\parallel(\vec{\lambda}(x)) \right] \right\} \quad (6.6)$$

with

$$\vec{\lambda}(x) = \vec{\Delta} + \frac{x}{\eta} (\vec{\Delta}' - \vec{\Delta}) ; m_\perp = \frac{1}{4\pi\delta_0^2} , m_\parallel = \frac{m_\perp}{3} . \quad (6.7)$$

For $m_\parallel = m_\perp$ the quantity (6.5) has been discussed in (2a). For our more general case the discussion is given in Appendix C with the result

$$\langle \Delta^*(x) \Delta(0) \rangle_{0,2} = \sum_\sigma e^{-|x|(E_\sigma - E_0)/T} \left| \int d^2 \Delta \chi_\sigma^*(\vec{\Delta}) \Delta \chi_0(\vec{\Delta}) \right|^2 \quad (6.8)$$

where E_σ and $\chi_\sigma(\Delta)$ are eigenvalues and eigenfunctions of a Schrödinger-like equation in 2 dimensions with an anisotropic mass, which in polar coordinates, $\Delta = |\Delta| e^{i\phi}$, reads

$$\left\{ -\frac{T^2}{4} \left[\frac{1}{m_\perp} \frac{1}{|\Delta|^2} \frac{\partial^2}{\partial \phi^2} + \frac{1}{m_\parallel} \frac{1}{|\Delta|} \frac{\partial}{\partial |\Delta|} \left| \Delta \right| \frac{\partial}{\partial |\Delta|} \right] + \varepsilon_\ell(|\Delta|) \right\} \chi_\sigma(\Delta) = E_\sigma \chi_\sigma(\vec{\Delta}) \quad (6.9)$$

The equal time correlation function (6.4) is given by (6.8) as

$$\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle = \frac{a}{w_0^2} \sum_{\sigma} \frac{2 \frac{E_{\sigma} - E_0}{T}}{\left(\frac{E_{\sigma} - E_0}{T} \right)^2 + p^2} \left| \int d^2 \Delta \chi_{\sigma}^*(\vec{\Delta}) \Delta \chi_0(\vec{\Delta}) \right|^2 \quad (6.10)$$

For $T \ll \delta_0$ and low excited states Eq.(6.9) gives

$$\chi_{\sigma} = \chi_{n,m} = \mathcal{N}_n e^{-\theta^2/2} H_n(\theta) \cdot \frac{e^{im\phi}}{\sqrt{2\pi}} ; \quad \theta^2 = \frac{1}{\sqrt{3}} \frac{(|\Delta| - \delta_0)^2}{\pi T \delta_0}$$

$$E_{\sigma} = E_{n,m} = (2n+1)\sqrt{3}T\delta_0 + \pi T^2 m^2 ; \quad n=0,1,2,\dots \quad m=0,\pm 1,\pm 2,\dots \quad (6.11)$$

as shown in Appendix C. Here H_n are Hermite polynomials and $\mathcal{N}_n$ radial normalization factors.

Similar to (6.8) one can show that

$$\langle (|\Delta(0)| - \delta_0)^2 \rangle_{0,2} = \int d^2 \Delta |\chi_0(\vec{\Delta})|^2 (|\Delta| - \delta_0)^2 \quad (6.12)$$

which together with (6.11) proves our assumption (6.3).

Due to (6.11) only $m = 1$ contributes in the sum over $\sigma = (n,m)$ in (6.10). Since the radial part of the integral in (6.10)

$$\int_0^{\infty} d|\Delta| |\Delta| R_0 R_n |\Delta| = \delta_0 \delta_{n,0} + \int d|\Delta| |\Delta| R_0 R_n (|\Delta| - \delta_0), \quad (6.13)$$

$$R = \mathcal{N} e^{-\theta^2/2} H$$

is of order $\sqrt{T\delta_0}$ for $n \neq 0$, we may neglect $n \neq 0$ for $T, |p| \ll \delta_0$ in (6.10) to obtain

$$\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle = \frac{a}{w_0^2} \delta_0^2 \frac{2\pi T}{(\pi T)^2 + p^2} \quad \text{for } T, |p| \ll \delta_0 \quad (6.14)$$

The result (6.14) for the correlation is entirely due to phase fluctuations and as shown in Appendix C can be obtained in a very easy way if one neglects amplitude fluctuations from the outset.

It is notable that the harmonic expression (6.2), extrapolated for $\Delta_0(x) = \delta_0$ down to $T \ll |p| \ll \delta_0$, i.e. using (5.12) for $\delta = \delta_0$

$$\frac{a}{w_0^2} \frac{1}{2} \left(\frac{T}{f_p^\perp} + \frac{T}{f_p^\parallel} \right) \rightarrow \frac{a}{w_0^2} \cdot \frac{T}{2} \cdot \left[\frac{\pi}{4} \frac{p^2}{\delta_0^2} + \mathcal{O} \left(\left(\frac{p}{\delta_0} \right)^0 \right) \right], \quad (6.15)$$

coincides to leading order with the Ginzburg-Landau expression (6.14). This can be understood as follows: Going back from the second line of the Ginzburg-Landau expression (C12) we obtain immediately Eq.(C11) with the sin replaced by its argument and "uncoiled" ϕ 's running from $-\infty$ to $+\infty$. This expression can be rewritten in terms of the Fourier transform

$$\tilde{\phi}_p = \eta \sum_{\ell} \phi(\ell\eta) e^{-ip\ell\eta} \quad (6.16)$$

of the uncoiled phase and gives

$$\begin{aligned} \langle \Delta^*(x) \Delta(0) \rangle_{0,2} = & \quad (6.17) \\ \delta_0^2 \lim_{\eta \rightarrow 0} & \frac{\int_{-\infty}^{\infty} d\phi_p^{\perp} d\phi_p^{\parallel} e^{-\overline{\mathcal{H}}_{0,2}/T} \exp \left[-\frac{i}{L} \sum_p \phi_p (e^{ipx} - 1) \right]}{\int_{-\infty}^{\infty} d\phi_p^{\perp} d\phi_p^{\parallel} e^{-\overline{\mathcal{H}}_{0,2}/T}} \end{aligned}$$

Here the sum is extended from $-\frac{\pi}{\eta} < p < \frac{\pi}{\eta}$ and the Ginzburg-Landau energy

$$\overline{\mathcal{H}}_{0,2} = \frac{1}{L} \sum_{0 < p < \frac{\pi}{\eta}} \frac{|\gamma_p|^2 4 \sin^2 p \eta / 2}{2 \pi \eta^2} \quad (6.18)$$

is identical with the harmonic energy (5.11), (5.12) for transverse $d\Delta$ since both coincide to second order in p and $d\Delta$ and the translation $D_p^\perp = \sqrt{2} \delta_0 \gamma_p$ holds according to (5.18) linear in $d\Delta$. The leading term ($\sim T$) for small T of (6.4) is determined by expansion of the second exponential in (6.17) to second order

$$\int dx e^{ipx} \langle \Delta^*(x) \Delta(0) \rangle_{0,2} \Big|_{\text{linear in } T} = \delta_0^2 \frac{1}{L} \langle |\gamma_p|^2 \rangle_{0,2} \quad (6.19)$$

and therefore coincides with the corresponding transverse harmonic expression, $\frac{1}{2L} \langle |D_p^\perp|^2 \rangle_{\text{Harmonic}}$. Of course the full expression (6.17) again gives (6.14).

The harmonic expression for $\Delta_0(x) \equiv \delta_0$ therefore provides a convenient smooth interpolation for the displacement correlation between the exact harmonic expression for $p \gg \delta_0$ and the approximate Ginzburg-Landau expression for $p < \delta_0$. This is shown in Fig.8.

Let us now discuss the displacement correlation in direct space, $\langle s_n s_m \rangle$. The thermal weight (compare (6.1) for example) is invariant if $\{\gamma_p\} \rightarrow \{\gamma_p \cdot e^{ipx_0}\}$, x_0 independent of p , since $\mathcal{H}$ is invariant against $\Delta(x) \rightarrow \Delta(x+x_0)$ which according to (2.5)

simply implies $G(x, y) \rightarrow G(x+x_0, y+x_0)$ and since $\mathcal{H} - \mathcal{H}^0$ is harmonic and contains only $|\chi_p|^2$'s. Consequently

$$\langle \chi_p \chi_{p'}^* \rangle = \langle |\chi_p|^2 \rangle \delta_{pp'} \quad , \quad \langle \chi_p \chi_{p'} \rangle = 0 \quad (6.20)$$

in our model and therefore, according to (1.5), (1.8)

$$\langle s_n s_m \rangle = e^{i2k_F(n-m)a} \frac{1}{N} \sum_p e^{ip(n-m)a} \frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle + cc \quad (6.21)$$

with the sum extended over $0 < 2k_F + p < \frac{\pi}{a}$.

Let us consider first the Ginzburg-Landau contribution from
(6.14)

$$\begin{aligned} \langle s_n s_m \rangle_{GL} &= \overline{s^2} e^{i2k_F(n-m)a} \frac{T}{2} \int dp \frac{e^{ip(n-m)a}}{(\pi T)^2 + p^2} + cc \\ &= \overline{s^2} \cos 2k_F(n-m)a \cdot e^{-|n-m|a\pi T} \end{aligned} \quad (6.22)$$

with the integral extended over $0 < 2k_F + p < \frac{\pi}{a}$. Here $\overline{s^2} = 2a^2 \delta_0^2 / w_0^2$ is s_n^2 for the case of the pure Peierls distortion, $\Delta(x) \equiv \delta_0 e^{i\phi} = \text{const}$, averaged over the phase ϕ . For the calculation of the difference $\langle s_n s_m \rangle - \langle s_n s_m \rangle_{GL}$ we observe that the corresponding difference in p -space is appreciable only for $|p| \gtrsim \sqrt{2\delta_0 \cdot \pi T}$ (compare Fig.8). In this case we may use for $\langle s_n s_m \rangle$ the harmonic expression $\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle_H$ given by the left hand side of (6.15) for $|p| < k_F$ and (6.2) for $|p| \gg \delta_0$. On the other hand we may drop T in the denominator of (6.14) for the calculation of $\langle s_n s_m \rangle_{GL}$. Therefore

$$\begin{aligned} \langle s_n s_m \rangle - \langle s_n s_m \rangle_{GL} &= \overline{s^2} e^{i2k_F(n-m)a} \frac{T}{2\delta_0} \frac{k_F}{\delta_0} \int \frac{dp}{k_F} e^{ip(n-m)a} F_p + cc \\ F_p &= \frac{1}{2\pi T} \frac{w_0^2}{a} \frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle_H - \frac{\delta_0^2}{p^2} \end{aligned} \quad (6.23)$$

with the integral extended over $0 < 2k_F + p < \frac{\pi}{a}$ with $|p| > \sqrt{2\delta_0 \cdot \pi T}$. According to (6.15), (5.12) and (6.2) the function F_p varies on the scale of k_F , decreasing from 5/12 at $p=0$ via $[2 \ln p / \delta_0]^{-1}$ for $\delta_0 \ll |p| \ll k_F$ to the Einstein value $[2 \ln 4k_F / \delta_0]^{-1}$ for $2k_F + p \rightarrow 0, \frac{\pi}{a}$. Therefore (6.23) describes a correlation of a few lattice constants where the integral in (6.23) is of $\mathcal{O}(1)$. Qualitatively (6.23) behaves like the correlation in the bare Einstein lattice,

$$\overline{s^2} = \frac{T}{2\delta_0} \frac{\pi/a}{\delta_0} \frac{1}{\ln 4k_F/\delta_0} \delta_{nm} = \frac{T}{T} \delta_{nm} \quad . \quad (6.24)$$

7. Comparison with real substances

The compound KCP ⁽⁵⁾ shows certain features of an incommensurate Fröhlich model. Optical measurements can be interpreted with an essentially free electron band structure ⁽⁴⁾ with a small Peierls gap δ_{eff}

$$\frac{\delta_{\text{eff}}}{E_F} = \frac{1}{33} \quad , \quad \delta_{\text{eff}} = 1160 \text{ K} \quad (7.1)$$

and the Peierls distortion occurs at a wavevector ⁽⁷⁾

$$\pm (2k_F - \frac{2\pi}{a}) \quad , \quad 2k_F = \frac{1.70 \pm 0.01}{2} \cdot \frac{2\pi}{a} \quad (7.2)$$

where $2k_F$ is consistent with 1.70 electrons per Pt (corresponding to 0.30 Br per Pt) and shows no commensurability effect

$$(2k_F \pm \frac{5}{6} \frac{2\pi}{a} = 1.67 \frac{\pi}{a}).$$

Our single chain model only makes sense well above the inter-chain ordering temperature of $T_{3D} \approx 100 \text{ K}$ in KCP ⁽⁸⁾. According to Equ. (7.2), $\frac{\pi}{a} < 2k_F < \frac{2\pi}{a}$, and our model should be slightly modified by assuming $\tilde{v}_k$ nonvanishing also in the second Brillouin zone, at least up to $k=2k_F$. If one still assumes $\tilde{v}_k=0$ for $|k| \geq \frac{2\pi}{a}$, i.e. neglecting bandstructure effects, this can easily be done as shown in appendix D. The result is a change in the dependence of the equilibrium gap on $\tilde{v}_k$ and f_E , expressed by $\delta_o \rightarrow \delta_{\text{eff}}$ in (D4). Apart from $\delta_o \rightarrow \delta_{\text{eff}}$ the relation (6.22) remains unchanged.

From (6.22), (7.2) one obtains a correlation length

$$\zeta_{||}(T) = \frac{1}{\pi T} = \frac{2}{\pi k_F} \frac{E_F}{T} = \frac{4}{1.7\pi^2} \frac{E_F}{T} a \approx 0.25 \frac{E_F}{T} a. \quad (7.3)$$

Since $E_F \approx 38000K$, our correlation length at 100 K equals ≈ 100 Pt-Pt spacings corresponding to a full width at half maximum ("FWHM") in k-space of $\Delta k = 2/\zeta_{||} = 0.007 \text{ \AA}^{-1}$. Experimentally ⁽⁹⁾ an upper limit of $0.006 \text{ \AA}^{-1}$ has been set to the FWHM for $T < 160$ K. Thus the correlation length of our simple model is of the correct order of magnitude (but somewhat too small) to be compatible with the experimental resolution. Experiments with improved wavevector resolution would be extremely useful, to learn via the temperature dependence of $\zeta_{||}$ about the actual character of the phase fluctuations (free, pinned or even induced ⁽²³⁾ by the Br impurities) already well above the interchain ordering temperature.

According to our discussion in section 5 and appendix D we expect well defined harmonic modes $\hat{s}_k$ for k well outside the interval of width

$$\Delta k = 2\delta_{\text{eff}} = \frac{\pi}{a} \cdot \frac{ak_F}{\pi} \frac{\delta_{\text{eff}}}{E_F} \approx 0.03 \frac{\pi}{a} \quad (7.4)$$

(compare (7.1), (7.2)), centered around $\frac{2\pi}{a} - 2k_F = 0.3 \frac{\pi}{a}$. This is in qualitative agreement with experiment ⁽¹⁰⁾.

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Appendix A

Since

$$\begin{aligned} \frac{1}{2} \int_{-2\pi TN}^{2\pi TN} d\omega \sqrt{\omega^2 + \delta^2} &= \sum_{-(2N-1) \leq \alpha \leq (2N-1)} \frac{1}{2} \int_{-\pi T}^{\pi T} d\omega \sqrt{(\omega_\alpha + \omega)^2 + \delta^2} = \\ &= \pi T \sum_{-(2N-1) \leq \alpha \leq 2N-1} \sqrt{\omega_\alpha^2 + \delta^2} + \mathcal{O}(T^2) \end{aligned} \quad (A1)$$

for $T \ll \delta$ and

$$\frac{1}{2} \int_{-2\pi TN}^{2\pi TN} d\omega \sqrt{\omega^2 + \delta^2} = \frac{\delta^2}{2} \left[\left(\frac{2\pi TN}{\delta} \right)^2 + \frac{1}{2} + \ln \frac{4\pi TN}{\delta} + \mathcal{O}\left(\frac{\delta}{TN}\right) \right] \quad (A2)$$

one obtains

$$\begin{aligned} \lim_{N \rightarrow \infty} \pi T \sum_{-(2N-1) \leq \alpha \leq 2N-1} (|\omega_\alpha| + \frac{\delta^2}{2|\omega_\alpha|} - W_\alpha) &= \\ &= \lim_{N \rightarrow \infty} \left\{ 2(\pi TN)^2 + \frac{\delta^2}{2} \left[\psi\left(N + \frac{1}{2}\right) - \psi\left(\frac{1}{2}\right) \right] - \right. \\ &\quad \left. - \frac{\delta^2}{2} \left[\left(\frac{2\pi TN}{\delta} \right)^2 + \frac{1}{2} + \ln \frac{4\pi TN}{\delta} + \mathcal{O}\left(\frac{\delta}{TN}\right) \right] + \mathcal{O}(T^2) \right\} \\ &= - \frac{\delta^2}{2} \left[\frac{1}{2} + \ln \frac{4\pi T}{\delta} + \psi\left(\frac{1}{2}\right) \right] . \end{aligned} \quad (A3)$$

Eq. (3.10) is identical with Fröhlich's expression (2.42) for $U=0$ since his electron-phonon interaction D can be written

$$D^2 = \frac{w_0^2}{a^2} \frac{1}{2MN\omega_E} , \quad \omega_E = \sqrt{F_E/M} \quad (A4)$$

in terms of our parameters and therefore (compare his equation (2.7))

$$\frac{2}{3} F_V = \frac{1}{2} D^2 \frac{N_{e\ell}}{E_F \omega_E} = \frac{w_0^2}{a} \frac{1}{\pi} \frac{1}{f_E} \quad (A5)$$

since $N_{e\ell}/N = 4k_F a/2\pi$.

The left hand side of (3.14) for $T \ll \delta$ and $|q| < \delta$ is given by

$$\begin{aligned} & 2 \cdot \frac{L}{\pi} \lim_{P \rightarrow \infty} \left[\int_{-P}^{-\delta+q} d\hat{E} \hat{E} \frac{|\hat{E}-q|}{\sqrt{(\hat{E}-q)^2 - \delta^2}} - \int_{-P}^{-\delta} d\hat{E} \hat{E} \frac{|\hat{E}|}{\sqrt{\hat{E}^2 - \delta^2}} \right] = \\ & = 2 \cdot \frac{L}{\pi} \lim_{P \rightarrow \infty} \left[-q \int_{-P-q}^{-\delta} \frac{de e}{\sqrt{e^2 - \delta^2}} - \int_{-P-q}^{-P} \frac{de e^2}{\sqrt{e^2 - \delta^2}} \right] = \\ & = q \sqrt{(P+q)^2 - \delta^2} - \int_{-P-q}^{-P} de |e| \left(1 + \frac{\delta^2}{2e^2} + \mathcal{O}(e^{-4}) \right) = \frac{q^2}{2} + \mathcal{O}(P^{-1}) \end{aligned} \quad (A6)$$

which proves the relation (3.14).

Appendix B

Since

$$G_0(x', x, i\omega_\alpha) = [G_0(x, x', -i\omega_\alpha)]^{*,T} \quad (B1)$$

(T means: transpose in 2x2 space), Eqs. (5.4), (4.1) give for

$\mu = 2$

$$\Omega^{(2)} \hat{=} \int dx \frac{1}{L} \sum_p \frac{1}{L} \sum_Q e^{iQx} \quad (B2)$$

$$\cdot^T \sum_\alpha \frac{1}{L} \sum_K \text{tr} \tilde{G}_{0,K+p}(x, i\omega_\alpha) \begin{pmatrix} 0, \Delta_p \\ \Delta_{-p}^*, 0 \end{pmatrix} \left[\tilde{G}_{0,K}(x, -i\omega_\alpha) \right]^{*,T} \begin{pmatrix} 0, \Delta_{-p+Q} \\ \Delta_{p-Q}^*, 0 \end{pmatrix}$$

with $|p|, |p-Q| > p_c$. If $\Delta_0(x)$ varies slowly on the length $\tilde{W}_1^{-1}$,
then the local approximation (4.4) is applicable for G_0 and $\Omega^{(2)}$

becomes

$$\begin{aligned} \Omega_\ell^{(2)} \hat{=} & \int dx \frac{1}{L} \frac{1}{2} \sum_p \frac{1}{L} \sum_Q e^{iQx} \left\{ - D_p^\perp(x) D_{p-Q}^{*\perp}(x) \cdot \right. \\ & \cdot^T \sum_\alpha \frac{|\Delta_0(x)|^2}{\tilde{W}_\alpha(x) (\tilde{W}_\alpha^2(x) + \frac{p^2}{4})} + (D_p^\parallel(x) D_{p-Q}^\parallel(x) + D_p^\perp(x) D_{p-Q}^{*\perp}(x)) \cdot \\ & \cdot^T \sum_\alpha \frac{-\omega_\alpha^2}{\tilde{W}_\alpha(x) (\tilde{W}_\alpha^2(x) + \frac{p^2}{4})} \left. \right\} \quad (B3) \end{aligned}$$

where the variables $D_p^{\parallel,\perp}(x)$ are defined as in (5.8) but with $\Delta_0 \rightarrow \Delta_0(x)$.

The last frequency sum in (B3) can be properly defined by the method leading to (5.11). One obtains for $\mathcal{K}_\ell^{(2)}$ the expression

on the right hand side of (B3) with the last frequency sum replaced by

$$T \sum_{\alpha} \rightarrow \frac{1}{\pi} \ln \frac{T}{T_p} + T \sum_{\alpha} \left[\frac{1}{|\omega_{\alpha}|} - \frac{\omega_{\alpha}^2}{\bar{W}_{\alpha}^0(x) (\bar{W}_{\alpha}^0(x) + \frac{p^2}{4})} \right] \quad (B4)$$

For λ_p 's with $k_F \gg |p| \gg \bar{W}_1^0$ the quantity $\mathcal{H}_{\ell}^{(2)}$ as given by (B3) (B4) again reduces to (5.13) with $\pi f_p = \ln \frac{|p|}{\delta_0}$ apart from corrections of order $\frac{|\Delta_0|^2}{p^2} \ln \frac{p}{|\Delta_0|}$.

Let us now estimate the $|p| \gg \bar{W}_1^0$ -contribution to $\Omega^{(2)}$ beyond the local approximation: Denote the contribution to G_0 according to (4.6) with σ derivatives by G^{σ} . If Δ_0 is assumed to change appreciably over the length δ_0^{-1} , i.e. $|\partial_x \Delta| \sim \delta_0 |\Delta_0|$, the qualitative behaviour of G^{σ} according to (4.4), (4.6) is given by

$$G^{\sigma}_{\mathbf{k}} \sim \begin{cases} \frac{1}{|\mathbf{k}|} & \text{for } \sigma = 0 \\ \frac{1}{|\mathbf{k}|} \left(\frac{\delta_0}{|\mathbf{k}|} \right)^{\sigma+1} & \text{for } \sigma > 0 \end{cases} \quad \text{and } |\mathbf{k}| > \delta_0 \quad (B5)$$

where $\mathbf{k} = (K, \omega_{\alpha})$. The contribution to the frequency sum in (B2) with the first and second Green's function replaced by G^{σ} and G^{τ} respectively,

$$T \sum_{\alpha} \frac{1}{L} \sum_{\mathbf{k}} \left| \lambda_p \right|_{\sigma, \tau}^2 \sim |\lambda_p|^2 \int_0^{\infty} d|\mathbf{k}| |\mathbf{k}| G_{\mathbf{k}+p, \omega}^{\sigma} G_{\mathbf{k}, \omega}^{\tau} \quad (B6)$$

is estimated by separating the integration plane in regions I of diameter $p/2$ around 0, $-p$ and the rest II. Then the main correction to the local approximation of the frequency sum in (B2) is of order $|\lambda_p|^2 \frac{\delta_0}{|p|}$ as obtained from $\sigma=0, \tau>0$ in region I. For $|p| \gg \delta_0$ this is small compared to the Δ_0 -independent main contribution $|\lambda_p|^2 \ln \frac{|p|}{\delta_0}$ of the local expression.

After this qualitative discussion of $\hat{\Omega}^{(2)}$ for $d\Delta$ of short wavelength we wish to consider in more detail the special situation $\Delta_0(x) = \delta e^{i2qx}$ for $d\Delta$ arbitrary. For this situation G_0 is known explicitly (see (3.13)), only the q^0 -contribution to $\mathcal{K}^{(2)}$ has to be redefined properly as already done in passing from (B3) to (B4). The result is

$$\begin{aligned} \mathcal{K}^{(2)} = & \frac{1}{2} \frac{1}{L} \sum_p \left\{ -\frac{1}{2} (|\tilde{\lambda}_{p+2q}|^2 + |\tilde{\lambda}_{-p+2q}|^2 - \tilde{\lambda}_{p+2q} \tilde{\lambda}_{-p+2q} - \tilde{\lambda}_{-p+2q}^* \tilde{\lambda}_{p+2q}^*) \delta^2 \cdot \right. \\ & + T \sum_{\alpha} \frac{1}{W} \frac{1}{W^2 + \frac{p^2}{4}} + (|\tilde{\lambda}_{p+2q}|^2 + |\tilde{\lambda}_{-p+2q}|^2) \left[\frac{1}{\pi} \ln \frac{T}{T_p} + \right. \\ & \left. \left. + T \sum_{\alpha} \left(\frac{1}{|\omega_{\alpha}|} - \frac{(\omega_{\alpha} + iq)^2}{W(W^2 + \frac{p^2}{4})} \right) \right] + (|\tilde{\lambda}_{p+2q}|^2 - |\tilde{\lambda}_{-p+2q}|^2) T \sum_{\alpha} \frac{ip/2 (\omega_{\alpha} + iq)}{W(W^2 + \frac{p^2}{4})} \right\} \end{aligned} \quad (B7)$$

with $W = \sqrt{(\omega_{\alpha} + iq)^2 + \delta^2}$ in the right half of the complex plane. We note two special cases : For $\delta \rightarrow 0$, q drops out and (B7) reduces to (5.13). If $q \rightarrow 0$, (B7) reduces to (5.11). For $T \ll \delta$ and $|q| < \delta$

$$\begin{aligned} \mathcal{K}^{(2)} = & \frac{1}{2L} \sum_p \left\{ \frac{1}{2} (|\tilde{\lambda}_{2q+p}|^2 + |\tilde{\lambda}_{2q-p}|^2 + \tilde{\lambda}_{2q+p} \tilde{\lambda}_{2q-p} + \tilde{\lambda}_{2q-p}^* \tilde{\lambda}_{2q+p}^*) \cdot \right. \\ & \left. \cdot f_{p,T=0}^{\parallel} + \frac{1}{2} (|\tilde{\lambda}_{2q+p}|^2 + |\tilde{\lambda}_{2q-p}|^2 - \tilde{\lambda}_{2q+p} \tilde{\lambda}_{2q-p} - \tilde{\lambda}_{2q-p}^* \tilde{\lambda}_{2q+p}^*) \cdot f_{p,T=0}^{\perp} \right\} \end{aligned} \quad (B8)$$

with the f 's of Eq. (5.12). We want to study the influence of thermally excited $\tilde{\lambda}_p$'s with $p \gg p_c \sim \delta_0$ on the Δ_0 -dependence of the energy. To this end we calculate

$$\begin{aligned} F_c[\Delta_0(x)] = & - T \ln \prod_{|p| > p_c} \int d\tilde{\lambda}_p' d\tilde{\lambda}_p'' \exp \frac{(-)}{T} \mathcal{K}^{(2)} ; \\ \tilde{\lambda}_p = & 0 \text{ for } |p| < p_c \end{aligned} \quad (B9)$$

which has to be considered as a correction to the "bare" Ginzburg-Landau energies (4.5), (4.11) which strictly hold for $d\Delta = 0$ only. The quantity F_c is an even function of q and is given for $q \geq 0$ up to an additive constant (q and δ independent) by

$$F_c = T \frac{L}{2\pi} \left[\int_{p_c-2q}^{p_c+2q} dp \ln \frac{f_p^{\parallel} + f_p^{\perp}}{2} + \int_{p_c+2q}^{\infty} dp \ln f_p^{\parallel} \cdot f_p^{\perp} \right]. \quad (B10)$$

The first terms in an expansion for small $|q|$, $\delta - \delta_0$ are

$$F_c = T \frac{L}{\pi} \left[|q| \ln \left(1 + \frac{1}{4\kappa_c^2 (1+\kappa_c^2)} \right) + (\delta - \delta_0) \int_{\kappa_c}^{\infty} \frac{d\kappa}{\kappa \sqrt{1+\kappa^2} \ln(\sqrt{1+\kappa^2} + \kappa)} + \dots \right] \quad (B11)$$

with $\kappa_c = p_c/2\delta_0$. This result shows again that the influence of short wavelength modes ($\kappa_c \gg 1$) on Δ_0 is negligible.

Appendix C

We want to construct eigenvectors χ of M in leading orders in η . Eq.(6.6) gives with $y = x/\eta$ and $\vec{a} = (\vec{\Delta}' - \vec{\Delta})/\sqrt{\eta}$

$$M(\vec{\Delta}, \vec{\Delta}') = \exp \frac{(-)}{T} \int_0^1 dy \{ a_i a_j m_{ij}(\vec{\Delta} + y\sqrt{\eta} \vec{a}) + \eta \epsilon(|\vec{\Delta} + y\sqrt{\eta} \vec{a}|) \} \quad (C1)$$

where m_{ij} is the square bracket in (6.6). Expanding (C1) and $\chi(\vec{\Delta}') = \chi(\vec{\Delta} + \sqrt{\eta} \vec{a})$ in terms of $\sqrt{\eta}$ one obtains

$$\begin{aligned} & \left(\sqrt{\eta} \int_{-\infty}^{\infty} d\vec{a} \exp \frac{(-)}{T} a_i a_j m_{ij}(\vec{\Delta}) \right)^{-1} \cdot \int_{-\infty}^{\infty} d\vec{\Delta}' M(\vec{\Delta}, \vec{\Delta}') \chi(\vec{\Delta}') = \\ & = \left\{ 1 - \frac{\eta}{T} \left[\frac{1}{2} m_{ij,\ell}(\vec{\Delta}) \overline{a_i a_j a_\ell \cdot a_s} \partial_s - \frac{T}{2} \overline{a_s a_t} \partial_s \partial_t + \epsilon(|\vec{\Delta}|) + \right. \right. \\ & \left. \left. + \frac{1}{6} m_{ij,\ell n}(\vec{\Delta}) \overline{a_i a_j a_\ell a_n} - \frac{1}{T} \frac{1}{2!} \left(\frac{1}{2} m_{ij,\ell}(\vec{\Delta}) a_i a_j a_\ell \right)^2 \right] \right\} \chi(\vec{\Delta}) + \mathcal{O}(\eta^2) \end{aligned} \quad (C2)$$

where the bar denotes

$$\bar{A} = \frac{\int_{-\infty}^{\infty} d^2 a \exp \frac{(-)}{T} a_i a_j m_{ij}(\vec{\Delta})}{\int_{-\infty}^{\infty} d^2 a \exp \frac{(-)}{T} a_i a_j m_{ij}(\vec{\Delta})} \quad (C3)$$

and $\partial = \partial/\partial\Delta$. The last line in (C2) gives T^2 -corrections to ϵ which can be neglected for low temperature. Since $d^2 a = da_{\parallel} da_{\perp}$ and

$$m_{ij}(\vec{\Delta}) a_i a_j = m_{\parallel} a_{\parallel}^2 + m_{\perp} a_{\perp}^2, \quad \frac{1}{2} m_{ij,\ell}(\vec{\Delta}) a_i a_j a_\ell = (m_{\parallel} - m_{\perp}) \frac{a_{\perp}^2 a_{\parallel}}{|\vec{\Delta}|} \quad (C4)$$

with

$$a_{\parallel}^2 = a_i a_j P_{ij}^{\parallel}(\Delta) \quad , \quad a_{\perp}^2 = \vec{a}^2 - a_{\parallel}^2 \quad) \quad (C5)$$

Eq. (C2) becomes $(P^{\perp} = 1 - P^{\parallel})$

$$\begin{aligned} & \left(\sqrt{\eta} \int_{-\infty}^{\infty} da_{\parallel} da_{\perp} \exp \frac{(-)}{T} (a_{\parallel}^2 m_{\parallel} + a_{\perp}^2 m_{\perp}) \right)^{-1} \cdot \int_{-\infty}^{\infty} d\vec{\Delta}' M(\vec{\Delta}, \vec{\Delta}') \chi(\vec{\Delta}') = \\ & = \left\{ 1 - \frac{\eta}{T} \left[-\frac{T^2}{4} \left(\frac{1}{m_{\perp}} \partial_s P_{st}^{\perp}(\vec{\Delta}) \partial_t + \frac{1}{m_{\parallel}} \partial_s P_{st}^{\parallel}(\vec{\Delta}) \partial_t + \epsilon(|\Delta|) \right] \right\} \cdot \\ & \cdot \chi(\vec{\Delta}) + \mathcal{O}(\eta^2) \end{aligned} \quad (C6)$$

Note the symmetric differential operator in agreement with the symmetric integral kernel M.

We use now the complete orthonormal set of functions χ_{σ} given by

$$\begin{aligned} & \left[-\frac{T^2}{4} \left(\frac{1}{m_{\perp}} \partial_s P_{st}^{\perp}(\vec{\Delta}) \partial_t + \frac{1}{m_{\parallel}} \partial_s P_{st}^{\parallel}(\vec{\Delta}) \partial_t \right) + \epsilon(|\Delta|) \right] \chi_{\sigma}(\vec{\Delta}) = \\ & = E_{\sigma} \chi_{\sigma}(\vec{\Delta}) \quad , \end{aligned} \quad (C7)$$

i.e. Eq.(6.9) of the main text, for the calculation of the multiple "matrix" product in (6.5) where M can be replaced by M times the prefactor of the first line in (C6) which is independent of $\vec{\Delta}, \vec{\Delta}'$. Eq.(6.5) involves products of the matrix $\mathcal{M}_{\sigma\tau} = (\chi_{\sigma}, M\chi_{\tau})$ of the form

$$\mathcal{M}^{|\mathbf{x}|/\eta} = \exp \frac{|\mathbf{x}|}{\eta} \ln \left[1 - \eta \frac{\mathcal{E}}{T} + \mathcal{O}(\eta^2) \right] \rightarrow \exp(-) |\mathbf{x}| \mathcal{E}/T \quad (C8)$$

which in the limit $\eta \rightarrow 0$ can be expressed by $\mathcal{E}_{\sigma\tau} = \delta_{\sigma\tau} E_{\sigma}$. As we shall see (C7) has a nondegenerate ground state which in the

thermodynamic limit $L \rightarrow \infty$ is the only state to survive in the product $\mathcal{M}^{(L-|x|)/\eta}$ and (6.5) is given by the expression (6.8) of the main text.

The hermitean differential operator, O , acting on χ on the left hand side of (6.9) is conveniently split into O^0 and a perturbation O'

$$O^0 = -\pi T^2 \frac{\partial^2}{\partial \phi^2} - 3\pi T^2 \delta_0^2 \frac{\partial^2}{\partial |\Delta|^2} + \frac{(|\Delta| - \delta_0)^2}{\pi} \quad (C9)$$

$$O' = -\pi T^2 \left(\frac{\delta_0^2}{|\Delta|^2} - 1 \right) \frac{\partial^2}{\partial \phi^2} - 3\pi T^2 \frac{\delta_0^2}{|\Delta|} \frac{\partial}{\partial |\Delta|} + \varepsilon_\ell \frac{(|\Delta| - \delta_0)^2}{\pi}$$

For $T \ll \delta_0$ and low excited states we may forget about the boundary $|\Delta| = 0$ in the radial part and obtain the unperturbed eigenfunctions and -values (6.11) in the main text. The corrections due to O'

$$\left| \frac{(\chi_{nm}, O' \chi_{n'm'})}{E_{nm} - E_{n'm'}} \right| \lesssim \sqrt{\frac{T}{\delta_0}} \quad \text{for } n, m = \mathcal{O}(1) \quad (C10)$$

are negligible.

The result (6.14) for the displacement correlation can be obtained very easily if one neglects amplitude fluctuations from the outset, i.e. $\Delta(\ell\eta) = \delta_0 e^{i\phi(\ell\eta)}$, $\int_{-\infty}^{\infty} d^2\Delta(\ell\eta) \rightarrow \int_{-\pi}^{\pi} d\phi(\ell\eta)$ in (6.5) and neglecting the $P^{\parallel}$ -term in (6.6). Then

$$\begin{aligned} & \langle \Delta^*(x) \Delta(0) \rangle_{0,2} = \\ & = \delta_0^2 \lim_{\eta \rightarrow 0} \frac{\prod_{\ell=0}^{(L/\eta)-1} \int_{-\pi}^{\pi} d\phi(\ell\eta) e^{-i(\phi(x) - \phi(0))} \exp \frac{(-)}{T} h \left[\phi((\ell+1)\eta) - \phi(\ell\eta) \right]}{\prod_{\bar{\ell}=0}^{(L/\eta)-1} \int_{-\pi}^{\pi} d\phi(\bar{\ell}\eta) \exp \frac{(-)}{T} h \left[\phi((\bar{\ell}+1)\eta) - \phi(\bar{\ell}\eta) \right]} \end{aligned} \quad (C11)$$

... $8\sin^2 \alpha/2$

For finite η this is a one-dimensional planar classical Heisenberg model. If in addition to $\phi(o)$ one introduces difference variables $a_\ell = \phi((\ell+1)\eta) - \phi(\ell\eta)$, these may be integrated from $-\pi$ to π too, because of the periodicity of the integrand. This gives

$$\begin{aligned}
 & \langle \Delta^*(x) \Delta(o) \rangle_{0,2} = \\
 & = \delta_0^2 \lim_{\eta \rightarrow 0} \left[\frac{\int_{-\pi}^{\pi} da e^{-ia} \exp(-h(a)/T)}{\int_{-\pi}^{\pi} da \exp(-h(a)/T)} \right]^{|x|/\eta} = \\
 & \hspace{25em} (C12) \\
 & = \delta_0^2 \lim_{\eta \rightarrow \infty} \left[\frac{\int_{-\infty}^{\infty} da e^{-ia} e^{-\frac{a^2}{4\pi\eta T}}}{\int_{-\infty}^{\infty} da e^{-\frac{a^2}{4\pi\eta T}}} \right]^{|x|/\eta} = \delta_0^2 \exp(-\pi|x|T)
 \end{aligned}$$

since for $\eta T \ll 1$ the sin may be replaced by its argument and the a -integral extended from $-\infty$ to $+\infty$.

Appendix D

If $2k_F$ is in the second Brillouin zone and $\tilde{v}_k$ is nonvanishing at least up to $k=2k_F$, then (1.4) gives

$$\begin{aligned}
 V(x) &= \frac{1}{L} \sum_{-\frac{\pi}{a} < k < 0} e^{ikx} \tilde{v}_k \frac{1}{L} \sum_{\frac{\pi}{a} < k < \frac{2\pi}{a}} e^{ikx} \tilde{v}_k + cc \\
 &= \frac{1}{L} \sum_{-\frac{\pi}{a} < k < 0} e^{ikx} \tilde{v}_k \frac{1}{L} \sum_p e^{i(2k_F+p)x} \tilde{\Delta}_p + cc.
 \end{aligned}
 \tag{D1}$$

Here we still assumed $\tilde{v}_k=0$ for $|k| > \frac{2\pi}{a}$. As independent dynamic variables we use $\hat{s}_k$ with $-\frac{\pi}{a} < k < 0$ or equivalently

$$\tilde{\Delta}_p = i w_p \hat{s}_{2k_F+p-\frac{2\pi}{a}}, \quad \frac{\pi}{a} < 2k_F+p < \frac{2\pi}{a}. \tag{D2}$$

This definition is slightly different from (1.8).

For slowly varying Δ , i.e. $|p| < \delta_{\text{eff}}$ (compare 5.1), the second terms in (D1) represent a potential with wavevectors near $\pm 2k_F$ which gives a Ginzburg-Landau energy (section 4), the first terms in (D1) contain wavevectors far away from $\pm 2k_F$ and, according to the discussion in section 5, give a harmonic energy (3.11) without the Einstein term. Therefore

$$\mathcal{H}[\Delta] = \mathcal{H}_0 + \mathcal{H}_2 + \dots + \frac{1}{L} \sum_p \frac{|\tilde{\Delta}_p|^2}{w_p} \int_{-(2k_F+p-\frac{2\pi}{a})} \tag{D3}$$

where $\overset{\circ}{\mathcal{H}}_0$, $\overset{\circ}{\mathcal{H}}_2$ are given by (4.5), (4.10) respectively and the p-sum runs over $|p| < \delta_{\text{eff}}$. The variation of $\mathcal{J}/w^2$ in (D3) with p is on the scale k_F , gives a negligible shift $\frac{\delta_{\text{eff}}^2}{k_F}$ in the Peierls wavevector and can otherwise be neglected compared to the gradient terms in $\overset{\circ}{\mathcal{H}}_2$. Therefore the last term in (D3),

$\frac{\mathcal{J} - (2k_F - \frac{2\pi}{a})}{w_0^2} \int dx |\Delta(x)|^2$ can be incorporated in $\overset{\circ}{\mathcal{H}}_0$ to give an effective gap

$$\frac{f_{E^a}}{w_0^2} + \frac{1}{w_0^2} \mathcal{J}_{-(2k_F - \frac{2\pi}{a})} = \frac{1}{\pi} \ln \frac{8E_F}{\delta_{\text{eff}}} \quad (D4)$$

An additional short wavelength $d\Delta$ (Equ. (5.1) with $p_c \sim \delta_{\text{eff}}$) represents an additional potential (D1) where the second terms in (D1) also contain only wavevectors well separated from $\pm 2k_F$ and lead to the harmonic energy (3.11); the first terms contribute as in (D3)

This gives

$$\mathcal{H} - \overset{\circ}{\mathcal{H}} = \frac{1}{L} \sum_p \frac{|\Delta_p|^2}{w_p^2} \left[f_{E^a} \mathcal{J}_{2k_F+p} + \mathcal{J}_{-(2k_F+p - \frac{2\pi}{a})} \right] \quad (D5)$$

with the p-sum running over $|p| > \delta_{\text{eff}}$ and $\frac{\pi}{a} < 2k_F + p < \frac{2\pi}{a}$. For $\delta_{\text{eff}} \ll |p| \ll k_F$ the square bracket equals $\frac{w_0^2}{\pi} \ln \frac{|p|}{\delta_{\text{eff}}}$ according to (D4).

With the philosophy of section 6, the displacement correlation for wavevectors near $2k_F - \frac{2\pi}{a}$ is given by (see (6.14))

$$\frac{1}{N} \left\langle \left| \hat{s}_{2k_F + p - \frac{2\pi}{a}} \right|^2 \right\rangle = \frac{1}{N w_p^2} \left\langle \left| \tilde{\Delta}_p \right|^2 \right\rangle = \frac{a}{w_o^2} \delta_{\text{eff}}^2 \frac{2\pi T}{(\pi T)^2 + p^2} \quad (\text{D6})$$

for $T \ll \delta_{\text{eff}}$, $p \lesssim \delta_{\text{eff}}$.

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Figure captions

- Fig.1: The electron-phonon interaction w .
- Fig.2: The giant Kohn effect (essentially, polarizability of onedimensional electrons as a function of the wave-vector k).
- Fig.3: Two plane waves (empty circles) with momentum $-k_F+k$ (-) and k_F+k (+) are combined to Bloch states (full circles) $k, \pm$ with energies $\pm \epsilon_k$. For $|k| \gg \delta$ the Bloch state reduces to the single plane wave connected with it by the broken line.
- Fig.4 : Dispersion of the harmonic expansion around $s \equiv 0$ for $T = 0$.
- Fig.5 : Dispersion for amplitude and phase mode
- a) $T = 0, \delta = \delta_0$: the difference in curvature for $|p| \ll \delta_0, \frac{\omega_p^2}{\omega_E^2} \ln \frac{8E_F}{\delta_0} = \pi f'' = 1 + \frac{1}{3} \left(\frac{p}{2\delta_0} \right)^2, \frac{\omega_p^2}{\omega_E^2} \ln \frac{8E_F}{\delta_0} = \pi f' = \left(\frac{p}{2\delta_0} \right)^2, \omega_E^2 = f_E/M$, is in agreement with the anisotropy in the Ginzburg-Landau energy (4.11).
- b) $T = T_p, \delta = 0$: $\pi f \approx 0.67 \left(\frac{p}{2\delta_0} \right)^2$ for $|p| \ll \delta_0$
 For $|p| \gg \delta_0$ all πf 's tend to the universal value $\ln \frac{|p|}{\delta_0}$.
- Fig.6 : Diagonal (a) and nondiagonal (b,c) contributions to Ω (2)
 for $dV \sim \tilde{\Delta}_p e^{i(2k_F+p)x} + \tilde{\Delta}_{p-2k_F} e^{ipx} + \tilde{\Delta}_{-p}^* e^{i(-2k_F+p)x} + \text{h.c.},$

$p > 0$ and for Δ_0 constant. Contributions b2)-b4) and c2)-c4) are not shown. Full circles and squares denote Bloch states which are composed of plane waves (open circles and squares), the arrows are phonon wavevectors k, k' . The diagrams 1, 2 contribute only for $k > 0$ or $k < -p$, the diagrams 3, 4 for $-p < k < 0$.

Fig.7 : Functions used to calculate the functional integral (6.5).

Fig.8 : The quantity $\frac{1}{N} \langle |\hat{s}_{2k_F+p}|^2 \rangle \cdot \frac{w_0^2}{a} \cdot \frac{2}{\pi T}$ versus $\kappa = p/2\delta_0$ for $\pi T = \delta_0/5$ and $|p| \ll k_F$ (see Eq.(6.15)). The analytic behaviour is given by $\left[\left(\frac{\pi T}{2\delta_0} \right)^2 + \kappa^2 \right]^{-1}$ and $\ln^{-1}(\sqrt{1+\kappa^2} + \kappa) \left(\frac{\sqrt{1+\kappa^2}}{\kappa} + \frac{\kappa_0}{\sqrt{1+\kappa^2}} \right)$ for $\kappa \ll 1$ and $\frac{k_F}{\delta_0} \gg \kappa \gg \frac{T}{\delta_0}$ respectively. For $\frac{k_F}{\delta_0} \gg \kappa \gg 1$ it tends to the universal harmonic behaviour $2 \ln^{-1} 2\kappa$.

Fig. 1

Fig. 2

Fig . 3

Fig. 4

Fig.5

Fig. 6

Fig. 7

Fig. 8