Mesoscopic charge-density-wave junctions

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We investigate theoretically charge-density waves (CDW's) in mesoscopic heterostructures for the configuration where the one-dimensional chains are oriented normal to the interfaces. Based on Bogoliubov–de Gennes equations and suitable boundary conditions, ground state properties of phase coherent CDW systems are calculated in the mean-field approximation. It is shown that in a charge-density-wave/normal-metal/charge-density-wave junction the CDW condensates couple through the normal metal region by means of Friedel oscillations. Geometrical resonance effects are predicted. We relate the phase-dependent energy of the junction to a momentum current, carried by electron-hole pairs. The effects of pinning potentials at the interfaces are also considered. Finally, we discuss the analogies with superconductor and ferromagnet junctions. [S0163-1829(96)07924-6]

I. INTRODUCTION

The coupling of spatially separated ground states in phase-coherent heterostructures is known to cause many remarkable effects. The Josephson effect and Andreev reflection in superconductor junctions,[1,2] the nonlocal exchange coupling,[3] and the associated giant magnetoresistance[4] in magnetic multilayers are only a few examples of the striking phenomena that occurr in such systems. In this context it is surprising that the concept of charge-density waves (CDW's) in mesoscopic junctions has apparently escaped attention. In the mesoscopic regime the coherence length of the CDW becomes comparable to the sample size. A search for alternate quantum size effects in mesocopic devices like heterostructures of CDW's and normal metals might lead to fundamental insights into the physics of charge-density waves.

In the 1950s, Peierls suggested that strongly anisotropic metals are unstable with respect to lattice deformations. This instability is known as the Peierls transition. The ground state consists of a periodic electron density modulation, called the charge-density wave, accompanied by a static periodic lattice distortion. Fröhlich[5] noted that in incommensurate systems the degeneracy of the condensate with respect to rigid translations generates a symmetry restoring collective mode of transport. The sliding motion of the CDW produces remarkable electrical behavior, like non-Ohmic conductivity[6] and narrow band noise.[7]

Charge-density waves in bulk systems have already received much attention in the last few decades (for an overview see Grüner[8]). Unlike mesoscopic superconducting devices, there has not been much work reported on CDW's in mesoscopic systems so far. We are only aware of sporadic contributions in charge-density-wave tunnel junctions within a tunneling Hamiltonian approach.[9–11] Experiments on mesoscopic CDW samples are expected to be conducted in the near future.[14] Stimulated by these experimental efforts, we investigate theoretically the ground state properties of various heterostructures in the mean-field approximation. Transport properties such as quasiparticle conductance and sliding CDW motion will be treated subsequently in Refs. 12 and 13.

The basis for our calculations are the Bogoliubov–de Gennes[15] (BdG) equations for CDW's. The BdG equations are known to successfully explain many experiments on spatially inhomogeneous superconductor structures. In Sec. II the Bogoliubov–de Gennes equations for CDW systems are derived from the mean-field approximation. We also propose boundary conditions which are necessary to solve the BdG equations in heterostructures. In the geometry where the one-dimensional chains are oriented normal to the interfaces, we calculate in Sec. III the density of states and the pinning energy of normal-metal/charge-density waves (N/C) and (C/N/C) junctions with barrier potentials of arbitrary strength at the interfaces. We consider the CDW proximity effect and the mechanism of phase coupling by Friedel oscillations. In Sec. IV we will point out the analogies with ferromagnet and superconductor junctions. Section V summarizes our conclusions.

II. MEAN-FIELD THEORY

A. Bogoliubov–de Gennes equations

In strongly anisotropic or quasi-one-dimensional materials, the particular shape of the band structure causes a nesting of electron-hole states near the Fermi surface. The backscattering of electrons near the Fermi energy produces a divergence in the response of the charge-density to lattice deformations. As a consequence, a charge-density-wave ground state is formed spontaneously at a critical temperature T_c, which is rigidly coupled to a periodic lattice distortion. The ground state consists of a condensate of electron-hole pairs and is characterized by a complex order parameter Δ. Because the effective mass of the electrons in the transverse direction is much larger than the effective mass in the direction along the chains, it is reasonable to assume that the only effect of neighboring chains is the suppression of thermal fluctuations of the order parameter. In this approximation, the main features of the Peierls transition and of the associated collective mode can be captured by the mean-field

treatment of the one-dimensional free electron gas coupled to the underlying lattice by electron-phonon interaction, as described by the Fröhlich Hamiltonian. In mean-field theory, the interaction with the phonons at $Q=2k_F$ is singled out, and the effective single-particle Hamiltonian reads

$$H=-\frac{\hbar^2}{2m}\partial_x^2-\epsilon_F+U(x)+\{\Delta(x)e^{iQx}+\Delta^*(x)e^{-iQx}\}, \quad (1)$$

where the first term describes the kinetic energy and $U(x)$ is an external potential, which is assumed to vary slowly on the scale of $1/k_F$. The last terms represents the phonon field, which consists of the product of a slowly varying pair potential $\Delta(x)$ and a term which oscillates with the CDW wave vector $Q=2k_F$. To solve the Schrödinger equation, $H\psi=\epsilon\psi$, the wave function close to the Fermi energy may be split into right (R) and left (L) going electron parts:

$$\psi(x)=\psi_R(x)e^{ik_Fx}+\psi_L(x)e^{-ik_Fx}. \quad (2)$$

ψ_R and ψ_L are also slowly varying. Disregarding second derivatives of ψ_R and ψ_L as well as terms which oscillate rapidly like $\exp(3ik_Fx)$, the Schrödinger equation can be cast into the eigenvalue equation:

$$\begin{pmatrix} -i\hbar v_F\partial_x+U(x) & \Delta(x) \\ \Delta^*(x) & i\hbar v_F\partial_x+U(x) \end{pmatrix}\Psi_k=\epsilon_k\Psi_k, \quad (3)$$

where the spinor Ψ_k is defined as

$$\Psi_k=\begin{pmatrix} \psi_{R,k} \\ \psi_{L,k} \end{pmatrix}. \quad (4)$$

These are the Bogoliubov–de Gennes equations for CDW systems. Right and left going wave functions are coupled by the pair potential $\Delta(x)$. Since the matrix operator is Hermitian, the eigenfunctions form a complete orthonormal set. The quasiparticle excitation spectrum is given by the energy eigenvalues. Note the subtle difference with the BdG equations in superconductivity: in superconductors the quasiparticle wave functions are linear combinations of electron-hole pairs, whereas here we have linear combinations of right and left going electrons. These equations have to be solved together with the self-consistency equation

$$\Delta(x)=g_{\rm ep}\sum_k \psi^*_{L,k}(x)\psi_{R,k}(x)\tanh(\beta\epsilon_k/2), \quad (5)$$

where the sum is taken over all k states, $g_{\rm ep}$ is the electron-phonon coupling constant, and $\beta=1/k_BT$.

In a uniform CDW system $U(x)=0$, $\Delta(x)=\Delta e^{i\varphi}$, and the BdG equations are easily solved. The energy eigenvalues $\epsilon_k\equiv\epsilon_\pm(k)$ are then given by

$$\epsilon_\pm(k)=\mathrm{sgn}(k)\sqrt{\Delta^2+(\hbar v_Fk)^2}, \quad (6)$$

where the wave vector k is measured relative to the Fermi wave vector $k\Rightarrow|k|-k_F$. The energy spectrum contains a gap 2Δ at k_F and the energies $\epsilon_\pm$ describe the conduction and valence band, see Fig. 1. The eigenfunctions are

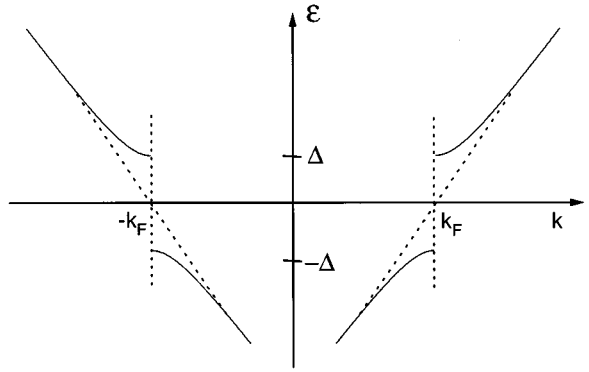

FIG. 1. The electron dispersion in the Peierls ground state. A gap 2Δ is formed at the Fermi wave vector k_F.

$$\Psi_-(x)=\begin{pmatrix} v_k \\ u_ke^{-i\varphi} \end{pmatrix}e^{ikx}, \quad \Psi_+(x)=\begin{pmatrix} u_k \\ -v_ke^{-i\varphi} \end{pmatrix}e^{ikx}, \quad (7)$$

where v_k and u_k are the standard BCS coherence factors

$$v_k^2=\frac{1}{2}\left(1-\frac{\sqrt{\epsilon_k^2-\Delta^2}}{\epsilon_k}\right), \quad u_k^2=\frac{1}{2}\left(1+\frac{\sqrt{\epsilon_k^2-\Delta^2}}{\epsilon_k}\right), \quad (8)$$

which satisfy the relation $v_{-k}=u_{k.}$

At $T=0$ all states below the gap are filled and all states above the gap are empty. The electronic energy gain by creating a gap overcomes the increased elastic energy at the critical temperature and induces the phase transition. The electron density in the ground state at $T=0$ is

$$n(x)=s\sum_k |\psi(x)|^2=s\sum_k \{v_k^2+u_k^2+2u_kv_k\cos(Qx+\varphi)\}. \quad (9)$$

Spin degeneracy s is now included. The product u_kv_k is called the condensation amplitude in state k and is appreciable only in an interval around k_F, which is inversely proportional to the CDW coherence length $\xi_0=\hbar v_F/\pi\Delta$. ξ_0 corresponds to the spatial dimension of the electron-hole pairs in the condensate. Integrating Eq. (9) and using Eq. (5) leads to the well-known density modulation

$$n(x)=s\left\{\frac{k_F}{\pi}+\frac{2\Delta}{g_{\rm ep}}\cos(Qx+\varphi)\right\}. \quad (10)$$

This is the charge-density wave. The modulation is proportional to the pair amplitude, the wavelength is given by $\lambda=2\pi/Q$, and the phase φ determines the position of the CDW.

B. Boundary conditions

For a theory of heterostructures based on the BdG equations, we have to determine boundary conditions at interfaces. Let us consider first the boundary condition at a short range impurity potential, modeled by a δ function $V(x)=H\delta(x)$. Adding this term to Eq. (1) and integrating the Schrödinger equation, the conventional boundary conditions for the wave function and its derivative are obtained:

$$\psi(0^+)=\psi(0^-), \quad (11)$$

$$\partial_x\psi|_{0^+}-\partial_x\psi|_{0^-}=\frac{2m}{\hbar^2}H\psi(0). \tag{12}$$

By substituting Eq. (2) into these conditions we obtain the boundary condition for the spinor wave function

$$\Psi(0^+)=\mathbf{M}\Psi(0^-) \tag{13}$$

in terms of the transfer matrix

$$\mathbf{M}=\begin{pmatrix}1-iZ & -iZ\\ iZ & 1+iZ\end{pmatrix}, \tag{14}$$

where $Z=H/\hbar v_F$ is the dimensionless scattering strength. In general, the transfer matrix also includes effects of potential steps. A difference in electron densities left and right of the interface can be modeled by a potential step $V(x)=\theta(x)(\epsilon_{F_L}-\epsilon_{F_R})$, where θ is the Heaviside step function. In this case the transfer matrix reads

$$\mathbf{M}=\frac{1}{\sqrt{4\alpha}}\begin{pmatrix}1+\alpha & 1-\alpha\\ 1-\alpha & 1+\alpha\end{pmatrix}, \tag{15}$$

where $\alpha=v_{F_L}/v_{F_R}$. For an ideal interface without impurity or potential step, $\mathbf{M}$ is the unit matrix and no mixing of right and left going electrons occurs. It will be shown that the off-diagonal terms due to defects or density mismatch leads to the pinning of the CDW. Given these boundary conditions, we have all the ingredients to calculate the ground state properties of CDW heterostructures.

III. HETEROSTRUCTURES

In spatially nonuniform electron systems, scattering due to band mismatch, interfaces, or impurities will change the density of states. The perturbed density of states ρ is expressed in terms of the scattering matrix $\mathbf{S}$ by the general relation[16]

$$\rho=\frac{1}{2\pi i}\frac{\partial}{\partial\epsilon}\ln\det\mathbf{S}+\rho_0, \tag{16}$$

where ρ_0 is the unperturbed density of states. This equation has been applied by Beenakker[2] to superconductor/normal-metal/superconductor (S/N/S) junctions. Here we will construct the scattering matrix for CDW heterostructures using the eigenfunctions of the BdG equations as a basis. The wave functions should be normalized to carry the same amount of quasiparticle current to ensure current conservation, which is equivalent to a unitary $\mathbf{S}$ matrix. The elements of the scattering matrix can be calculated from the boundary conditions at the scattering sites. Using the expression

$$E(\varphi)=\frac{1}{2\pi i}\int\epsilon\frac{\partial}{\partial\epsilon}\ln\det\mathbf{S}(\epsilon,\varphi)\,d\epsilon \tag{17}$$

we can calculate the phase-dependent total energy at low temperatures from the scattering matrix. The interaction between the CDW and the nonuniformities in the system results in a position- or phase-dependent force on the CDW. This force pins the CDW and in order to observe a sliding CDW motion a threshold voltage is necessary to overcome the associated pinning potential. The pinning force is expressed as

$$F=-Q\frac{dE}{d\varphi}. \tag{18}$$

We will now apply this formalism to the single impurity problem in Sec. III A, to the normal-metal/charge-density-wave (N/C) junction in Sec. III B, and to the C/N/C junction in III C.

A. Single impurity pinning

The interaction between a CDW and a single impurity has been investigated extensively by Tüttö and Zawadowski.[17] In their model only backscattering with momentum transfer Q is taken into account. In principle, we cover both forward and backward scattering using the boundary conditions discussed in Sec. II B. This problem is treated here mainly to demonstrate the simplicity of our formalism. The impurity is again modeled by a δ function potential $V(x)=H\delta(x)$. The wave functions to the left and right of the impurity at $x=0$ are

$$\Psi(x)=\begin{cases}A\begin{pmatrix}v_k\\ u_ke^{-i\varphi}\end{pmatrix}e^{ikx}+B\begin{pmatrix}u_ke^{i\varphi}\\ v_k\end{pmatrix}e^{-ikx}, & x<0\\ C\begin{pmatrix}v_k\\ u_ke^{-i\varphi}\end{pmatrix}e^{ikx}+D\begin{pmatrix}u_ke^{i\varphi}\\ v_k\end{pmatrix}e^{-ikx}, & x>0\end{cases} \tag{19}$$

and have the same macroscopic phase φ. The scattering matrix $\mathbf{S}$ relates the incoming amplitudes A and D to the outgoing amplitudes B and C via

$$\begin{pmatrix}B\\ C\end{pmatrix}=\mathbf{S}\begin{pmatrix}A\\ D\end{pmatrix}=\begin{pmatrix}r_{11} & t_{12}\\ t_{21} & r_{22}\end{pmatrix}\begin{pmatrix}A\\ D\end{pmatrix}, \tag{20}$$

where r stands for the reflection and t for the transmission amplitude. Matching the wave functions using Eq. (13) we obtain after some algebra

$$r_{11}=-iZe^{-i\varphi}\left\{\frac{v_k^2e^{i\varphi}+u_k^2e^{-i\varphi}+2u_kv_k}{(1+iZ)v_k^2-(1-iZ)u_k^2+2iZu_kv_k\cos\varphi}\right\},$$

$$r_{22}=-iZe^{i\varphi}\left\{\frac{v_k^2e^{-i\varphi}+u_k^2e^{i\varphi}+2u_kv_k}{(1+iZ)v_k^2-(1-iZ)u_k^2+2iZu_kv_k\cos\varphi}\right\},$$

$$t_{12}=t_{21}=\frac{v_k^2-u_k^2}{(1+iZ)v_k^2-(1-iZ)u_k^2+2iZu_kv_k\cos\varphi}. \tag{21}$$

It is easily verified that the scattering matrix is unitary. The determinant of the scattering matrix becomes

$$\det\mathbf{S}(\epsilon,\varphi)=-\frac{(1-iZ)v_k^2-(1+iZ)u_k^2-2iZu_kv_k\cos\varphi}{(1+iZ)v_k^2-(1-iZ)u_k^2+2iZu_kv_k\cos\varphi}, \tag{22}$$

and we obtain for the energy-phase relation

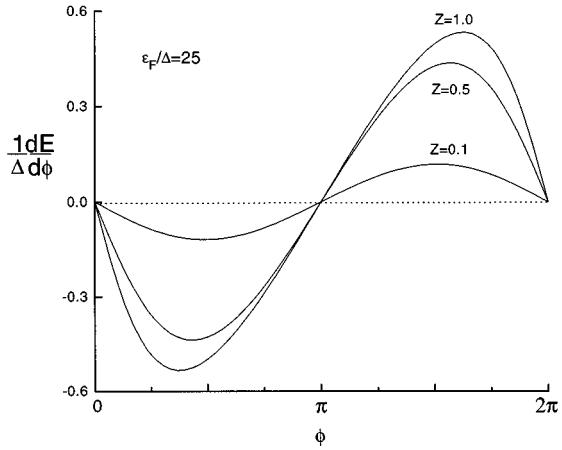

FIG. 2. The dependence of the pinning force from a single impurity as a function of the CDW position for different barrier strengths Z.

$$\frac{dE}{d\varphi}=-\frac{2Z\sin\varphi}{\pi}\times\int_{-\epsilon_F}^{-\Delta}u_kv_k\left\{\frac{(v_k^2-u_k^2)}{(v_k^2-u_k^2)^2+Z^2(1+2u_kv_k\cos\varphi)^2}\right\}d\epsilon, \tag{23}$$

where we have used the Fermi energy ϵ_F as integration cutoff. For weak impurity potentials, $Z\ll 1$, we may disregard the Z^2 term in the denominator. Carrying out the integral in this limit by using Eq. (5) the classical result

$$\frac{dE}{d\varphi}=-\frac{\Delta}{\pi}\frac{Z}{\hat{g}}\sin\varphi \tag{24}$$

is recovered, where the dimensionless coupling constant $\hat{g}=g_{\rm ep}/2\pi\hbar v_F$ is introduced. If the scattering potential is repulsive ($Z>0$), the energy minimum configuration corresponds to $\varphi=\pi$ and the electron density at the impurity site is minimal. For stronger impurity potentials the integral has to be calculated numerically. Figure 2 shows the pinning force for different scattering strengths. For small Z the pinning force is sinusoidal. For stronger potentials a deviation occurs, which leads to higher harmonics in the Fourier spectrum. The behavior of the pinning force is qualitatively the same as calculated by Ref. 17.

B. N/C junction

Consider a normal-metal/charge-density wave (N/C) junction with an interface at $x=0$. In the CDW region the order parameter $\Delta(x)$ near the interface is not constant, but decays smoothly over a finite length of the order of the coherence length, as indicated schematically in Fig. 3. This is the CDW proximity effect. To determine $\Delta(x)$ near the interface one has to solve the gap equation (5).[18] Here we disregard the proximity effect and assume a step function pair potential, which is a common assumption in S/N junctions. A δ function potential is added to the interface to model an interface defect or impurity. For simplicity we assume the CDW and the normal-metal to be one dimensional and the average electron densities to be equal. Mismatch in electron densities

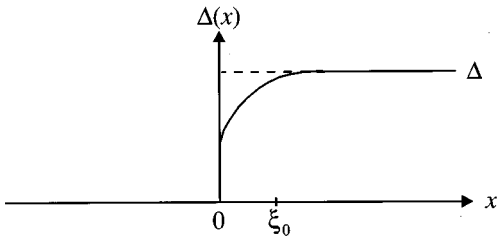

FIG. 3. The proximity effect at a N/C interface (schematic). In the CDW $\Delta(x)$ recovers its bulk value Δ at a distance of the order of ξ_0 from the interface.

will result in an additional potential barrier, which can readily be included by using the transfer matrix **M** as defined in Eq. (15).

The wave functions in both regions are

$$\Psi(x)=\begin{cases}\dfrac{A}{\sqrt{k'}}\begin{pmatrix}1\\0\end{pmatrix}e^{ik'x}+\dfrac{B}{\sqrt{k'}}\begin{pmatrix}0\\1\end{pmatrix}e^{-ik'x}, & x<0\\ \dfrac{C}{\sqrt{k}}\begin{pmatrix}v_k\\u_ke^{-i\varphi}\end{pmatrix}e^{ikx}+\dfrac{D}{\sqrt{k}}\begin{pmatrix}u_ke^{i\varphi}\\v_k\end{pmatrix}e^{-ikx}, & x>0\end{cases} \tag{25}$$

with wave vector $k'=\epsilon/\hbar v_F$ in the normal-metal and $k=\sqrt{\epsilon^2-\Delta^2}/\hbar v_F$ in the CDW region. The wave function in the normal-metal region is decoupled ($\Delta=0$ implies $v_k=1$ and $u_k=0$). Matching the wave functions using Eq. (13) we obtain after some algebra

$$r_{11}=\frac{(1-iZ)u_ke^{-i\varphi}-iZv_k}{(1+iZ)v_k+iZu_ke^{-i\varphi}},$$

$$r_{22}=-\frac{(1+iZ)u_ke^{i\varphi}+iZv_k}{(1+iZ)v_k+iZu_ke^{-i\varphi}},$$

$$t_{12}=t_{21}=\frac{\sqrt{v_k^2-u_k^2}}{(1+iZ)v_k+iZu_ke^{-i\varphi}}, \tag{26}$$

where we have used the relation $\sqrt{k/k'}=\sqrt{v_k^2-u_k^2}$. Figure 4 shows the reflection and transmission probabilities for $Z=0$ and $Z=1$ ($\varphi=0$). Electron states in the gap ($-\Delta<\epsilon<0$)are totally reflected. If $\Delta=0$ the normal reflection and transmission probabilities are obtained: $T=(1+Z^2)^{-1}$ and $R=1-T$. Note that in contrast to the Blonder-Tinkham-Klapwijk model[1] of superconductor junctions the transmission probability depends on the macroscopic phase of the CDW. This phase dependence has important consequences for the quasiparticle conductance, which will be treated in Ref. 12. The determinant of the scattering matrix is

$$\det\mathbf{S}(\epsilon,\varphi)=-\frac{(1-iZ)v_k-iZu_ke^{+i\varphi}}{(1+iZ)v_k+iZu_ke^{-i\varphi}}. \tag{27}$$

For a perfect interface with $Z=0$ the expression obviously does not depend on φ. Therefore, the CDW is not pinned and the translational degeneracy of the CDW is conserved. For $Z\neq 0$ the CDW *is* pinned.

Calculation of the electron density in the normal-metal region ($x<0$) for $Z=0$ yields

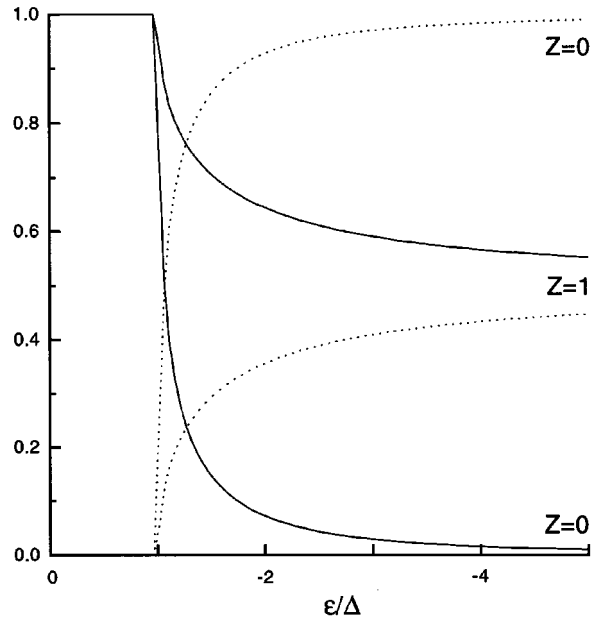

FIG. 4. Reflection (solid) and transmission probabilities (dotted) at the N/C interface for barrier strengths $Z=0$ and $Z=1$ as a function of energy.

$$n(x)=s\left\{\frac{k_F}{\pi}+\int_0^{k_F}2u_kv_k\cos(2kx+\varphi)dk\right\}. \tag{28}$$

We see that the electron density consists of a constant term and a rapidly oscillating term which decays algebraically like $1/x$. The last term is very similar to a Friedel oscillation caused by a potential defect in the electron gas. Here the Friedel oscillation is not induced by an impurity, but by the CDW system, and depends on its phase.[17]

C. C/N/C junction

The coupling of phase-coherent ground states which are spatially separated by a normal metal has strong effects on the physical properties of the system. We will now investigate the mechanism and the consequences of phase coupling in a C/N/C junction. Consider two one-dimensional CDW materials separated by a normal metal with length L, as sketched in Fig. 5(a). As in the previous section we approximate this C/N/C junction by a step model for the pair-potential shown in Fig. 5(b). The spatial dependence of the order parameter is then

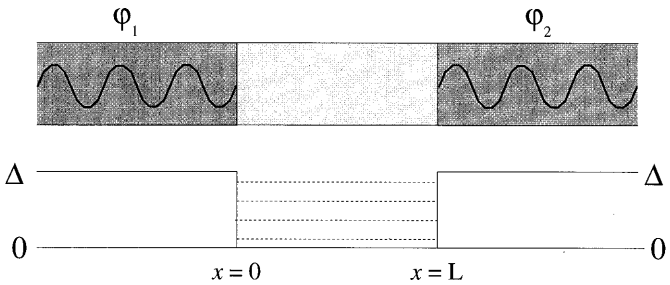

FIG. 5. (a) Schematic picture of the C/N/C junction. (b) Scattering potential which describes a mesoscopic junction. Bound states are formed in the gap.

$$\Delta(x)=\begin{cases}\Delta e^{i\varphi_1}, & x<0\\ 0, & 0<x<L\\ \Delta e^{i\varphi_2}, & x>L.\end{cases} \tag{29}$$

There is a total phase difference, $\varphi=\varphi_2-\varphi_1$, over the junction. For simplicity we assume again that the average electron densities are the same in the normal-metal and the CDW. The energy spectrum of this double junction is given by the eigenvalues of the BdG equation. There will be bound states in the gap and a scattering continuum below and above the gap, which is modified by the presence of the junction.

As before, solving the BdG equations and matching the wave functions results in the reflection and transmission coefficients. The determinant of the scattering matrix is

$$\det\mathbf{S}(\epsilon,\varphi)=-\frac{v_k^2e^{ik'L}-u_k^2e^{-ik'L-i\varphi}}{v_k^2e^{-ik'L}-u_k^2e^{ik'L+i\varphi}}, \tag{30}$$

where k' is the wave vector in the normal-metal region. The energy-phase relation becomes

$$\frac{dE}{d\varphi}=-\frac{1}{2\pi}\int_{-\epsilon_F}^{-\Delta}d\epsilon\left\{1-\frac{v_k^2-u_k^2}{v_k^4+u_k^4-2u_k^2v_k^2\cos(2k'L+\varphi)}\right\}+\sum_n\frac{d\epsilon_n}{d\varphi}. \tag{31}$$

The first term is an integration over the continuous energy spectrum and the sum is taken over all bound states. The second term in the brackets of this equation, which we will call ν in the following, is the factor by which the density of states of the normal region is modified by the presence of the CDW's. The total term is thus the difference in the density of states of the normal region. Note that ν has a maximum when $2k'L+\varphi=2\pi n$ (n, an integer) and a minimum when $2k'L+\varphi=\pi(2n+1)$. The maximum corresponds to the resonant scattering condition

$$\nu_{\max}=\frac{1}{v_k^2-u_k^2}=\frac{\epsilon}{\sqrt{\epsilon^2-\Delta^2}}=\frac{N_{\mathrm{CDW}}(\epsilon)}{N_0(\epsilon)}, \tag{32}$$

where N_{CDW} and N_0 denote the bulk density of states in the CDW and normal-metal regions, respectively. The bound states ϵ_n formed in the gap of this junction are given by the poles of the scattering matrix and satisfy

$$2\arccos\left(\frac{\epsilon}{\Delta}\right)+2k_FL+\frac{2}{\pi}\frac{\epsilon}{\Delta}\frac{L}{\xi_0}+\varphi=2\pi n. \tag{33}$$

The first term is due to the penetration of the gap states into the CDW's. Above Δ the bound states broaden into the resonant scattering continuum. This can be seen from the transmission probability

$$T(\epsilon)=\frac{\left(\frac{\epsilon}{\Delta}\right)^2-1}{\left(\frac{\epsilon}{\Delta}\right)^2-\cos^2\left(\frac{\epsilon}{\pi\Delta}\frac{L}{\xi_0}+\chi\right)}\quad\text{for }\epsilon>\Delta, \tag{34}$$

where $\chi=k_FL+\varphi/2$, which is plotted in Fig. 6. Oscillations with period $\pi^2\xi_0/L$ are identified and explained as a quasi-

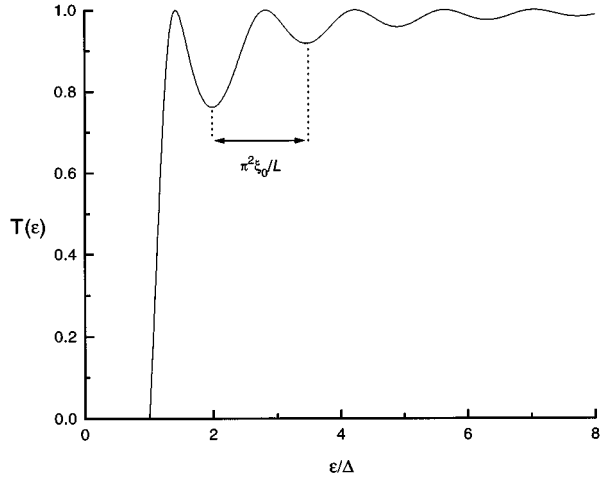

FIG. 6. The transmission probability as a function of energy. Geometrical resonances with period $\pi^2\xi_0/L$ are identified as Tomasch oscillations.

particle interference effect caused by scattering from the gap structure. In the field of superconductivity similar geometrical resonances are known as Tomasch oscillations.[20] The modulation of the quasiparticle conductance could be observed in the d^2V/dI^2 analysis of an I-V transport measurement. It is emphasized that these expressions are very similar to those for the Josephson junction as calculated in Refs. 21–23, where the resonant states correspond to the transfer of a Cooper pair. One crucial difference is that in our system, $dE/d\varphi$, does not express a zero bias electrical Josephson current. The electrical current is zero in a C/N/C junction, since the transmission coefficient from left to right equals the transmission coefficient from right to left. In Sec. IV we will relate $dE/d\varphi$ to a flow of electron-hole pairs, which carry zero charge but momentum Q.

Phase coupling is determined by scattering states in the continuous spectrum ($\epsilon<-\Delta$) and by localized states ($-\Delta<\epsilon<0$). The total energy depends only on the phase difference over the junction. This means that at an ideal interface there is no intrinsic pinning. If one CDW is moved adiabatically, dissipationless sliding CDW transport through the normal region is possible. This is equivalent to a supercurrent flowing in a S/N/S junction. As shown in Sec. III B, an N/C contact will modulate the electron density in the normal metal, which resembles a Friedel oscillation, but depends on the phase of the CDW. The phase coupling in the C/N/C junction can thus be understood as a phase locking of Friedel oscillations, arising from both interfaces. The mechanism is similar to the nonlocal exchange Ruderman-Kittel-Kasuyan-Yosida (RKKY) interaction in magnetic multilayers via spin-density oscillations.[3]

For future experiments it should be relevant to include impurities or defects at the interfaces. We now include two δ function potentials $V(x)=H_1\delta(x)+H_2\delta(x-L)$ at the interfaces of the C/N/C heterostructure, with $L=5\xi_0$. Figure 7 shows the response of phase φ_2 as a function of phase φ_1 for which the energy is minimal ($H_1=H_2$). If φ_1 is changed adiabatically slow in time, the change of φ_2 in time is nonlinear and shows a phase jump.

IV. THREE MESOSCOPIC JUNCTIONS

We have already mentioned similarities between the phase coupling in the S/N/S and the C/N/C junctions. We

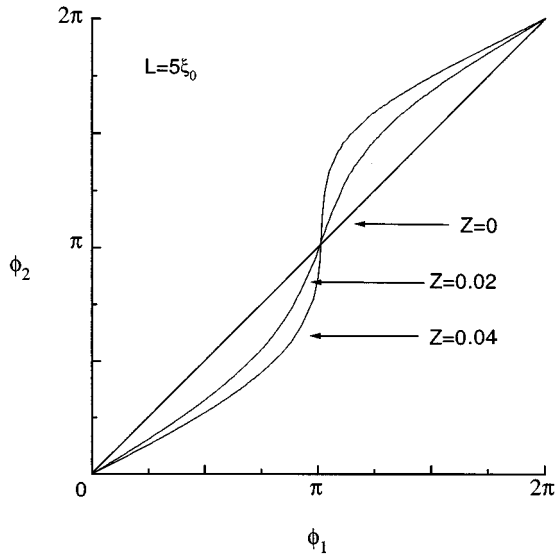

FIG. 7. The response of the phase ϕ_2 to an adiabatic change of the phase ϕ_1 for different impurity strengths Z. The change of ϕ_2 is nonlinear for $Z\neq 0$.

will now investigate these analogies further and also compare them with the ferromagnet/normal-metal/ferromagnet (F/N/F) junction. Mathematically the phase coupling is calculated almost identically for all three systems, namely by solving Bogoliubov–de Gennes type of equations in the three regions and by matching of the wave functions. The physics is very different, however. A phase difference over the junction results in a current. In S/N/S junctions, Andreev scattering generates a supercurrent through the normal metal region in response to a phase difference over the junction.[2] In F/N/F junctions, depending on the width of the normal-metal, nonlocal exchange coupling of the magnetization directions may cause a stable antiparallel (π) coupling via spin-density oscillations.[24] In Refs. 3 and 24 it has been shown that a difference in magnetization moments results in a net spin current flowing through the normal layer. We argue that the phase coupling in the C/N/C junction can be formulated in terms of a momentum current, or to put it differently, by coherent transport of electron-hole pairs.

In Sec. II we have linearized the energy spectrum near the Fermi energy. If we keep the quadratic dependence of the energy dispersion, the BdG equations are given by

$$\begin{pmatrix} H & \Delta \\ \Delta^* & H \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}=\epsilon\begin{pmatrix} f \\ g \end{pmatrix}=i\hbar\,\partial_t\begin{pmatrix} f \\ g \end{pmatrix}, \tag{35}$$

where $H=-\hbar^2\partial_x^2/2m-\epsilon_F+U(x)$ and $\Delta=\Delta(x)\exp(iQx)$. The quasiparticle current $j_{\rm qp}$ can directly be calculated as

$$j_{\rm qp}=\frac{\hbar}{m}\{\mathrm{Im}(f^*\partial_x f)+\mathrm{Im}(g^*\partial_x g)\}. \tag{36}$$

In the approximation that the one-dimensional electron gas is perturbed only in the vicinity of the Fermi energy, a widely used expression for the momentum p per particle is

$$p=\hbar k_F\{|f|^2-|g|^2\}, \tag{37}$$

where the terms in brackets are the difference between right and left going electron states. The force $\partial_t p$ can be calculated using the BdG equation and this procedure results in

$$\partial_t p + \partial_x j_p = 4k_F \mathrm{Im}(\Delta f^* g), \tag{38}$$

where j_p is defined as

$$j_p = \frac{\hbar^2 k_F}{m}\{\mathrm{Im}(f^*\partial_x f) - \mathrm{Im}(g^*\partial_x g)\}. \tag{39}$$

In this one-dimensional model, j_p corresponds to the T_{xx} component of the stress tensor and is equivalent to the flow of x-momentum density in the x direction. Note that this equation only differs by a minus sign from Eq. (36). In bulk CDW systems, $j_{\mathrm{qp}}=0$ at the gap edge $\epsilon=\Delta$, whereas the momentum current $j_p \sim k_F$. This is similar to bulk superconductors where $j_{\mathrm{qp}}=0$, but the electrical current $j_e \sim k_F$. Equation (38) is equivalent to the conservation law for the quasiparticle *charge* in a superconductor.[1] Here it is the conservation law for the quasiparticle *momentum*. The right-hand side is a source (or drain) term connecting the quasiparticles with the condensate. In one dimension j_p is related to the pinning force [Eq. (18)] via

$$\frac{dE}{d\varphi} = -\frac{\hbar}{2} J_p, \tag{40}$$

where the total momentum current $J_p$is the sum over all occupied states $J_p = 1/\hbar k_F \Sigma j_p$.

The phase coupling in the three junctions under consideration can be summarized by the following ''universal'' identities:

$$\text{F/N/F:} \quad \frac{dE}{d\varphi} = -\frac{\hbar}{2} J_s,$$

$$\text{S/N/S:} \quad \frac{dE}{d\varphi} = -\frac{\hbar}{2} J_e,$$

$$\text{C/N/C:} \quad \frac{dE}{d\varphi} = -\frac{\hbar}{2} J_p. \tag{41}$$

The currents are determined by

$$J_s = \frac{\hbar}{m}\sum_k \{\mathrm{Im}(f^*\partial_x g) - \mathrm{Im}(g^*\partial_x f)\},$$

$$J_e = \frac{\hbar}{m}\sum_k \{\mathrm{Im}(f^*\partial_x f) + \mathrm{Im}(g^*\partial_x g)\},$$

$$J_p = \frac{\hbar}{m}\sum_k \{\mathrm{Im}(f^*\partial_x f) - \mathrm{Im}(g^*\partial_x g)\}, \tag{42}$$

where f and g represent spin up and spin down electrons in magnetic junctions, electron and hole like states in the superconductor junctions and right and left going electrons in the charge-density wave junctions. These wave functions are calculated from the following equations

$$\text{F/N/F:} \quad \begin{pmatrix} H_+ & \Delta \\ \Delta^* & H_- \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix} = \epsilon\begin{pmatrix} f \\ g \end{pmatrix},$$

$$\text{S/N/S:} \quad \begin{pmatrix} H & \Delta \\ \Delta^* & -H^* \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix} = \epsilon\begin{pmatrix} f \\ g \end{pmatrix}, \tag{43}$$

$$\text{C/N/C:} \quad \begin{pmatrix} H & \Delta \\ \Delta^* & H \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix} = \epsilon\begin{pmatrix} f \\ g \end{pmatrix},$$

where H_+, H_-, and Δ in the F/N/F junction are defined by $H_\pm = H \pm h_z$ and $\Delta = h_x + i h_y$, with $h_{x,y,z}$ the components of the magnetization vector. The magnetic junction is simpler as far as the self-consistency condition is concerned, because spin-up and spin-down electrons have the same mass, whereas in the superconductor and charge-density-wave junction the effective mass of the quasiparticles and quasiholes has to be taken into account.

V. SUMMARY

We have investigated coherence effects of charge-density waves in mesoscopic systems by solving the CDW Bogoliubov–de Gennes equations with suitable boundary conditions. The scattering matrix theory, using the BdG solutions as a basis, provides a simple method for ground state energy calculations. From this model, transport properties like quasiparticle conductances can easily be extracted.[12] We have studied the N/C interface, with and without an impurity. It is found that an ideal interface will not pin the CDW. The interaction between the impurity potential and the CDW has a strong effect on the transmission and reflection probabilities. The electron density in the normal region is modulated like a Friedel oscillation, but is induced by the CDW and depends on its phase. These Friedel oscillations are the origin of the phase coupling in a C/N/C junction, analogous to exchange coupling in magnetic systems via spin-density oscillations. Tomasch-like oscillations due to quantum size effects are identified in the C/N/C junction. The phase-dependent energy is related to a momentum current, indicating a coherent flow of electron-hole pairs.

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