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Paramagnetic spin splitting of the conductances for tunnel junctions between partially gapped metals with charge density waves and normal metals or ferromagnets

A M Gabovich¹, Mai Suan Li², M Pękała³, H Szymczak²
and A I Voitenko¹

¹ Institute of Physics, Prospekt Nauki 46, 03028 Kiev-28, Ukraine

² Institute of Physics, Aleja Lotnikow 32/46, PL-02-668 Warsaw, Poland

³ Department of Chemistry, University of Warsaw, Aleja Zwirki i Wigury 101, PL-02-089 Warsaw, Poland

E-mail: collphen@iop.kiev.ua (A M Gabovich)

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Abstract

We consider tunnelling between a metal partially gapped by charge density waves (CDWM) and an ordinary metal (M) or a ferromagnet (FM) separated by an insulator (I) in an external magnetic field H . Zeeman paramagnetic splitting is assumed to dominate in the CDWM over orbital magnetic effects. The quasiparticle tunnel current J and relevant differential conductance G are calculated as functions of the bias voltage V . The peaks of $G(V)$, originating from the electron density of states singularities near the charge density wave gap edges, were shown to be split in the magnetic field, each peak having a predominant spin polarization. This effect is analogous to the H -induced splitting of $G(V)$ peaks obtained by Tedrow and Meservey for junctions between normal metals and superconductors (S). Thus, it is possible to electrically measure the polarization of current carriers in such a set-up, although the behaviours of $G(V)$ in the two cases are substantially different. The use of M–I–CDWM junctions instead of M–I–S ones has certain advantages. The absence of the Meissner effect, which weakens the constraints upon the junction geometry and electrode materials, comprises the main benefit. The other advantage is the larger energy range of the charge density wave gaps in comparison to that for superconductors' gaps, so that larger H s may be applied.

1. Introduction

Electron tunnelling between superconducting (S) and ferromagnetic (FM) electrodes in a magnetic field provides a powerful method for studying both electron properties of the

paired states and the spin-split band structure of the itinerant electron spectrum [1, 2]. The main practical goal of those investigations consists in the determination of the electron spin polarization P inside the ferromagnet at its Fermi level, which is defined as

$$P = \frac{N_{\text{FM}-} - N_{\text{FM}+}}{N_{\text{FM}-} + N_{\text{FM}+}}, \quad (1)$$

where $N_{\text{FM}s}$ ($s = \mp$) is the density of states (DOS) of the ‘majority’ (–) or ‘minority’ (+) of electrons at the Fermi level of the FM with spins directed opposite to (along) the direction of the magnetic field H , respectively. At the same time, the corresponding ‘majority’ of electron magnetic moments μ_{el} are directed *along* H , since $\mu_{\text{el}} = -\mu_{\text{B}}^* < 0$. Here, $\mu_{\text{B}}^* = e\hbar/2m^*c$ is the effective Bohr magneton, e is the elementary charge, \hbar is Planck’s constant, c is the velocity of light and m^* is the effective mass of the current carriers in the FM. Definition (1) is not unique, and transport properties may be described, e.g., by a similar combination but involving majority and minority current densities rather than $N_{\text{FM}\mp}$ [3]. A proper choice is important for calculations in specific cases, but for the aspects of the problem discussed here all changes might be reduced to a renormalization of the free parameter P of the theory.

According to the seminal idea of Tedrow and Meservey [1, 4], the polarization P may be expressed in terms of the differential tunnel conductivity $G(V) \equiv dJ/dV$ taken at definite voltages V and measured in a non-zero external magnetic field H . Here J is the tunnel current through a S–I–FM junction (I stands for an insulator). The method should work in this set-up because the initially identical peaks of conductivities $G_-(V)$ and $G_+(V)$ from the two spin subbands shift due to the Zeeman effect in the superconducting films [5] and their amplitudes deform downwards and upwards non-symmetrically when the field is switched on.

Unfortunately, the application of this scheme, promising in principle, led to a deduced P of the wrong positive sign (i.e. the majority of the magnetic moments of tunnelling electrons were found to be in the field direction) for the junctions Al–Al₂O₃–FM, with FM = Ni and Co, whereas the band calculations predicted that the minority spin electrons should give the prevailing contribution to the DOS at the Fermi energy level and, hence, to the overall current [1, 6]. To solve the apparent controversy, a number of theoretical studies were carried out, changing the starting naive picture of the tunnelling process. First, it was recognized that the tunnelling spin-split DOSs for ferromagnets differ from the band ones because the probability of the electron penetration into the barrier region depends on the kind of intermediate electronic states involved [1, 6–8]. The second required modification makes allowance for the non-ohmic (Fowler–Nordheim) character of conductivity caused by the electric field distortion of the primordial barrier’s rectangular shape [9]. Finally, the Zeeman splitting of the $G(V)$ peak in the superconducting electrode is drastically diminished by spin–orbit interactions especially effective for heavy elements, with the respective scattering rate proportional to Z^4 , where Z is the atomic number [1, 10]. Broadly speaking, the modern approaches treat the whole junction as a single entity and take into account the interface states and possible structural disordering [6, 11]. Moreover, one should take into account that d electrons in the FMs may be not only localized but also itinerant, the latter participating in tunnelling [7].

One should also bear in mind that the paramagnetic mechanism of the superconductivity suppression [5, 12–14], with the spin splitting of $G(V)$ being its clear indication, can dominate over the orbital (Meissner) depairing [15, 16] only in special situations. Thin film superconducting electrodes of the Al–Al₂O₃–FM sandwich with the magnetic field parallel to the junction plane exhibit a typical example of such a behaviour, since the orbital depairing quantity $\alpha_{\text{parallel}} = e^2 d^2 DH^2/6\hbar$ is small for thin enough films and a small enough mean free path l [1, 16, 17]. Here d is the film thickness, $D = v_{\text{F}}l/3$ is the diffusion constant,

v_F is the Fermi velocity of the electrons in Al. In the general case, all the listed factors act simultaneously and their interplay is rather complicated.

Hence, it becomes clear that the resources for selecting proper superconducting covers are not very numerous. At the same time, the use of the paramagnetic effect in non-magnetic electrodes to probe the ferromagnetic properties of the counter-electrodes seems quite helpful. Therefore, we propose a new class of tunnelling partners for the ferromagnetic materials, namely, metals partially gapped by charge density waves (CDWs)—CDWMs [18–23]. So, the tunnelling scheme now has the form CDWM–I–FM. An external magnetic field stimulates a paramagnetic effect in the CDWM analogous to that in superconductors [24–26]. On the other hand, the giant diamagnetic (Meissner) response does not appear for CDWMs at all because this state lacks superfluid properties [27, 28]. As for the spin–orbit coupling, which leads to harmful spin flips [10], its role can be diminished by an adequate choice of the light-atom constituents for CDW materials.

But in any case, since the critical temperature T_d of the CDW transition usually is much larger than its superconducting counterpart T_c and the same remains true for the corresponding energy gaps Σ and Δ , a much larger Zeeman splitting can be obtained for CDWMs in comparison to that in superconductors from the viewpoint of the paramagnetic limit. Then, the existing spin–orbital smearing, determined in either case by a dimensionless parameter $b = \hbar/3\Gamma\tau_{so}$ (here Γ means Δ or Σ) [1, 17, 29, 30], would not totally suppress the separation between the $G_+(V)$ and $G_-(V)$ CDW peaks for the same magnitude of the spin–orbital scattering amplitudes \hbar/τ_{so} as in superconductors.

Below, our reasoning is supported by specific calculations of the paramagnetic splitting. It is shown that characteristic features of $G(V)$ for CDWM–I–FM junctions in the magnetic field are unlike those for S–I–FM ones revealing, in particular, much intrinsic asymmetry with respect to the bias voltage.

2. Behaviour of CDW metals in a magnetic field

The properties of the partially gapped CDWM electrode are characterized in the framework of the Bilbro–McMillan model [23, 35, 36], originally applied to CDW superconductors. According to this approach, which describes with equal success the Peierls insulating state in quasi-one-dimensional substances [18, 37] and the excitonic insulating state in semimetals [28, 38], the Fermi surface (FS) consists of three sections. Two of them ($i = 1, 2$) are nested, with the corresponding fermion quasiparticle spectrum branches obeying the equation

$$\xi_1(\mathbf{p}) = -\xi_2(\mathbf{p} + \mathbf{Q}), \quad (2)$$

where \mathbf{Q} is the CDW vector. So, the electron spectrum here becomes degenerate (d) and a CDW-related order parameter appears. The rest of the FS ($i = 3$) remains undistorted under the electron–phonon (the Peierls insulator) or Coulomb (the excitonic insulator) interaction and is described by the non-degenerate (n) spectrum branch $\xi_3(\mathbf{p})$. A uniform dielectric (CDW) order parameter $\tilde{\Sigma}$ appears only on the nested FS sections. The extent to which the FS is dielectrically gapped is described by the parameter

$$\mu = \frac{N_d(0)}{N_d(0) + N_{nd}(0)}, \quad (3)$$

where $N_{d(nd)}(0)$ is the electron DOS at the d(nd) FS section above T_d . In essence, it is a relative portion of the FS, which is gapped and can be determined, in principle, by resistive, specific heat, or optical experiments (see the relevant references and discussion in our review [23]).

The CDWM phase, characterized by a matrix dielectric order parameter $\tilde{\Sigma}_{im}^{\alpha\gamma}$, is described, in the presence of the external magnetic field H and without making allowance for any orbital diamagnetism, by a system of Dyson equations for the normal \mathcal{G}_{ij} temperature Green functions [39]. Latin subscripts in $\tilde{\Sigma}_{im}^{\alpha\gamma}$ correspond to the FS sections, while Greek superscripts reflect the spin structure of the order parameters.

The orbital influence of the magnetic field on CDWM thermodynamics, being not so large as for superconductors, can nevertheless exist, at least in principle. That is, if the nesting conditions are imperfect (which is always the case) and the Zeeman splitting effects are negligible, a transverse magnetic field, which reduces the quasiparticle spectrum dimensionality, results in an increase of T_d . We note that a similar growth was also observed for the critical temperature T_N of the spin density wave (SDW) state [40–42]. Moreover, field-induced SDWs were predicted [40, 43–45] and observed for organic substances [46, 47]. The situation for CDWs is more complicated, since in that case the magnetic field acts not only diamagnetically but also paramagnetically [25, 26].

In any case, for present purposes one can disregard the diamagnetic effect while investigating the spin-split peaks of the differential conductivity for normal metals with CDW distortions. Of course, this does not mean that T_d itself does not depend on H if one goes beyond the approximation adopted in this publication. Since theoretical analysis of a simultaneous action of orbital and Pauli terms may lead to ambiguous results for $T_d(H)$ or $\Sigma(H)$, it is more useful to look at the available experimental data.

For the majority of CDW substances, T_d is of the order of hundreds of kelvins [18, 19, 23, 35] (for SmTe_3 , the estimated $T_d \approx 1300$ K is even substantially higher than the melting temperature of 1096 K [48]) and, as a consequence, the magnetic fields necessary for conspicuously altering T_d are inaccessible to experimentalists. There are, however, several compounds with smaller T_d , for which both the DOS spin splittings and the dependences $T_d(H)$ can be observed relatively easily. First of all, the A15 compound V_3Si with $T_d(H = 0) = 20.15$ K should be mentioned. Its investigation in the magnetic field showed [49] that the field-induced CDW suppression $\Delta T_d \propto -H^2$ and is small indeed: even for a very large $H = 156$ kOe the correction was only 0.6 K. Organic substances $\alpha\text{-(ET)}_2\text{MHg(SCN)}_4$ ($M = \text{K, Tl, Rb, etc}$) with $T_d = 8\text{--}10$ K (at the pressure $p = 1$ bar and $H = 0$) constitute another promising class of CDW objects [26, 50–52] with an interplay of orbital and Pauli effects in the magnetic field [53]. There is even a point of view [54, 55] that the diamagnetic orbital response in those compounds is connected to non-equilibrium persistent currents. It should be particularly emphasized that the quadratic decrease of T_d with H , similar to that in V_3Si , was found [56] for the extremely anisotropic Peierls quasi-one-dimensional metal $\text{Per}_2[\text{Au(mnt)}_2]$ ('Per' and 'mnt' mean perylene and maleonitriledithiolate) with $T_d(H = 0) = 12.2$ K. Later, experimentalists managed to completely suppress the CDW state in this substance [57] and the related one $\text{Per}_2[\text{Pt(mnt)}_2]$ with $T_d(H = 0) = 8$ K [58]. These observations are in accordance with the theory [59, 60] based on a close analogy between CDW insulators and superconductors.

Mathematically, the similarity between paramagnetic properties of two collective states that manifest drastically different kinetic behaviour is described by the famous equation

$$\ln\left(\frac{T}{T_0}\right) + \text{Re} \psi\left(\frac{1}{2} + i\frac{\mu_B^* H}{2\pi T}\right) - \psi\left(\frac{1}{2}\right) = 0, \quad (4)$$

where $\psi(x)$ is the digamma function and T_0 is equal either to T_d for Peierls insulators or to T_c for superconductors. Recall that for the latter the Pauli spin energy term reduces T_c gradually until $T_c(H)/T_c(H = 0)$ becomes 0.566, when the temperature-driven phase transition becomes of the first kind [5, 61–63].

Unfortunately, the type of the CDW phase transition in the magnetic field for $\text{Per}_2[\text{Au}(\text{mnt})_2]$ was not studied in [57, 58]. It is remarkable that after the initial CDW state in $\text{Per}_2[\text{Pt}(\text{mnt})_2]$ has been suppressed above $H \approx 200$ kOe, further enhancement of H leads to the emergence of new field-induced CDW states, which in their turn disappear when H exceeds 400 kOe [58].

All the aforesaid concerned thermodynamics and it does not mean that the magnetic field exerts no influence on various bulk transport properties of the CDWMs. On the contrary, diamagnetic (orbital) effects in extremely high quantizing H may be strongly pronounced, as was shown, e.g., for NbSe_3 , nominally pure and doped by 3d ferromagnetic metals [64–66]. But we emphasize that the observed non-linear and oscillatory galvanomagnetic phenomena reveal themselves for H larger than and comparable to the paramagnetic limit, whereas the spin splitting investigated become apparent and should be studied at smaller fields.

Thus, while studying the Pauli paramagnetic splitting in normal CDW materials, no restrictions from above appear on the H amplitude except the natural limit $\mu_B^* H < \Sigma_0/\sqrt{2}$, where the quantity $\Sigma_0 \equiv \frac{\pi}{\gamma} T_d$ is an amplitude of the CDW order parameter at the temperature $T = 0$, $\gamma = 1.78 \dots$ is the Euler constant. The inequality above represents the paramagnetic limit H_p^{CDWI} for a CDW insulator [24, 25, 50, 67], which in a first approximation has the same form as and similar origin to its counterpart H_p^{BCS} for superconductors. For a *partially gapped* CDWM, the paramagnetic limit is somewhat smaller [68], namely,

$$H_p^{\text{CDWM}} = \frac{\Sigma_0}{\mu_B^*} \sqrt{\frac{\mu}{2}}, \quad (5)$$

because $0 \leq \mu \leq 1$ (see equation (3)). The Pauli paramagnetic suppression of the CDW order parameter is due to the fact that such electron–hole pairing couples the bands (in the excitonic insulator) or the different parts of the one-dimensional self-congruent band (in the Peierls one) with the same spin direction, in contrast to the SDW case, where current carriers with the opposite spin directions are paired. When the magnetic field is switched on, both the congruent FS sections having the chosen spin projection shift either up or down in energy. Therefore, the nesting CDW vectors \mathbf{Q}_+ and \mathbf{Q}_- do not coincide any more, and the initial CDW state is gradually destroyed [24]. One should bear in mind that the limiting value equation (5) is a consequence of the basic mean-field theory making no allowance for specific CDW structures, commensurability effects or rearrangement of CDWs in the magnetic field (see above). If those phenomena are taken into account, actual CDWs may survive the fields larger than H_p^{CDWM} . Indeed, such a robustness of the CDW state was recently observed in $\text{Per}_2[\text{Au}(\text{mnt})_2]$ [69].

In the conjectured absence of the orbital magnetism, the thermodynamics of the CDWM in a magnetic field is similar to that of the Bardeen–Cooper–Schrieffer (BCS) superconductor, where the diamagnetic phase with the homogeneous Δ and the initial T_c survives for low enough T with growing H until H reaches the Clogston–Chandrasekhar value H_p [63, 70] and the first-kind field-induced transition into the normal state occurs. Since we are going to deal with smaller fields, the intriguing problem of the non-homogeneous state [24] analogous to the Larkin–Ovchinnikov–Fulde–Ferrel one in ordinary superconductors for $H \geq H_p$ will be not touched upon. Hence, making allowance for the spin-singlet structure (CDWs) of the matrix self-energy part $\tilde{\Sigma}_{ij}^{\alpha\beta} = \tilde{\Sigma} \delta_{\alpha\beta}$ in the weak coupling limit, we are to consider an equation for the order parameters $\tilde{\Sigma}$ in the case $H = 0$. We assume the function $\tilde{\Sigma}(T)$ to be a BCS-like one, although in experiment it usually shows a ‘generalized’ BCS-like form. That is, in the coordinates $\tilde{\Sigma}(T)/\tilde{\Sigma}(T = 0)$, versus T/T_d , the data follow the Mühlischlegel curve, whereas the ratio $2\Sigma_0/k_B T_d$ essentially exceeds the BCS weak coupling limit (such a behaviour is described by the phenomenological scheme [71]). Here k_B is the Boltzmann constant. For example, in NbSe_3 with its two CDW transitions at $T_d^{\text{low}} = 59$ K and $T_d^{\text{high}} = 145$ K [23, 35],

the respective ratios, as was shown by direct tunnelling studies [72], fall into the ranges of 11.8–14.3 and 11.4–14.4.

3. Current–voltage characteristics. Theory

While examining current–voltage characteristics (CVCs), for the sake of definiteness, the bias voltage V is chosen as the difference between voltages at the itinerant (Stoner) FM and a CDWM: $V \equiv V_{\text{FM}} - V_{\text{CDWM}}$.

It is presumed that for H high enough to produce experimentally resolved splitting of the electron DOS peaks, all domains inside the ferromagnet are completely aligned in the field direction [1]. We also anticipate that the initial bulk polarization of a quasiparticle is preserved during the tunnelling process, i.e. the influence of the FM–I interface on the tunnel current is totally neglected. We fully recognize that, generally speaking, such is not the case, the boundary and disorder effects being very important [2, 3, 6, 11, 31–34]. However, an account of these complications may be postponed until the specific CDWM–I–FM junctions are produced. The main goal of this publication is to consider the very possibility of the new type of counter-electrodes in tunnel junctions for studying magnetic materials.

Making use of the BCS function $\tilde{\Sigma}(T)$ and following the Green function method developed for BCS superconductors by Larkin and Ovchinnikov [73], we calculate a quasiparticle tunnel current $J(V)$ between a ferromagnet and a CDWM. The particular case of $P = 0$ and $H = 0$ was treated in our previous publications that contain necessary technical details [74, 75].

Under an assumption that there is no spin flipping while tunnelling, the overall tunnel current J can be described as consisting of different terms $J_{i\mp}$ having the same form

$$J_{i\mp} \propto \text{Re} \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega \frac{\text{Im} G_{i\mp}^{\text{CDWM}}(\omega' \pm \mu_{\text{B}}^* H) G_{\mp}^{\text{FM}}(\omega \pm \mu_{\text{B}}^* H)}{\omega' - \omega + eV + i0} \quad (6)$$

and corresponding to various combinations of the CDWM and FM spin-dependent temporal Green functions. The upper (lower) sign corresponds to the ‘majority’ (‘minority’) spin orientation, respectively. In the basic approach adopted here, there is no problem with $G_{\mp}^{\text{FM}}(\omega)$. At the same time, there emerge six quantities $G_{i\mp}^{\text{CDWM}}(\omega)$ instead of a unique spin-projection pair $G_{\mp}^{\text{BCS}}(\omega)$ specifying the BCS state [5, 14]. The former can be obtained from the temperature Green functions of the CDWM:

$$\mathcal{G}_{nd}^{\mp}(\mathbf{p}, \omega_n) = \frac{i\omega_n \pm \mu_{\text{B}}^* H + \xi_3(\mathbf{p})}{(i\omega_n \pm \mu_{\text{B}}^* H)^2 - \xi_3^2(\mathbf{p})}, \quad (7)$$

$$\mathcal{G}_d^{\mp}(\mathbf{p}, \omega_n) = \frac{i\omega_n \pm \mu_{\text{B}}^* H + \xi_1(\mathbf{p})}{(i\omega_n \pm \mu_{\text{B}}^* H)^2 - \xi_1^2(\mathbf{p}) - \Sigma^2}, \quad (8)$$

$$\mathcal{G}_c^{\mp}(\mathbf{p}, \omega_n) = \frac{\tilde{\Sigma}}{(i\omega_n \pm \mu_{\text{B}}^* H)^2 - \xi_1^2(\mathbf{p}) - \Sigma^2}. \quad (9)$$

After the straightforward procedure [73, 75], we arrive at the current

$$J(V) = \sum_{f=n,d,c;s=-,+} J_{fs}(V), \quad (10)$$

where

$$J_{n\mp} = \frac{(1 - \mu)(1 \pm P)V}{2eR}, \quad (11)$$

$$J_{d\mp} = \frac{\mu(1 \pm P)}{4eR} \int_{-\infty}^{\infty} d\omega K(\omega, V, T) |\omega \pm \mu_{\text{B}}^* H| f_{\pm}(\omega, H, \Sigma); \quad (12)$$

$$J_{c\mp} = \frac{\mu (1 \pm P) \tilde{\Sigma}}{4eR} \int_{-\infty}^{\infty} d\omega K(\omega, V, T) \text{sign}(\omega \pm \mu_B^* H) f_{\pm}(\omega, H, \Sigma). \quad (13)$$

Here

$$K(\omega, V, T) = \tanh \frac{\omega}{2T} - \tanh \frac{\omega - eV}{2T}, \quad (14)$$

$$f_{\pm}(\omega, H, \Sigma) = \frac{\theta(|\omega \pm \mu_B^* H| - \Sigma)}{\sqrt{(\omega \pm \mu_B^* H)^2 - \Sigma^2}}, \quad (15)$$

R is the ‘normal state’ (above T_d) resistance of the junction, $\theta(x)$ denotes the Heaviside theta function. Note that the signs in the variables $\omega \pm \mu_B^* H$, involved in the current components, are inverse to s . It should be borne in mind that the current components depend on the phase φ of $\tilde{\Sigma} = \Sigma e^{i\varphi}$, whereas the thermodynamic properties of CDW superconductors are degenerate with respect to φ [39, 76]. We suggested that quasiparticles originating from all FS sections make their contributions to the total current proportionally to the DOS of the relevant section. That means an absence of any kind of directional tunnelling, which is possible, in principle [77–82]. Such an assumption may be justified by an inevitable spatial averaging over CDW domains with different wavevector orientations.

The important difference between the problem at hand and its counterpart appropriate to the BCS superconductivity is the emergence of the terms $J_{c\mp}$. They reflect the existence of the electron–hole pairing [23, 28], originating from the interband Green function \mathcal{G}_c (see equation (9)), and have a different structure to the remaining terms induced by conventional normal Green functions \mathcal{G}_d and \mathcal{G}_n (see equations (7) and (8) as well as detailed discussion in [83, 84]). To a large extent, \mathcal{G}_c is analogous to the anomalous Gor’kov Green function \mathcal{F} , which, however, determines a Josephson rather than quasiparticle tunnel current [85]. The appearance of terms (13) leads to the drastic *asymmetry* of the CVC of non-symmetrical tunnel junctions involving CDWMs [84] as opposed to *symmetrical* CVC for similar non-symmetrical junctions based on conventional superconductors [86, 87]. In incommensurate CDWMs, the order parameter phase φ is arbitrary [37]. However, to understand the picture qualitatively it is enough to restrict oneself to the particular case of commensurate CDWs, when φ is either 0 or π . Then, relevant equations describe tunnelling between, e.g., excitonic insulators [28, 38], for which the phase is pinned by the interband four-fermion interaction [88]. In principle, another situation is also possible, when a tunnel contact area is large enough to span several zones with varying φ . As a consequence, term (13) would be averaged to some extent and the CVC asymmetry would be substantially reduced. Nevertheless, even then the distinctions from superconducting junctions would be significant due to the existence of n FS sections. Henceforth, we shall consider only the most interesting cases with $\varphi = 0$ or π .

It should be noted that the very existence of the CVC-symmetry-breaking phase-dependent contributions, such as our term J_c (see also similar terms in [74, 75, 84, 89–98]), to the quasiparticle current were discarded in some earlier publications dealing with tunnelling between electrodes with CDWs [99, 100]. In particular, the tunnel current terms dependent on the left-or right-hand-side φ s were rejected [99] as artefacts of the tunnel Hamiltonian approach, because they ‘unphysically’ depend on the CDW location in the bulk. This point of view is not correct, since the relevant calculations based on the microscopic method [85, 101] result in wiping out the disputed terms only by means of averaging over the potential barrier values randomly distributed over the junction plane.

At the same time, a similar procedure can be easily carried out in the simple tunnel Hamiltonian approach [85, 86]. The validity of our approach stems from the calculations of the tunnel conductances $G(V)$ in CDW insulator (CDWI)–I–M junctions [91–93] carried out

on the basis of the generalized Bogoliubov–de Gennes equations [102], previously applied to superconductors [103]. (The account of the original Bogoliubov–de Gennes approach can be found in [15, 101].) It turned out that for the interfacial barrier $W\delta(x)$, where $\delta(x)$ is the Dirac delta function, the phase dependence of the $G(V)$ is preserved for *arbitrary* non-zero values of the dimensionless barrier strength $Z_{\text{BTK}} = W/\hbar v_F$ [91–93]. The tunnel Hamiltonian results for contacts involving CDWs [74, 75, 84, 94–98] can be straightforwardly reproduced for $Z_{\text{BTK}} \rightarrow \infty$, similarly to the situation for superconducting junctions [103]. At the same time, in the latter case $G(V)$ does not depend upon the phase φ for isotropic superconductors [85], contrary to what is appropriate to CDWM–I–M junctions. It is remarkable that tunnel junctions involving anisotropic superconductors demonstrate the dependences of $G(V)$ on the angles between the tunnel direction and the crystalline axes [104].

The qualitative distinction between CDW- and superconductor-based junctions consists in the different meaning of the phase φ for the corresponding order parameters. Indeed, the Fröhlich current density j , associated with the CDW motion, is proportional to the temporal, t , phase derivative $d\varphi/dt$, whereas the concomitant electron density change δn varies directly with $d\varphi/dx$, x being the coordinate along the Peierls chain [37, 105]. On the other hand, just the opposite happens in superconductors (and superfluids): $v_s \sim \nabla\varphi$ and $n_s \sim d\varphi/dt$, where v_s and n_s are the superfluid velocity and density, respectively [85, 106]. These distinctions are related to the fact that superconductors are described by the so-called off-diagonal long-range order (ODLRO) and Gor’kov Green functions \mathcal{F} , while CDWs are described by the diagonal long-range order (DLRO) and ‘normal’ Green functions \mathcal{G} (see the discussion in [23, 28, 38, 107]). That is why the phase φ appears explicitly in the expressions for tunnel currents in CDWI–I–M and CDWM–I–M junctions [74, 75, 84, 89–98]. The phase is pinned by a boundary of the CDWI (or the CDWM), thus inducing a position- and phase-dependent force on the CDW [93, 102]. As was mentioned above, the quantity φ for the Peierls insulator may take an arbitrary value at random. In the excitonic insulator, the randomness also arises but the choice is restricted to 0 or π . This result is adequately described both by the Bogoliubov–de Gennes–Visscher–Bauer approach and the tunnel Hamiltonian method. The situation when the tunnel junction properties are sensitive to the phases of either or both CDW order parameters is not at all weird. This junction can be considered as an analogue of a Josephson one with the main difference that the Josephson current flows between two superconductors, while the *quasiparticle* current J_c may also link one normal and one CDW electrode. In actual practice, the tunnel current originates from a CDW superficial area, which, nevertheless, preserves the CDW properties (see, e.g., [23, 72, 108–110]).

The dependence on φ of the quasiparticle current $J(V)$ in the framework of the tunnel Hamiltonian approach and when the potential barrier at the interface between the CDWM (CDWI) and the insulating interlayer is infinite is not at all strange if one looks at this phenomenon from a more general viewpoint. Indeed, the partial coherence survival obtained in this work is to some extent similar to the incomplete suppression of the quantum-mechanical Friedel oscillations [111] at the metal–vacuum interface in the simple non-self-consistent infinite-barrier [112] and semi-classical infinite-barrier [113] models (see a discussion of the relationship between these models in [114, 115]). Although metal electrons in the framework of these models do not penetrate into vacuum, an interface-induced oscillating exchange–correlation hole does exist in such a metal, so the deviation of the electron density $n(z)$ from its bulk asymptotics is proportional to $3j_1(2k_F z)/2k_F z$ [112, 116, 117]. Here $j_1(x)$ is the spherical Bessel function, k_F is the Fermi wavenumber and z is the distance from the metal–vacuum interface. The equation $n(z) = 0$ holds true at the interface. A similar kind of a hole also survives in the semi-classical approach when the barrier is finite and electrons spill out beyond the metal [118]. Of course, the characters of the exchange–correlation hole near the

interface are different for finite and infinite barrier heights. In particular, $n(z = 0) \neq 0$ for finite barriers. This means that the phase of the static Friedel wave changes depending on the interface properties, whereas the quantum-mechanical interference persists. Returning to the CDWM-based junctions, it is natural to expect that for each type of the barrier the phase φ entering equation (13) should have its proper value. However, the terms $J_{c\mp}$ should not disappear unless contributions of different current-carrying channels are averaged out.

Therefore, the phase averaging may or may not occur in specific experiments. But if it holds, the apparent properties of the tunnel junction are radically modified. It is worth mentioning that the current component proportional to $\cos(\varphi_1 - \varphi_2)$ in CDWM–I–CDWM junctions [96, 99, 100, 119] should be averaged out on the same basis as the other phase-dependent terms, contrary to what was stated in [99, 100]. Nevertheless, if the phases of the CDW order parameters hold constant in each electrode for the CDWM–I–CDWM set-up or only one constant phase exists in the corresponding electrode of the CDWM–I–M junction, the J_c component retains its primordial unaveraged form (see equation (13) and respective expressions in [75, 119]). There is some evidence that the aforementioned CVC-symmetry-breaking terms might have already been observed in a number of tunnel structures involving CDWMs (see the discussion in [23, 84, 120, 121]). In this paper we restricted ourselves to the ‘pure’ situation, where there is no need to average over the phase values, although the possibility of the opposite ‘dirty’ case, when J_c totally disappears, should be kept in mind. We stress that the predicted polarization-dependent spin splitting survives *any kind* of phase averaging, including the scenario of different transfer-matrix elements [99, 100].

Conductivities $G_{fs}(V) = dJ_{fs}/dV$ can be obtained by differentiating relevant equations (11)–(13). At $T = 0$, the corresponding analytical expressions read

$$G_{n\mp}(V) = \frac{(1 - \mu)(1 \pm P)}{2R}, \quad (16)$$

$$G_{d\mp}(V) = \frac{\mu(1 \pm P)}{2R} \text{sign}(V) (eV \pm \mu_B^* H) f_{\pm}(eV, H, \Sigma), \quad (17)$$

$$G_{c\mp}(V) = \frac{\mu(1 \pm P)\tilde{\Sigma}}{2R} \text{sign}(V) f_{\pm}(eV, H, \Sigma). \quad (18)$$

Naturally, the sum of the G_n terms gives the constant $\frac{(1-\mu)}{R}$.

4. Numerical results and discussion

Below, we show the results obtained for the dependences of the dimensionless conductance RdJ/dV of the CDWM–I–FM junction on the dimensionless bias voltage eV/Σ_0 . The dimensionless parameters of the problem are the reduced external magnetic field $h = \mu_B^* H/\Sigma_0$, the reduced temperature $t = k_B T/\Sigma_0$ and the polarization P . The key result of this paper is represented by figure 1 for $\tilde{\Sigma} > 0$. It is readily seen that $G(V)$ is highly asymmetrical, contrary to the symmetrical patterns appropriate to tunnel junctions involving superconductors no matter whether those junctions are symmetrical or not [86, 87]. Mathematically this stems from an almost total compensation between $G_d(V)$ and $G_c(V)$ peculiarities at voltages of one sign and their enhancement at voltages of the other sign (for the adopted choice $\tilde{\Sigma} > 0$, this means negative and positive V , respectively). In the absence of the external magnetic field and spin polarization, such an asymmetrical behaviour of $G(V)$ was obtained by us earlier [75, 84, 121]. When H is switched on, the electronic DOS peak splits as in the case of superconductors [1, 17]. The spin splitting is noticeable, however, only for one CVC branch ($V > 0$ in the case $\tilde{\Sigma} > 0$ —the other branch contains only remnants of the gap-related features; also see below). Thus, a simple algebraic procedure of Tedrow and Meservey for finding P

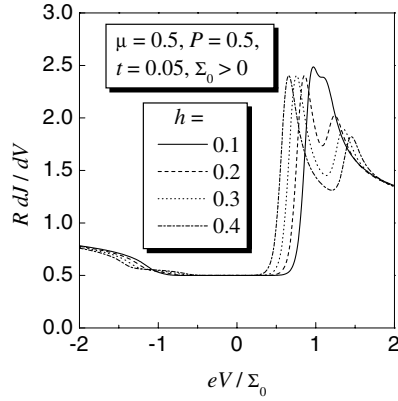


Figure 1. Dependences of differential conductances on the bias voltage V across the tunnel junction made up of a charge density wave metal and a ferromagnet for various external magnetic fields H . See the explanations in the text.

from a set of G values measured for certain V and H , successful for S–I–FM junctions [1, 4], seems to fail for CDWM–I–FM ones, because this method needs the values of conductances on both voltage branches. Nevertheless, the advantage of the set-up, proposed here for detecting spin-polarization-induced changes, consists in the amplification of the spin-splitting effect for one CVC branch and a larger scale of Σ in comparison to Δ .

The dependences $G(V)$ are very sensitive to the value of P . Moreover, they crucially depend on the sign of $\tilde{\Sigma}$ in the CDWM. Let us first consider the case $\tilde{\Sigma} > 0$ (figure 2, panel (a)). One can see how the phenomenon of spin splitting reveals itself under the action of the magnetic field when a CDWM constitutes a tunnel junction with a non-magnetic electrode ($P = 0$) and how this picture is distorted for a ferromagnetic counter-electrode ($P \neq 0$), with the minority spin peak, which is positioned further from zero bias than the majority one, disappearing with increasing P , so that for the complete polarization ($P = 1$; this limit is attainable in half-metallic ferromagnets [122–125]) only one (majority) peak survives.

When $\tilde{\Sigma} < 0$ (figure 2, panel (b)), the minority spin peak disappears with increasing P , similarly to the opposite case for $\tilde{\Sigma} > 0$, but now it is situated closer to the zero bias than the majority one. Hence, the ‘modified’ symmetry relationship

$$G(-\tilde{\Sigma}, V) = G(\tilde{\Sigma}, -V), \quad (19)$$

obtained [84, 121] for junctions involving normal or superconducting CDW electrodes and non-ferromagnetic normal metal counter-electrodes (cf $P = 0$ curves on both panels) is no longer valid. Then different signs of $\tilde{\Sigma}$ can be distinguished by CVC measurements. It is worth underlining once more that the actual $\tilde{\Sigma}$ sign for a specific junction might occur at random, induced by unpredictable fluctuations, since the bulk thermodynamic free energy of normal or superconducting CDW metals does not depend on this sign [39, 76, 126].

One should also bear in mind the possibility of CVC fluctuation-induced ‘symmetrization’ if a hypothetical small extra term $\delta\hat{H}$ proportional to $\tilde{\Sigma} \text{sign}(eV)$ exists in the system Hamiltonian [75]. Then the measured CVC would consist of different bias branches for $\tilde{\Sigma} > 0$ and $\tilde{\Sigma} < 0$ cases, respectively. For non-magnetic electrodes, this phenomenon, due to equation (19), might result in a totally symmetrical CVC (see figure 3, dashed curves). But for $P \neq 0$, relation (19) is not fulfilled and the non-symmetric form of CVCs becomes unavoidable (solid curves). The infinitesimal term $\delta\hat{H} \propto \tilde{\Sigma} \text{sign}(eV)$ may lead to an unusual crypto-CDW

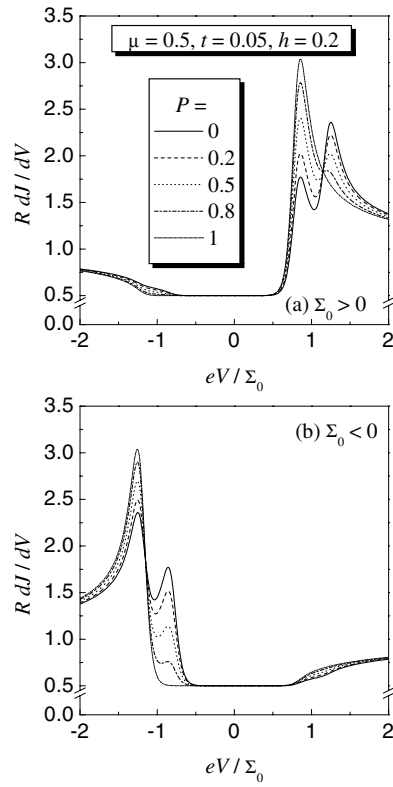


Figure 2. The same as figure 1 but for various polarizations P of electrons on the FM Fermi level. Panels correspond to different signs of the dielectric order parameter $\tilde{\Sigma}$ of the CDWM. See the explanations in the text.

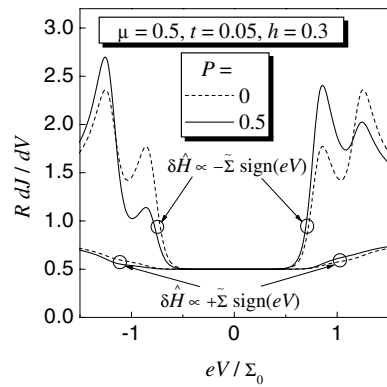


Figure 3. The hypothetical ‘symmetrization’ effect for the CDWM–FM tunnel junction. See the explanations in the text.

situation, when observed CVCs possess almost inconspicuous peculiarities, although the amplitude Σ of the CDW order parameter $\tilde{\Sigma}$ might be arbitrarily large.

It is obvious that all many-body features discussed above are due to the FS gapping, so that when the gapping degree μ decreases, the spin splitting and the very $G(V)$ peculiarities at

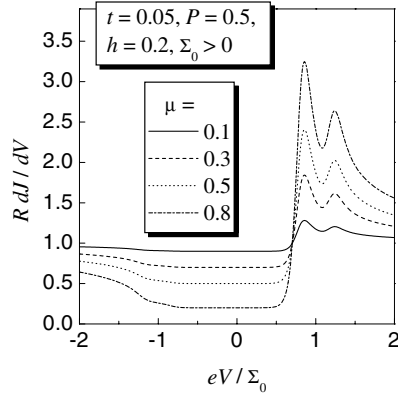


Figure 4. The same as in figure 1 but for various degrees μ of the Fermi surface gapping in the CDWM.

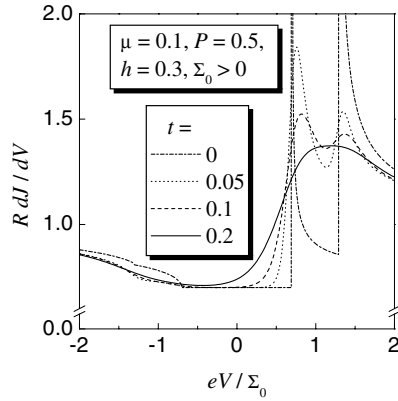


Figure 5. The same as figure 1 but for various temperatures T .

$eV = \Sigma \pm \mu_B^* H$ are reduced and finally disappear, as is demonstrated in figure 4. The control parameter μ can be changed *in situ*, e.g., by an external pressure. Furthermore, CVCs might be a sensitive probe of μ .

The smoothing effect of the temperature is shown in figure 5. The Zeeman splitting already becomes unobservable at a relatively small value $t = 0.2$. However, CDW metals with T_d s of the order of 10–15 K are now available [51, 57] with the corresponding destructive magnetic fields $H \approx 180$ –270 kOe, which are attainable experimentally. Hence, the separation between the gap-induced peaks of $G(V)$ becomes so large for H slightly below the respective paramagnetic limit H_p^{CDWM} that temperatures required to detect paramagnetic effects will be quite reasonable from the technical point of view.

Thus, we have predicted a new type of the tunnel junction, where magnetic field-driven splitting of the differential conductivity peaks is to appear. The splitting has a paramagnetic (spin) origin and its very existence is ensured by the correlative gap Σ appropriate to the material of one of the electrodes. The spectrum of specific tunnel processes may be very rich because the current components depend on the CDW phase in this electrode. If the counter-electrode is ferromagnetic, its polarization P should influence the resulting $J(V)$ and $G(V)$ in the manner similar to but not coinciding with that for the sandwich involving superconductors [1].

To be certain that the predicted spin splitting can be observed, let us consider the spin-orbit smearing in 2H-NbSe₂ with the superconducting critical temperature $T_c = 7.2$ K and $T_d = 33.5$ K [23] and compare it with that in Al where a clear-cut spin-splitting effect was found [1]. We shall confine the consideration for 2H-NbSe₂ to the CDW-induced peaks only. The spin-orbit scattering in superconductors is governed by a single parameter $b = \hbar/(3\tau_{so}\Delta) \propto Z^4/\Delta$, where \hbar/τ_{so} is the spin-orbit scattering rate, Z is the material atomic number and Δ is the superconducting gap. For Al, $Z_{Al} = 13$, $\Delta_{Al} \approx 0.4$ meV and $b_{Al} \approx 0.05$, while even the value of 0.2 ensures a satisfactory spin splitting of the Δ -driven peaks [1, 17]. On the other hand, using the same ideas, $b_{2H-NbSe_2} \propto Z_{Nb}^4/\Sigma$ for 2H-NbSe₂, where $\Sigma \approx 34$ meV is the measured dielectric gap [127] and $Z_{Nb} = 41$ ($Z_{Se} = 34$, which may only improve our estimation). Assuming the elastic scattering rates to be of the same order of magnitude in the two materials, we obtain $b_{2H-NbSe_2} \approx 1.2b_{Al} \approx 0.06$. Thus, even if the spin splitting of the Δ -induced peaks in 2H-NbSe₂ is smeared, that of the CDW-triggered ones should remain resolved—even more so because the superconductivity- and CDW-induced CVC peaks are well separated from one another (cf the values of T_c and T_d for 2H-NbSe₂ quoted above).

One can indicate several other possible candidates for the CDW partner of FMs in tunnel sandwiches. These are organic CDW metals α -(ET)₂MHg(SCN)₄ ($M = K, Tl, Rb$) [26, 51] and Per₂[M(mnt)₂] ($M = Au, Pt$) [57, 58]. The main weak point of those materials is the presence of heavy elements Hg, Tl, Au or Pt, which is dangerous because of a possible spin-orbit smearing of the spin-split $G(V)$ peaks. A two-leg ladder compound Sr_{14-x}Ca_xCu₂₄O₄₁ also seems very promising. Really, Ca doping alters T_d and Σ over a remarkably wide range from 210 K and 130 meV, respectively, for $x = 0$ down to 10 K and 3 meV for $x = 9$ [128].

On the whole, the application of the fruitful ideas, earlier developed for superconductors [1], to normal partially CDW-gapped metals seems useful for studying those strongly correlated objects.

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