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COMMENSURABLE CHARGE-DENSITY WAVES IN A RANDOM POTENTIAL

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We study commensurable charge-density wave systems in the presence of random impurities. The results of the microscopic theory, especially the contributions of second order in the impurity fields, are briefly discussed. The lifetime of the excitations is calculated, as well as the response of a soliton to an external field.

1. Introduction

During the last few years, many experimental investigations[1] have demonstrated the fascinating properties of quasi-onedimensional metals at low temperatures. The observed effects are related to the formation of a charge-density wave (CDW), as predicted by Peierls and Fröhlich, and the pinning of the CDW by impurities, or the underlying lattice. The results have been interpreted theoretically by various models[2-6]; here, we only wish to remark that the perturbational treatment of the impurities[7-9] has been criticised[10].

In this note, we study the behavior of a commensurable CDW in the presence of disorder. We consider situations where the commensurability effects dominate the random potential, allowing for a perturbational treatment of the latter. To be definite, we describe the impurity potential by random Gaussian fields, $\eta(x)$, and $\xi(x)$, $\xi^*(x)$, whose means are zero, and correlations are given by $< \eta\xi > = < \xi\xi > = 0$, and

$$< \eta(x)\,\eta(x') > = \Gamma_\eta \times \delta(x - x') \tag{1}$$

$$< \xi(x)\,\xi^*(x') > = \Gamma_\xi \times \delta(x - x') \tag{2}$$

In one dimension, we have $\Gamma_\eta = v_F/2\tau_1$, $\Gamma_\xi = v_F/2\tau_2$, with $\tau_1(\tau_2)$ the electron scattering times with changes in momentum close to zero and $\pm 2p_F$, respectively. (p_F, v_F: Fermi momentum/velocity). If three dimensional effects are to be included, we will use Eqs. (1,2) with $x \to \vec{x}$, and the above expressions for $\Gamma_{\xi,\eta}$ have to be multiplied by d^2, where d is the distance between the conducting chains. Note that, if the impurity potential is a sum of randomly distributed δ-functions of strength v, we have $\Gamma_{\xi,\eta} \sim n_{imp} \times v^2$, where n_{imp} is the impurity density.

2. Microscopic Theory

The microscopic theory can be formulated by using the path integral representation[9,11-14] of the generating functional (or partition function) for imaginary times. In the first step, one integrates over the phonon variables, and introduces a complex order parameter, $\Delta = -i \mid \Delta \mid \exp(-i\chi)$. Fluctuations in $\mid \Delta \mid$, however, are suppressed by large energies, and its equilibrium value can be inserted. The result is an effective action for the relevant variable, the phase χ, which has a contribution from the phonons, $\sim m_F\dot{\chi}^2$, where m_F is the Fröhlich mass divided by the band mass, and an electronic contribution given by tr log $\hat{G}$, where $\hat{G}$ is the electron Green's function. Commensurability pinning is included[15] by extending $\hat{G}$ to a $M \times M$ matrix. Finally, log $\hat{G}$ is expanded in second order with respect to $v_F(\partial_x\chi)/2 - e\phi$, where ϕ is the electric potential, and with respect to the impurity fields. In view of the inequality $m_F >> 1$, we can neglect time derivatives of χ in the electron contribution. From the resulting effective action, the real time equation for χ is derived, following the method described in Ref. 14. We obtain (ignoring noise terms) the following equation of motion:

$$\partial_t^2\chi - c^2\partial_x^2\chi + \frac{\omega_o^2}{M}\sin M\chi = I_1 + I_2 - \gamma\dot{\chi} \tag{3}$$

Here, $c^2 = v_F^2/m_F$, ω_o is the characteristic frequency of the commensurability potential[15], and the coupling between chains can be included[9] by $c^2\partial_x^2 \to c^2\partial_x^2 + c_\perp^2\partial_\perp^2$. For I_1, we obtain

$$I_1 = 2\pi v_F \rho_1 m_F^{-1}\,\mathrm{Re}\,(\xi \exp i\chi) + 2e^* v_F(E - \partial_x\eta/e) \tag{4}$$

Here, ρ_1 is the density of electrons condensed in the CDW state, $e^* = e/m_F$, and E the electric field. For finite temperatures, some coefficients depend on T through $\mid \Delta \mid$; in addition, c^2 and e^* have to be multiplied by $1 - Y$, where $Y(T)$ is the Yoshida function.

We now discuss in more detail the second order impurity contributions, which lead to $I_2 - \gamma\dot{\chi}$. The effective action has a contribution

$$-\frac{1}{4}\int dx dx' d\tau d\tau'\, \beta(x - x', \tau - \tau') \times \tilde{\xi}(x,\tau)\tilde{\xi}(x',\tau') + c.c. \tag{5}$$

where $\tilde{\xi}(x,\tau) = \xi(x)\exp i\chi(x,\tau)$, and a similar one with $\tilde{\xi}\tilde{\xi}^*$. As in the theory of Josephson tunneling, the first term is related to the supercurrent, and the second one ($\tilde{\xi}\tilde{\xi}^*$) to the normal current and thus to dissipation. We evaluate (5) in the limit of small frequencies and long wave-lengths, compared to $|\Delta|$ and $\xi_o \sim v_F/|\Delta|$, respectively, and find I_2 to be given by:

$$I_2 = 2\pi v_F\, m_F^{-1}\, \mathrm{Re}\,(i\mu \exp 2i\chi) \tag{6}$$

Note the similarity to the first term in I_1, but also the factor two multiplying the phase[16]. The random field $\mu(x)$ is given by

$$\mu(x) = \int dy\, \xi(x+y/2)\,\xi(x-y/2)\,\beta_0(y) \tag{7}$$

Here, $\beta_0(y)$ is the zero frequency component of $\beta(y,\tau)$, which we find to be given by

$$\beta_0(y) = \frac{T}{v_F^2}\sum_n \frac{|\Delta|^2}{\omega_n^2 + |\Delta|^2} \times \exp[-2\,(\omega_n^2 + |\Delta|^2)^{1/2}\,|y|\,/v_F] \tag{8}$$

where $\omega_n = (2n+1)\pi T$ is the Matsubara frequency. Obviously, this quantity decreases exponentially for $y \gtrsim \xi_o$ (for low temperatures). Especially

$$\beta_o(0) = |\Delta|/2v_F^2 \times \tanh(|\Delta|/2T) \tag{8'}$$

which is proportional to the critical current in Josephson junctions[17]. Note that $\mu(x)$ is not a Gaussian field, but all correlation functions can be calculated. For example, we find

$$<\mu(x)\,\mu^*(x')> = \Gamma_\mu\, \delta(x-x') \tag{9}$$

with $\Gamma_\mu \simeq \xi_o \times [\Gamma_\xi \times \beta_o(0)]^2$. Clearly, if simple coarse graining arguments apply, an effective averaged force can be derived[16] from (6), in the same way as from the first term in I_1. A measure of their relative importance is $X = \rho_1^2\Gamma_\xi/\Gamma_\mu \sim 10 \times (\rho_1/\rho_o)^2 E_F^2 \tau_2/|\Delta|$, where ρ_o is the total electron density. Inserting, e.g., $\rho_1/\rho_0 \sim 0.1$, $|\Delta| \sim 0.1\,E_F$, we obtain $X \gg 1$ provided $E_F\tau_2 \gg 1$. Close to the critical temperature, this factor will be even larger. Thus, in contrast to other estimates[16], the present model leads to the conclusion that the "classical" term is typically larger than the "Josephson" contribution. The same estimate holds for quasi-onedimensional situations. We remark, however, that the result may be different in systems with true three-dimensional coherence. In this case, roughly speaking, X has to be multiplied by $(d/\xi_\perp)^2 << 1$, where $\xi_\perp$ is the perpendicular coherence length. Note, also, that the two contributions have non-vanishing correlations.

The other second order term is similar to the normal current in Josephson junctions. We consider this contribution averaged with respect to the impurities: Then we may apply known results[14], and obtain for example γ from the low frequency behavior of the normal current:

$$\gamma = (\tau_2 m_F)^{-1}\int_{-\infty}^{\infty} dE\,(-\frac{\partial f_o}{\partial E})\,[N(E)]^2 \tag{10}$$

where, f_o is the Fermi function, and $N(E)$ the (normalised) density of states. N(E) includes effects of inelastic as well as impurity scattering, which we here treat in an approximate way, by introducing a line-width Γ_o. For $\Gamma_o >> |\Delta|$, we find $N(E) \simeq 1$, and $\gamma = (\tau_2 m_F)^{-1}$. For $\Gamma_o << |\Delta|$, γ decreases exponentially with decreasing T, reflecting the decrease in the number of excitations, and approaches for T=0 the limit $\gamma = (\tau_2 m_F)^{-1}[N(0)]^2$, $N(0) = \Gamma_o/|\Delta|$.

3. Lifetime of Small Amplitude Modes

In this section we wish to demonstrate that the classical impurity term in I_1 leads to a damping of the small amplitude fluctuations of high enough frequency, by decay into other phasons. We consider three dimensions, and $I_2 = 0$, $\gamma \to 0$. The contribution to the action quadratic in χ has the following form:

$$S = \frac{m_F}{4\pi v_F d^2}\int d^3x\, d^3y \times T\sum_n \chi_{-n}(\vec{x})\,\kappa^{-1}(\vec{x},\vec{y},\omega_n)\,\chi_n(\vec{y}) \tag{11}$$

where $\chi_n(\vec{x}) = \chi(\vec{x},\omega_n)$, $\omega_n = 2n\pi T$, and the factor $(\pi v_F d^2)^{-1}$ is the density of states at the Fermi surface (which consists of two parallel planes). Without impurities, the correlation function, κ, depends only on the coordinate difference, and its Fourier transform is given by $\kappa_o^{-1}(\vec{q},\omega_n) = \omega_n^2 + \omega_q^2$, where $\omega_q^2 = \omega_o^2 + c^2q_x^2 + c_\perp^2 q_\perp^2$. In the presence of the random potential, on the other hand, we obtain

$$\kappa^{-1}(\vec{x},\vec{y},\omega_n) = \kappa_o^{-1} - \tilde{\rho}_1\, \mathrm{Re}\,(i\xi(\vec{x}))\,\delta(\vec{x}-\vec{y}) \tag{12}$$

where $\tilde{\rho}_1 = \rho_1 \times 2\pi v_F d^2/m_F$. Here, ρ_1 is the *three-dimensional* density of condensed electrons. We treat the impurities by perturbation theory, and expand κ with respect to ξ; in the approximation which neglects intersecting impurity lines, we find for the inverse of the *averaged* correlation function

$$<\kappa>^{-1}(\vec{q},\omega_n) = \kappa_o^{-1} - \Sigma(\omega_n) \tag{13}$$

where the self energy, $\Sigma(\omega_n)$, is given by

$$\Sigma(\omega_n) = \frac{1}{2}\tilde{\rho}_1^2\Gamma_\xi \int \frac{d^3q}{(2\pi)^3}\,\kappa_o(\vec{q},\omega_n) \tag{14}$$

Especially, we want to point out that

$$\mathrm{Im}\,\Sigma(\omega_n \to -i\omega + 0) = \gamma_{ph}\,(\omega^2 - \omega_o^2)^{1/2}\,\mathrm{sgn}\,\omega \tag{15}$$

for $\omega^2 > \omega_o^2$, and zero elsewhere. This quantity determines the damping of the phasons; it is non-zero only above the minimum phason frequency, ω_o, and becomes linear in ω for $\omega >> \omega_o$. The damping constant, given by $\gamma_{ph} = \tilde{\rho}_1^2\Gamma_\xi/8\pi c c_\perp^2$, is just the Fukuyama-Lee-Rice frequency[18] characteristic for impurity pinning.

4. Motion of Solitons

To investigate the motion of solitons in the random potential, we use a scaled version of (3), ignoring I_2 and η (the latter can be included without difficulty). We put $\varphi = M\chi$, and measure time, length, and electric field in units of ω_o^{-1}, $L_o = c/\omega_o$, and $E_o = \omega_o^2/2e^* v_F M$, respectively. In addition, $\xi \to \Gamma_\xi^{1/2}\xi$, such that now $<\xi(x)\xi^*(x')> = \delta(x-x')$. Then (3) transforms into

$$\ddot{\varphi} - \varphi'' + \sin\varphi = \alpha\,\mathrm{Re}\,(\xi\, e^{i\varphi/M}) + E - \gamma\dot{\varphi} \qquad (16)$$

where $\alpha = M(L_o/L_\xi)^{3/2}$, with L_ξ the characteristic length for the impurities[18]; generally, $\alpha \sim L_\xi^{(d-4)/2}$, where d is the dimension. We assume α, E, $\gamma << 1$, and employ standard methods of perturbation theory[19–21] to evaluate the effect of the r.h.s. in (16). Dissipation is due to transfer of momentum to the impurities: Therefore, we start from the momentum conservation law which is a direct consequence of (16). With $P = -\dot{\varphi}\varphi'$, $\Pi = \frac{1}{2}(\dot{\varphi}^2 + \varphi'^2) - U$, and $U = -\cos\varphi + \alpha M\,\mathrm{Re}\,(i\xi\, \exp i\varphi/M)$, we obtain

$$\partial_t P + \partial_x \Pi = -(\partial_x U)_\varphi - \varphi' E - \gamma P \qquad (17)$$

where $(\partial_x U)_\varphi$ is the derivative of U for constant φ. A well-known example[19] is $\alpha = 0$, in which case, for a constant field, a stationary situation arises with a kink moving at constant velocity, v, given by

$$\frac{\pi}{4}E = \pm\gamma v\,(1 - v^2)^{-1/2} \qquad (18)$$

for an anti-soliton (soliton). This result can be arrived at by inserting the anti-soliton, $\varphi_o(y) = 4 \times \tan^{-1}\exp(-y)$, where $y = (x - vt)/(1 - v^2)^{\frac{1}{2}}$, into (17) and integrating with respect to the coordinate.

In the first step, we consider the translational mode in more detail. For small velocities, we may use the ansatz[20] $\varphi = \varphi_o(x - z)$ where the location of the kink is taken time dependent: $z = z(t)$. Then we obtain, the following equation of motion:

$$\ddot{z} + \gamma\dot{z} = -V'(z) + \pi E/4 \qquad (19)$$

$$V'(z) = \frac{\alpha}{8}\int dx\, \varphi_o'\, \mathrm{Re}\,[\xi\, e^{i\varphi_o/M}] = \frac{\alpha}{8}\int dk\, \bar{\xi}_k\, e^{ikz} \qquad (20)$$

We assumed E to depend on time only. Clearly (19) describes the motion of the kink in the random impurity field, which is integrated with the shape of the kink. Accordingly, we find that the correlations of $\bar{\xi}_k$ ($\bar{\xi}_k$ is the Fourier transform of a real Gaussian field with average mean) decay exponentially for $k \gtrsim 1$. With $< \bar{\xi}_k \bar{\xi}_{k'} >= \Gamma_k \delta(k + k')$, we obtain, for example, $\Gamma_k = \pi k^4[\mathrm{sech}^2(\pi k/2) + \mathrm{csch}^2(\pi k/2)]$ for M=1, and $\Gamma_k = \pi\,\mathrm{sech}^2(\pi k/2)$ for $M \to \infty$. In the long wave-length limit, Γ_k remains finite except for $M = 1$, with the result $\Gamma_{k=0} = M^2[1 - \cos(2\pi/M)]/2\pi$. As a characteristic of the potential, note that

$$< [V(z) - V(o)]^2 >= \frac{\alpha^2}{32}\int dk\, \frac{\Gamma_k}{k^2}(1 - \cos kz) \qquad (21)$$

which, for large $|\, z \,|$, is finite ($\sim \alpha^2$) for $M = 1$, and increases $\sim |\, z \,|$ for $M > 1$.

As an application of (19), we study the linear response to a field $E(t) = E_\omega \exp(-i\omega t)$. Let z_o be a local minimum of V(z), and define the response function by $\chi_\omega(z_o) = z_\omega/E_\omega$. Instead of $\chi_\omega(z_o)$, we consider a weighted sum over different minima, averaged with respect to the impurities, of this quantity. We write

$$\chi_\omega = \frac{\pi}{4}\int_o^\infty d\omega_o\, \frac{P(\omega_o)}{-\omega^2 - i\omega\gamma + \omega_o^2} \qquad (22)$$

where

$$P(\omega_o) = N^{-1} \times 2\omega_o < \sum_{z_o} \delta(\omega_o^2 - V''(z_o))\, W(z_o) > \qquad (23)$$

The constant, N, is determined such that $P(\omega_o)$ is normalized (and thus (22) gives the correct response for high frequencies). Here, we consider only $W(z_o) = 1$, i.e. all minima are taken into account with equal probability; in this case, N is the average number of minima. We obtain the following result:

$$P(\omega_o) = 4\omega_o^3/\bar{\omega}^4 \exp(-\omega_o^4/\bar{\omega}^4) \qquad (24)$$

where $\bar{\omega}^2 = (2A_2)^{1/2}\alpha/8$, $A_2 = \int_{-\infty}^{\infty} dk\, k^2\, \Gamma_k = 4 \times (1 + 8/M^2)/3$. The relation $\bar{\omega}^2 \sim \alpha$ is clear from (19), and the exponential decrease of $P(\omega_o)$ for large ω_o is related to the Gaussian distribution of the random field. For $\gamma \to 0$, $\omega << \bar{\omega}$, we obtain

$$\begin{aligned} \mathrm{Re}\,\chi_\omega &\simeq \pi^{3/2}/4\bar{\omega}^2 \\ \mathrm{Im}\,\chi_\omega &\simeq \pi^2\omega^2/2\bar{\omega}^4 \times \mathrm{sgn}\,\omega \end{aligned} \qquad (25)$$

The response function, χ_ω, is directly related to the dielectric function and the conductivity, σ_ω, the latter being proportional to $-i\omega\,\chi_\omega$. Especially, $\mathrm{Re}\,\sigma_\omega \sim \omega^3 \times \mathrm{sgn}\,\omega$ for small frequencies.

In the next step, we include dissipation due to scattering in the random potential, by calculating the correction to the kink, $\varphi = \varphi_o(x - z) + \varphi_1, \varphi_1 \sim \alpha$. Note that φ_1 is perpendicular to the translational mode. We do not study the general result, but only the *impurity average* (for fixed $z(t)$) of the correction due to φ_1. As a result we have to add the following expression to the l.h.s. of (19):

$$H_c[z] = \int_{-\infty}^{t} dt' \int \frac{d\kappa}{2\pi}\, \gamma_\kappa(t - t')\, e^{i\kappa[z(t) - z(t')]} \qquad (26)$$

Here, $\gamma_\kappa(t - t')$ is related to the Green's function of the linearised sine-Gordon equation. If the kink moves with constant velocity, $z = vt$, we find (note $v << 1$)

$$H_c(v) \equiv H_c[vt] = \alpha^2 h_M\, v^{-(3/2 + 4/M)} e^{-\pi/v} \qquad (27)$$

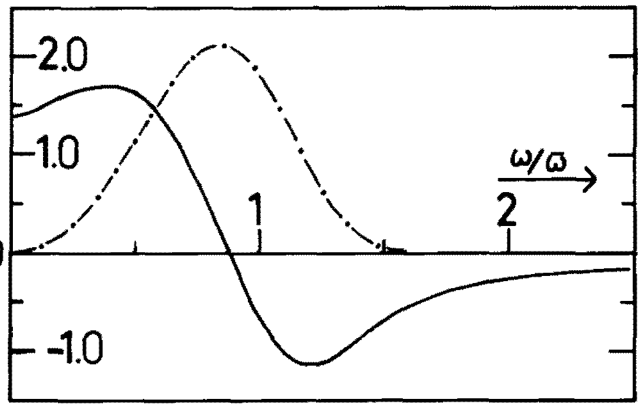

Fig. 1 : Real part (—) and imaginary part (– · – · –) of the response funktion, χ_ω (see Eq.(22)).

and, for example, $h_1 = h_2 = \pi/4\sqrt{2}$, $h_\infty = h_1/2$. As expected, the gap in the excitation spectrum leads to an exponentially small damping for small velocities.

Finally, we have examined the motion of a kink in a large constant field (presumably $E >> \alpha$) , using the ansatz $\varphi = \varphi_o(y) + \tilde{\varphi}_1$, where $\tilde{\varphi}_1$ is determined by perturbation theory. $\tilde{\varphi}_1$ is inserted into (17), which is then integrated over x, and averaged. We consider $\gamma \to 0$; in this case, however, the perturbation theory works only for M=1 (for $M > 1$, the potential is not "flat" enough, see (21)), and for not too small velocities, $v^2 >> \alpha$, which follows from an analyis of the translational mode in $\tilde{\varphi}_1$. We obtain, for high velocities, a relation similar to (18):

$$(\pi/4)E = \gamma_s v(1 - v^2)^{-1/2}, \qquad v \to 1 \qquad (28)$$

where $\gamma_s = \alpha^2/6$ is the damping constant. Note that, although M=1 is meaningful within our model, the relevant cases for CDWs are $M > 2$.

In conclusion, we have discussed in this section some aspects of the motion of solitons in a random potential. We expect that a model like the one presented here can further enhance our understanding of the role impurities play in CDW systems. Further details will be discussed elsewhere[22].

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