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Charge Conservation in the Incommensurate-Commensurate Transition of Charge Density Waves

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CHARGE CONSERVATION IN THE INCOMMENSURATE-
COMMENSURATE TRANSITION OF
CHARGE DENSITY WAVES

by
Jörg Kastrop

A Thesis
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
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Department of Physics

Western Michigan University
Kalamazoo, Michigan
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CHARGE CONSERVATION IN THE INCOMMENSURATE-
COMMENSURATE TRANSITION OF
CHARGE DENSITY WAVES

Jörg Kastrop, M.A.

Western Michigan University, 1992

With the complex continuation method, introduced by Gupta and Sutherland (1976), the grand partition function for the sine-Gordon model of charge density waves may be calculated without violation of charge conservation. Contrary to previous works by Okwamoto, Takayama and Shiba (1979) and Turkevich and Doniach (1982) the chemical potential becomes temperature dependent. By direct comparison of numerical results with those of the above mentioned authors it is shown that the incommensurate-commensurate transition does not occur in the previously predicted temperature range.

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How do I thank the people who have encouraged me, a student of a one-year exchange program from the University of Paderborn (Germany), to fulfill my dream of getting a master's degree during my stay in Kalamazoo? What can I say to those who kindly explained everything I needed to know about my new environment and thereby enabled me to finish this thesis? I would like to express my deepest appreciation for all the members of the Physics Department at Western Michigan University for their great support.

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Finally, I would like to express my gratitude to my parents. Without their loving support this work would simply not exist.

Jörg Kastrup

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INTRODUCTION

The theory of charge density waves (CDW's) has evolved to a well established means to describe the low temperature behavior of conductors. McMillan (1975) was the first who examined the incommensurate-commensurate (lock-in) transition and predicted discommensurations in the commensurate CDW. The natural one-dimensional description of a CDW bearing system turned out to be the sine-Gordon model. It has been used by Okwamoto, Takayama and Shiba (1979) and Turkevich and Doniach (1982) to predict various properties of the CDW's in the incommensurate-commensurate transition region. In their investigations both groups used the free energy functional that was introduced by McMillan. A slightly different approach was taken by Guyer and Miller (1978) treating the sine-Gordon chain as a system of torsion coupled pendula. They found that the mechanical variable conjugate to the phase in the CDW is the torque and concluded that a boundary condition on the phase must enter their calculation as an external torque on the pendula. But where do the boundary conditions, that are imposed by the law of charge conservation, enter the calculations of Okwamoto et al. and Turkevich and Doniach? They set the chemical potential μ , which is the equivalent to Guyer and Miller's external torque, to zero and thereby allow their system to create the charge carrying phase solitons freely; thus violating the charge conservation.

The purpose of this work is to show how their results change if one works with a non-zero chemical potential conjugate to the charge of the system. Sections two and three give a microscopic introduction of a model Hamiltonian for a lock-in transition and review the zero temperature behavior of the model. The following sections focus on the $T \neq 0$ case. With the help of the transfer matrix method (Scalapino, Sears, & Ferrell, 1972) the problem of calculating the functional integral

in the partition function is reduced to the evaluation of a simple matrix eigenvalue problem. By applying the complex continuation trick of Gupta and Sutherland (1976) the grand partition function is calculated. Special attention is given to the connection between the chemical potential and the boundary condition. The analysis of the grand partition function finds its firm basis in the equivalence between the Gupta and Sutherland method and the Guyer and Miller approach (see the simultaneously appearing master's thesis by Johlen, 1992). The following sections are devoted to the calculation of the phase-phase correlation function and the structure factor. Finally the results of the numerical calculations are presented and compared with the previous results. The last section finishes this work with a conclusion.

THE MODEL HAMILTONIAN

With the help of the charge density wave order parameter $\psi(x) = \rho_0 e^{i\varphi(x)}$ the incommensurate CDW may be written

$$\begin{aligned}\rho(x) &= \bar{\rho} + \text{Re}\psi(x_0) \\ &= \bar{\rho} + \rho_0 \cos(qx + \Phi).\end{aligned}\tag{1}$$

The phase is set to $\varphi = qx + \Phi$ to suggest the picture of a distorted plane wave with $q = 2k_F$. The CDW is called commensurate when the reciprocal lattice vector G is a rational multiple of the CDW vector q . Inspired by measurements at $2H - TaSe_2$ (see Suits, Couturié, & Slichter, 1980), where the CDW-length has been found to be about 1% longer than three times the Lattice constant, we define

$$\delta = \frac{q - G/n_0}{G/n_0}.\tag{2}$$

For the case of $2H - TaSe_2$ we set $n_0 = 3$ because the incommensurate CDW is close to three-fold commensurability. The local velocity of a phase disturbance in the CDW is $v = -\frac{1}{q}\dot{\Phi}$. With the effective mass m^* of the electrons in the CDW condensate and the number density n of electrons per spin, the kinetic energy per unit length may be written as $K.E. = nm^* \left(\frac{1}{q}\dot{\Phi}\right)^2$. Guided by the microscopic theory of Lee, Rice and Anderson (1974) the elastic energy is chosen to be $E.E. = \frac{v_F}{4\pi}\phi_x^2$ where v_F is the Fermi velocity. Note that by writing down the elastic energy we have set Planck's constant \hbar to unity. For an interaction between the CDW and the underlying lattice we consider a phenomenological commensurability energy density

$$\begin{aligned}
C.E. &= d \operatorname{Re} (e^{-iGx} e^{in_0\phi}) \\
&= d \cos [n_0(\Delta qx + \Phi)],
\end{aligned} \tag{3}$$

where $\Delta q = q - G/n_0$ and n_0 an integer. The form of the interaction term was initially proposed by McMillan (1975) and later used by Turkevich and Doniach (1981). The C.E. is minimal when the CDW length is exactly n_0 times the lattice constant so that an n_0 -fold commensurability is favored. Substituting

$$n_0(\Delta qx + \Phi) = \phi \tag{4}$$

we obtain the model Hamiltonian

$$\mathcal{H}[\phi] = \int_0^L dx \left\{ \frac{m^*}{2\pi q n_0^2} \phi_x^2 + \frac{v_F}{4\pi n_0^2} (\phi_x - n_0 \Delta q)^2 + d(1 - \cos \phi) \right\}. \tag{5}$$

It is important to notice that the concept of charge conservation imposes a boundary condition on ϕ . The continuity equation $\dot{\rho} + \nabla j = 0$ demands that the local current density $j = -\frac{2ne}{q} \dot{\Phi}$ is accompanied by a charge density $\rho = \frac{2e}{2\pi} \Phi_x$. The net charge of a system of length L is then

$$Q = \frac{2e}{2\pi} (\Phi(L) - \Phi(0)). \tag{6}$$

By defining $Q = 0$ as the charge reference state, and using eq.4, we arrive at the boundary condition

$$\phi(L) - \phi(0) = n_0 \Delta q L \equiv 2\pi N. \tag{7}$$

Since solitons and antisolitons, elementary excitations in the system (5), change the phase by $\pm 2\pi$, the constant $N = n_0 \Delta q L / 2\pi$ represents the net number of solitons ($N > 0$) or antisolitons ($N < 0$). It is interesting to note that each soliton carries a charge of $2e/n_0$.

ZERO TEMPERATURE PROPERTIES

From the Hamiltonian (5) the phase dynamics is described by the well known sine-Gordon equation:

$$\frac{m^*}{\pi q n_0^2} \phi_{tt} - \frac{v_F}{2\pi n_0^2} \phi_{xx} + d \sin \phi = 0 \quad (8)$$

Note that we have degenerate vacua $\phi_0 = 0, \pm 2\pi, \pm 4\pi, \dots$. Solitons and antisolitons are elementary excitations of (8) connecting adjacent vacua:

$$\phi = 4 \arctan \left[\exp \left(\pm \sqrt{d} \sqrt{\frac{2\pi n_0^2}{v_F}} x \right) \right]. \quad (9)$$

Thus an estimate for the size of a soliton is given by

$$s = \sqrt{\frac{v_F}{2\pi d n_0^2}}. \quad (10)$$

Other elementary excitations are the so called breather modes. These are bound states of a soliton-antisoliton pair oscillating with the period

$$\tau = \sqrt{\frac{m^*}{\pi d q n_0^2}}. \quad (11)$$

It is now convenient to use s and τ as length and time scales by defining $\tilde{t} \equiv t/\tau$ and $\tilde{x} \equiv x/s$. Substituting this into (8) we wind up with the dimensionless sine-Gordon equation

$$\phi_{\tilde{t}\tilde{t}} - \phi_{\tilde{x}\tilde{x}} + \sin \phi = 0. \quad (12)$$

At $T = 0$ we may neglect thermal fluctuations ($\phi_{\tilde{t}} = 0$) so that our boundary value problem reduces to

$$\phi_{\tilde{x}\tilde{x}} = \sin \phi \quad (13)$$

$$\phi(\tilde{L}) - \phi(0) = 2\pi N. \quad (14)$$

By assuming $\phi(0) = 0$, equation (13) may be rewritten in the form of an elliptic integral of the second kind.

$$\tilde{x} = \frac{K}{2} \int_0^{\phi/2} \frac{dy}{\sqrt{1 - K^2 \cos^2 y}}, \quad (15)$$

where the constant K can be calculated numerically by using condition (14) for given N and \tilde{L} . Here, as a measure of commensurability, we define

$$\eta \equiv \frac{L - Ns}{Ns}. \quad (16)$$

The ideal incommensurate state is then characterized by $\eta = 0$ and the commensurate state by $\eta = \infty$. It is important to notice that the soliton width s and the pinning strength d are related. It is seen from (10) that high commensurability η means small soliton width and strong pinning

$$d = \frac{v_F}{2\pi n_0^2} \frac{1}{s^2} = \frac{v_F}{2\pi n_0^2} \left((1 + \eta) \frac{N}{L} \right)^2. \quad (17)$$

This may be confirmed by comparing Figures 1 and 2, where the umklapp-process is much stronger for higher η . Contrary to earlier works the concept of charge conservation (14) forces the number of kinks to stay constant over the length L for different η . It is this seemingly little difference that will later produce a significant change in the low temperature behavior of the structure factor.

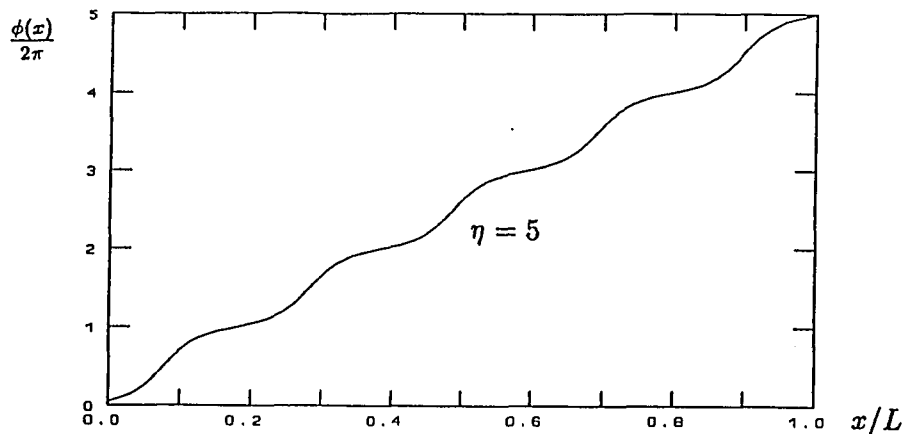


Figure 1. $\phi(x)/2\pi$ for Commensurability $\eta = 5$.

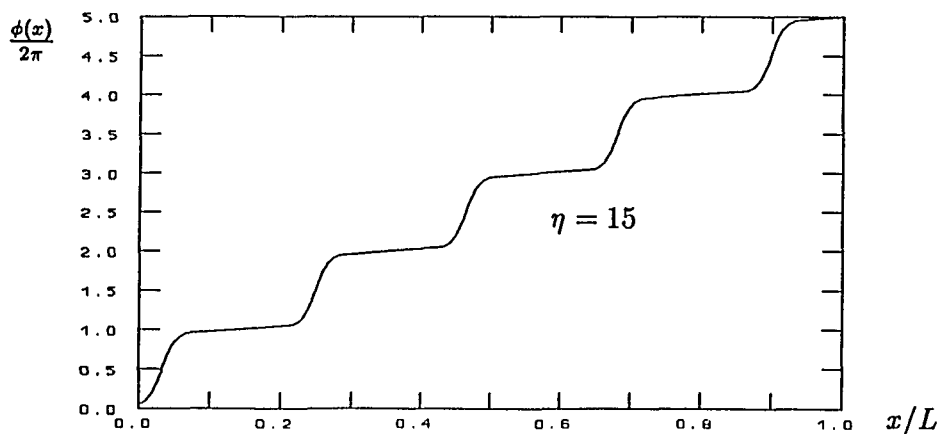


Figure 2. $\phi(x)/2\pi$ for Commensurability $\eta = 15$.

THE PARTITION FUNCTION

It is obvious that the simple form of $\phi(x)$ (see Figures 1 and 2) is going to break down at $T > 0$. The soliton lattice "melts." For small η ($\Rightarrow s$ small) and low densities N/L , the system may be treated as a dilute soliton gas (Currie, Krumhansl, Bishop, & Trullinger, 1980). However, at higher temperatures and arbitrary densities, the dilute gas picture is certainly irrelevant, and thermal properties of the system have to be explored through the analysis of correlation functions.

From the Hamiltonian (5), we get the canonical momentum

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \frac{m^*}{\pi q n_0^2} \dot{\phi}. \quad (18)$$

Now the kinetic energy part in (5) can be rewritten as

$$K.E. = \frac{\pi q n_0^2}{2m^*} \Pi^2. \quad (19)$$

The classical partition function separates into a space part and a momentum part:

$$Z_N = \int \delta\phi \delta\Pi e^{-\beta \mathcal{H}[\phi, \Pi]} = Z_\phi Z_\Pi. \quad (20)$$

The functional integration may be performed by dividing L into M segments of length Δx . The momentum part is then calculated easily to give

$$\begin{aligned} Z_\pi &= \prod_{i=1}^M \int_{-\infty}^{\infty} d\Pi_i e^{-\beta \Delta x \frac{\pi q n_0^2}{2m^*} \Pi_i^2} \\ &= \left(\frac{2m^*}{\beta q \Delta x n_0^2} \right)^{M/2}. \end{aligned} \quad (21)$$

By using the transfer matrix method (Scalapino et al.,1972) we can reduce the problem of calculating the space part of the partition function to an eigenvalue problem.

$$Z_\phi = \int_{-\infty}^{\infty} d\phi_1 \cdots d\phi_{M+1} \delta(\phi_{M+1} - \phi_1 - 2\pi N) \prod_{i=1}^M K(\phi_i, \phi_{i+1}), \quad (22)$$

where the transfer integral operator $K(\phi_i, \phi_{i+1})$ has been defined as

$$K(\phi_i, \phi_{i+1}) = e^{-\beta \Delta x \left\{ \frac{v_F}{4\pi n_0^2} \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} - n_0 \Delta q \right)^2 + d(1 - \cos \phi_{i+1}) \right\}}. \quad (23)$$

The δ -function in (22), which takes care of the boundary condition $\phi_{M+1} - \phi_1 = 2\pi N$, is now expanded as

$$\delta(\phi_{M+1} - \phi_1 - 2\pi N) = \sum_n \Phi_n^*(\phi_{M+1} - 2\pi N) \Phi_n(\phi_1). \quad (24)$$

The complete orthonormal set $\{\Phi_n\}$ has to be chosen to satisfy the transfer integral eigenvalue equation

$$\int d\phi_i K(\phi_i, \phi_{i+1}) \Phi_n(\phi_i) = \sqrt{\frac{4\pi^2 \Delta x n_0^2}{\beta v_F}} e^{-\beta \Delta x \epsilon n} \Phi_n(\phi_{i+1}). \quad (25)$$

An important thing to note is that the transfer integral operator is non-hermitian, as we will see below, and therefore does not guarantee the existence of an orthonormal set of eigenfunctions. In fact the eigenfunctions obtained by solving a resulting pseudo Schrödinger equation are highly non-orthogonal. Fortunately, the master's thesis by Johlen (1992) appearing simultaneously with this work shows that orthonormalizing the eigenvectors with the Gram-Schmidt orthogonalization method leaves the partition function unchanged. Thus we may

safely assume the existence of a set $\{\Phi_n\}$ with the desired properties.

Inserting (24) into (22) and using the fact that the Φ_n are eigenfunctions of the transfer integral equation (25) we have

$$Z_\phi = \sqrt{\dots}^M \sum_n e^{-\beta L \epsilon_n} \int_{-\infty}^{\infty} d\phi \Phi_n^*(\phi - 2\pi N) \Phi_n(\phi), \quad (26)$$

where we have used $L = M\Delta x$ and replaced ϕ_{M+1} by ϕ . In order to calculate the Φ_n and the corresponding ϵ_n we have to solve the transfer integral equation (22). A Taylor expansion of $\Phi_n(\phi_i)$ about ϕ_{i+1} enables us to rewrite the left part of equation (25)

$$\int d\phi_i K(\phi_i, \phi_{i+1}) e^{(\phi_i - \phi_{i+1}) \frac{d}{d\phi}} \Phi_n(\phi_{i+1}). \quad (27)$$

After substituting $y = \phi_i - \phi_{i+1}$ and collecting the coefficients of y and y^2 in the exponent, we can perform the y -integral to get

$$\{-32t^2 \frac{d^2}{d\phi^2} + 16\pi t \frac{d}{d\phi} + (1 + \eta)^2 (1 - \cos \phi)\} \Phi_n(\phi) = \frac{\epsilon_n}{d_c} \Phi_n(\phi). \quad (28)$$

In writing down equation (28) we have measured the temperature in units of the $\eta = 0$ soliton energy

$$t = \frac{T}{8s_c d_c}, \quad (29)$$

where $s_c = L/N$ and $d_c = \frac{v_F}{2\pi n_0 s_c^2}$. We have thus replaced the transfer integral equation (25) by a Schrödinger-like eigenvalue problem.

Now Floquet's theorem tells us that the eigenfunctions of (28) are of the form

$$\Phi_n(\phi) = e^{ik\phi} \psi_{\alpha k}(\phi) \quad (30)$$

$$\psi_{\alpha k}(\phi) = \psi_{\alpha k}(\phi + 2\pi), \quad (31)$$

where α is a band index and the wave number k is in the first Brillouin zone:

$$k \in \left[-\frac{\pi}{l}, \frac{\pi}{l}\right] = \left[-\frac{1}{2}, \frac{1}{2}\right]. \quad (32)$$

With equations (20), (21), (26) and (30) the partition function finally becomes

$$Z_N = \left(\frac{m^*}{m}\right)^{M/2} \left(\frac{8t}{n_0^2 s}\right)^M \frac{1}{2\pi} \sum_{\alpha} \int_{-1/2}^{1/2} dk e^{\beta L \varepsilon_{\alpha, k}} e^{ik2\pi N}. \quad (33)$$

THE GRAND PARTITION FUNCTION AND THE CHEMICAL POTENTIAL

Because of the rapidly oscillating factor $\exp(ik2\pi N)$ the k integral in (33) is not easy to evaluate in the thermodynamic limit $N \rightarrow \infty$. This problem may be avoided by considering the grand partition function:

$$\begin{aligned} \mathcal{Z} &= \sum_{N=-\infty}^{\infty} (e^{\beta\mu})^N Z_N \\ &= \left(\frac{m^*}{m}\right)^{M/2} \left(\frac{8t}{n_0^2 s}\right)^M \frac{1}{2\pi} \sum_n \int_{-1/2}^{1/2} dk e^{-\beta L \epsilon_n(k)} \\ &\quad \times \sum_{n=-\infty}^{\infty} e^{(\beta\mu + 2\pi ki)N}. \end{aligned} \quad (34)$$

Following a method introduced by Gupta and Sutherland (1976) we allow μ to take imaginary values

$$\beta\mu = -2\pi i\lambda. \quad (35)$$

The sum over N can be performed by using

$$\sum_{N=-\infty}^{\infty} e^{2\pi i N(k-\lambda)} = \delta(k-\lambda). \quad (36)$$

We get

$$\mathcal{Z} = \left(\frac{m^*}{m}\right)^{M/2} \left(\frac{8t}{sn_0^2}\right)^M \frac{1}{2\pi} e^{-\beta L \epsilon_0(\lambda)}. \quad (37)$$

Note that only the lowest band $\alpha = 0$ contributes in the thermodynamic limit $L \rightarrow \infty$. Now the question is whether an analytic continuation of $\mathcal{Z}(k)$ to an

Equations (38) and (39) are then iteratively solved to give $\mu(t)$ and $\varepsilon_0(t)$. It is also noted that because of the non-hermiticity of the matrix the energy eigenvalues $\varepsilon_{\alpha k}$ are generally complex, while the lowest eigenvalue ε_{0k} turns out to be always real.

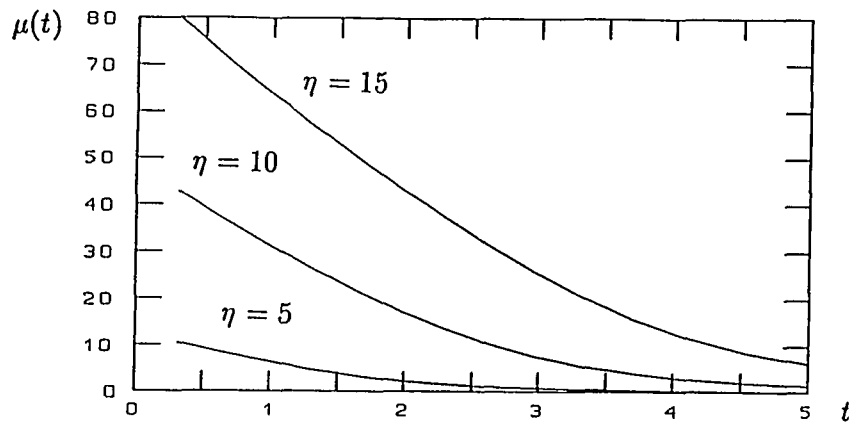


Figure 3. Chemical Potential Versus the Reduced Temperature.

In Figure 3 $\mu(t)$ is plotted versus the reduced temperature. It is important to notice the μ does not diverge at $t \rightarrow 0$. This is because at low temperatures μ may be interpreted as the creation energy of solitons which is certainly finite.

DERIVATION OF THE PHASE-PHASE CORRELATION FUNCTION

To get an idea of the degree of thermal disordering along the chain we calculate the phase-phase correlation function. It is defined as

$$\begin{aligned} H(x - x') &= \langle e^{i\varphi(x)} e^{-i\varphi(x')} \rangle \\ &= e^{i\frac{Q}{n_0}(x-x')} \langle e^{i\phi(x)/n_0} e^{-i\phi(x')/n_0} \rangle, \end{aligned} \quad (41)$$

where the average $\langle \dots \rangle$ is over the grand canonical ensemble:

$$\begin{aligned} \langle e^{i[\phi(x)-\phi(x')]/n_0} \rangle &= \frac{1}{\mathcal{Z}} \sum_{N=-\infty}^{\infty} e^{\beta\mu N} \int \delta\phi \delta\Pi e^{-\beta\gamma t[\phi, \Pi]} e^{i[\phi(x)-\phi(x')]/n_0} \\ &= \frac{1}{\mathcal{Z}} \sum_{N=-\infty}^{\infty} e^{\beta\mu N} Z_{\Pi} \tilde{Z}_{\phi}. \end{aligned} \quad (42)$$

\tilde{Z}_{ϕ} is a shorthand for the ϕ -integral which now takes the form

$$\tilde{Z}_{\phi} = \int d\phi_1 \cdots d\phi_{M+1} \delta(\phi_{M+1} - \phi_1 - 2\pi N) \prod_{i=1}^M K(\phi_i, \phi_{i+1}) e^{i(\phi_i - \phi_m)/n_0}. \quad (43)$$

In the above, we used

$$\begin{aligned} x &= (l-1)\Delta x, \\ x' &= (m-1)\Delta x, \\ \phi(x) &= \phi_l, \\ \phi(x') &= \phi_m. \end{aligned} \quad (44)$$

Expanding the δ -function as in (24) we can perform the first $l - 1$ integrals to get

$$\begin{aligned} \tilde{Z}_\phi &= \int d\phi_{M+1} \cdots d\phi_l \sqrt{\frac{4\pi^2 \Delta x n_0^2}{\beta v_F}}^{(l-1)} e^{i\phi_m/n_0} \\ &\times \sum_n e^{-\beta \epsilon_n \Delta x (l-1)} \prod_{i=l}^M K(\phi_i, \phi_{i+1}) \\ &\times \Phi_n^*(\phi_{M+1} - 2\pi N) \Phi_n(\phi_l) e^{i\phi_l/n_0}. \end{aligned} \quad (45)$$

Now the expansion

$$e^{i\phi_l/n_0} \phi_n(\phi_l) = \sum_j \langle \Phi_j | e^{i\phi_l/n_0} | \Phi_n \rangle \Phi_j(\phi_l) \quad (46)$$

allows us to perform the next $(m - l)$ integrals and a similar expansion for $e^{-i\phi_m/n_0} \Phi_j(\phi_m)$ allows us to perform the last $(M - m + 1)$ integrals. We thus have

$$\begin{aligned} \tilde{Z}_\phi &= \sqrt{\cdots}^M \sum_{n,j,j'} e^{-\beta \epsilon_n \Delta x (l-1)} e^{-\beta \epsilon_j \Delta x (m-l)} e^{-\beta \epsilon_j \Delta x (M-m+1)} \\ &\times \langle \Phi_j | e^{i\phi/n_0} | \Phi_n \rangle \langle \Phi_{j'} | e^{-i\phi/n_0} | \Phi_j \rangle \\ &\times \int d\phi \Phi_n^*(\phi - 2\pi N) \Phi_j(\phi) \\ &= \sqrt{\cdots}^M \sum_{n,j} |\langle \Phi_j | e^{i\phi/n_0} | \Phi_n \rangle|^2 \\ &\times e^{2\pi N i k} e^{-\beta \epsilon_n L} e^{-\beta(x-x')(\epsilon_j - \epsilon_n)} \end{aligned} \quad (47)$$

Now for macroscopic L , we may write $n = (0, k)$ and according to the selection rule $j = (\alpha, k + 1/n_0)$. Inserting the resulting expression back into equation (42) and proceeding as before for the sum over N and the k -integral, we finally obtain

$$H(x - x') = e^{i\frac{\sigma}{n_0}(x-x')} \sum_{\alpha} \overline{W}(\alpha) e^{-\beta(x-x')[\epsilon_{\alpha}(k+1/n_0) - \epsilon_0(k)]}, \quad (48)$$

where we have defined $\overline{W}(\alpha) = |\langle \psi_{\alpha, k+1/n_0} | \psi_{0, k} \rangle|^2$. It is now important to remember that the derivation was done under the assumption that $x < x'$. Because

$$H(x - x') = \left\langle e^{i\phi(x')} e^{-i\phi(x)} \right\rangle^* \quad (49)$$

we expect the real part of H to be symmetric under exchange of x and x' and the imaginary part to be antisymmetric. Hence we have in general

$$\begin{aligned} H(x - x') &= e^{i\frac{\sigma}{n_0}(x-x')} \sum_{\alpha} \overline{W}(\alpha) \\ &\quad \times e^{-\beta|x-x'|[\operatorname{Re} \epsilon_{\alpha}(k+1/n_0) - \epsilon_0(k)]} \\ &\quad \times e^{-i\beta(x'-x)\operatorname{Im} \epsilon_{\alpha}(k+1/n_0)}, \end{aligned} \quad (50)$$

where we have made use of the fact that ϵ_0 is always real. The result will be used in the next section.

THE STRUCTURE FACTOR AND NUMERICAL RESULTS

A directly measurable quantity is the x-ray scattering factor due to the charge density wave:

$$S(Q) = \langle \rho_Q^\dagger \rho_Q \rangle \quad (51)$$

with

$$\rho_Q = \frac{1}{\sqrt{L}} \int e^{-ixQ} \rho(x) dx \quad (52)$$

where $\rho(x) = \rho_0 \exp(i\varphi(x))$ is the charge density associated with the CDW. A straightforward calculation making use of result (50) leads to

$$\begin{aligned} S(Q) &= \frac{\rho_0^2}{L} \int dx dy e^{-i(x-y)Q} \langle e^{-i\varphi(y)} e^{i\varphi(x)} \rangle \\ &\propto \sum_{\alpha} \overline{W}(\alpha) \frac{\xi^{-1}}{\xi^{-2} + (Q - (G/n_0 + \Delta Q))^2} \end{aligned} \quad (53)$$

In (53) we have defined

$$\xi^{-1} = \beta [Re \varepsilon_{\alpha}(k + 1/n_0) - \varepsilon_0(k)] \quad (54)$$

$$\Delta Q = \beta Im \varepsilon_{\alpha}(k + 1/n_0) \quad (55)$$

Note that $\overline{W}(\alpha)$ in (53) quickly decreases with α and the lineshape is roughly a Lorentzian. Then the inverse correlation length ξ^{-1} represents the linewidth and ΔQ the shift of the peak. In Figures 4 and 6, ξ^{-1} and ΔQ have

been plotted against the temperature for various commensurability strengths η . For comparison, the previous results of Okwamoto et al. (1979) and Turkevich and Doniach (1982) are plotted in Figures 5 and 7. They have been obtained by setting $\mu \equiv 0$ (or $k \equiv 0$) in our calculations. We thereby reallocate the violation of charge conservation and thus recover the results of the above mentioned authors. The most striking result is that in the charge conserved case the scattering peak does not converge toward G/n_0 in the previously predicted temperature range. However, as can be seen from the definition of the correlation function and the fact that for $T = 0$ and large η the system is predominantly in the commensurate state, the peak must shift to G/n_0 when the temperature approaches zero. It is noted that at $\eta = 0$ we have $\mu \approx 0$ for all t and thus the two calculations lead to similar results. In comparing Figures 4 and 5, one notices that the correlation length becomes smaller in the charge conserved case than without charge conservation. This is a clear indication that the $t = 0$ soliton lattice state in the charge conserved case is rather fragile and "melts" easily. For all η the curves show a tendency to go to zero with temperature. This is because at $t = 0$ the correlation length must be infinitely large.

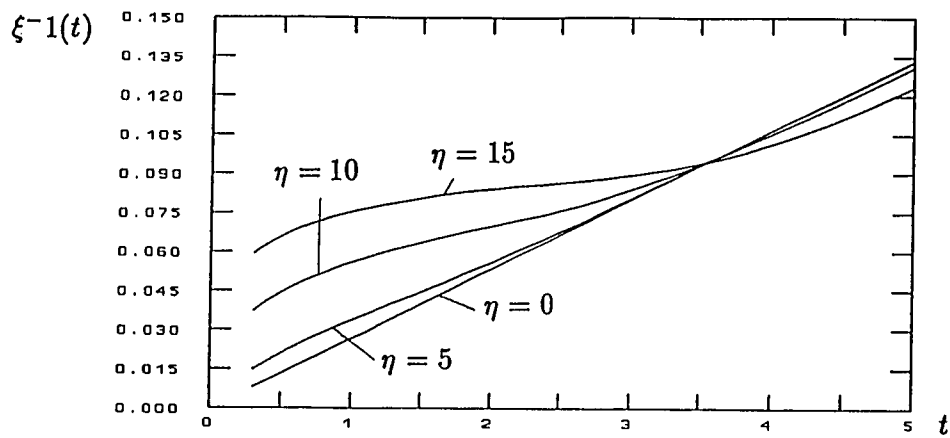


Figure 4. Charge Conserved Case: Inverse Correlation Length.

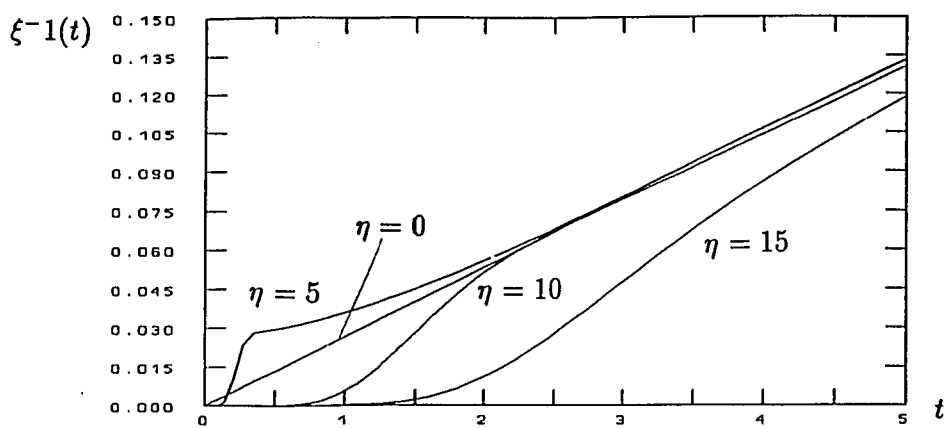


Figure 5. Charge Not Conserved ($\mu \equiv 0$): Inverse Correlation Length.

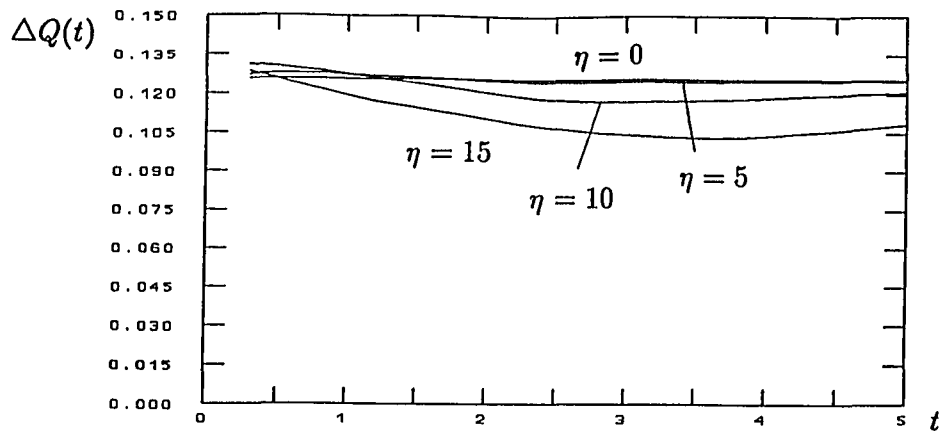


Figure 6. Charge Conserved Case: Shift ΔQ of the Scattering Peak.

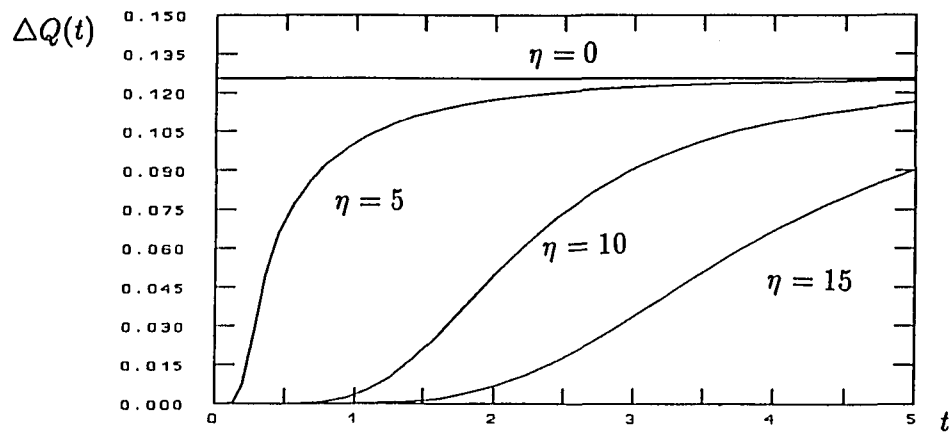


Figure 7. Charge Not Conserved: Shift ΔQ of the Scattering Peak.

CONCLUSION

We have shown that the charge conservation does play an important role in the low-temperature behavior of charge density waves. It turned out that in the examined temperature range the incommensurate-commensurate transition (for $\eta > 0$) does not occur and it is not clear if it does occur at finite temperatures. Because of convergence problems in the eigenvalue equation the calculation could not be extended to lower temperatures. To shed some light on this question a low temperature WKB expansion similar to the one given by Turkevich and Doniach (1982) (but explicitly including charge conservation) appears to be more promising than conducting more rather expensive numerical calculations in the low-temperature region.

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