Vortices in density-wave systems subject to transverse electric fields

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In this paper we predict many interesting properties of vortices in highly anisotropic density wave systems subject to strong transverse electric fields. We mainly concentrate on ground state properties. Besides electric field-induced vortices we consider also thermally activated vortices. A different type of temperature-driven transition between two different phases of density waves in strong fields is predicted and several properties of those phases are reported. [S0163-1829(98)09035-3]

I. INTRODUCTION

It is now well realized that the dynamics of topological defects plays an important role in low dimensional electronic systems. In a particular case of density wave (DW) ground states (for a review, see Ref. 1) it was found that topological defects are responsible for such interesting phenomena as the generation of narrow-band noise[2] and nonlinear current-voltage characteristics in strong fields (the phenomenon associated with the so-called ''phase slippage'').[3,4] More recently, quantum phase slip through creation of vortices was proposed[5] to explain low-temperature properties of the spin-density wave compound $(TMTSF)_2PF_6$.[6,7]

This paper was originally initiated by the prediction[8] that DW systems should possess a phase in strong electric fields applied transverse to the direction of highest conductivity. This phase was called a ''mixed state'' in analogy with the mixed state of type-II superconductors, and was characterized by the presence of vortices. We have undertaken an extensive study of the predicted transition. The possibility of transverse electric field-induced transition to metallic state (type-I-like) was also investigated and a temperature-driven transition between type-I and type-II regions of the phase diagram was predicted. We report these findings here as well as some interesting anticipated properties of the above-mentioned phases such as, e.g., nonexponential screening of electric fields by DW systems in a mixed state.

II. GINSBURG-LANDAU THEORY

We adopt a macroscopic mean-field description of the dynamics of DW systems and make use of a (time-independent) Ginsburg-Landau free energy[1] which is a functional of complex order parameter $\Delta(\mathbf{r})=|\Delta(\mathbf{r})|\exp(i\phi)$, the absolute value of which is a DW gap in the electronic spectrum. For the case of a highly anisotropic system with an open Fermi surface, $\mathbf{k}=[\pm k_F(1+\gamma\cos(bk_y)],k_y,k_z)$ (here x is the direction of highest conductivity—usually the direction along conducting chains, y is the direction of strongest Fermi surface wrapping, γ is the anisotropy parameter, and b is lattice constant along y; we neglect dispersion along z], this functional is[9]

$$F_{inhom}=\int d\mathbf{r}\,\frac{K}{2|\Delta_0|^2}[|\partial_x\Delta|^2+\gamma^2|\partial_y\Delta|^2]. \qquad (1)$$

We would like to emphasize the fact that the two terms in F_{inhom} are of totally different origin. As is well known,[1] in the system described above a (charge or spin) density modulation appears with the wave vector: $\mathbf{q}=\mathbf{q}_0=(2k_F,\pi/b,0)$: $\rho\propto\mathrm{Re}\,\Delta\exp(i\mathbf{q}_0\mathbf{r})$. A spatial variation of Δ gives rise to the effective shift in $\mathbf{q}$ by $\delta\mathbf{q}=\vec{\nabla}\phi$ where ϕ is the phase of the complex order parameter. Thus the gap is developed at the wave vector which is slightly off its optimal value $\mathbf{q}_0$. This costs extra energy: $\delta E\propto|\delta\mathbf{q}|$—it is linear with $\delta\mathbf{q}$ which is quite costly for small deviations. Instead the system rearranges its *electron density* in such a way that *locally* $2k_F$ coincides with the new DW wave vector. There is no more linear contribution to the energy, however another contribution arises—the energy of the nonhomogeneous electron density distribution. But the fact is that this density (per chain) is[1]

$$\rho=\frac{1}{\pi}\partial_x\phi \qquad (2)$$

and the extra energy is $\delta E\propto\rho^2\propto(\delta q_x)^2$—it is *quadratic* in δq_x and therefore wins for small distortions of DW gap. This phenomenon is usually described as follows: ''particle density follows the variations of the gap.'' At the same time the gradient in y direction does not lead to any change in the local charge density; its contribution to the free energy is of purely elastic character.

In this paper we shall be interested in the response of DW system to external *electric* fields. We take account of the effect of electric field by introduction of the following term into the free energy functional:[8]

$$F_{el}=\int d\mathbf{r}\left[Je\rho\varphi-\frac{1}{8\pi}(\epsilon|\vec{\nabla}\varphi|^2+\lambda_{qp}^{-2}\varphi^2)+\varphi\rho^{ext}\right]. \qquad (3)$$

Here the first term describes coupling of the electric field to the charge induced by DW distortion, the term in parentheses represents energy associated with electric field itself and with the coupling of electric field to free charge carriers excited over the DW gap. The last term represents the interaction of electric field with external charges.[11] Strictly speaking, Eq. (3) is the *action* of the system taken with a minus sign. However, we shall use the term ''free energy functional'' to denote a functional of which an extremum determines the ground state. We also emphasize that electric field couples only to x component of the gradient of the gap—only this component induces electric charge.

An important point here is that our action is essentially different from that of Ref. 8 in that it contains wave-vector-dependent dielectric constant $\epsilon=\epsilon(k)$. It appears because the ground state of DW, in complete analogy with the low-T ground state of *semiconductors*, is highly polarizable due to excitations of *virtual* electron-hole pairs. This should not be mixed either with the screening due to thermally excited quasiparticles, nor should it be mixed with the screening due to spatial distortion of the order parameter (see below). We stress that this dielectric function is *generic* for a gapped electronic system. It can be calculated using simple anisotropic two-band semiconductor model[1]

$$\epsilon(k)\sim\frac{\lambda_{TF}^{-2}}{k^2+\xi(k)^{-2}}. \tag{4}$$

Here, λ_{TF} is the Thomas-Fermi screening length in the metallic state, and $\xi(k)$ is anisotropic coherence length in DW state. [The value $\epsilon(0)$ is usually huge: for instance $\epsilon(0)\sim10^5$ for $(TMTSF)_2PF_6$]. Now we turn to the analysis of the response of DW systems to external electric fields.

III. WEAK FIELDS

Density wave is the state of broken translational invariance. In the absence of external fields the phase of the order parameter $\Delta=|\Delta|\exp(i\theta)$ is the so-called degeneracy parameter: the free energy is globally $U(1)$ invariant—it does not change if we make a global substitution $\theta\rightarrow\theta+$const which corresponds to a homogeneous displacement of the density wave along the x axis. Consequently, there is a *phason* (Goldstone) gapless mode associated with this degeneracy. At the same time the orthogonal *amplitudon* mode, in which $|\Delta|$ is varied, has a gap in the spectrum at $k=0$. Therefore we expect that in the limit of weak fields the response of the system is given by the excitation of phason mode only. Thus we set $|\Delta|$ to be constant. After Fourier transform,

$$\begin{aligned}F_{inhom}+F_{el}&=\int d\mathbf{r}\bigg[\frac{Kk_\gamma^2}{2}\bigg|\theta_k\bigg|^2+Je\varphi_k ik_x\theta_{-k}\\&\quad-\frac{1}{8\pi}(\epsilon k^2+\lambda_{qp}^{-2})\bigg|\varphi_k\bigg|^2+\varphi_k\rho_{-k}^{ext}\bigg]\\&=\int d\mathbf{r}\bigg[\frac{Kk_\gamma^2}{2}\bigg|\theta_k-i2ek_x\varphi_k/v_Fk_\gamma^2\bigg|^2\\&\quad-\frac{1}{8\pi}(\epsilon k^2+\Lambda_k^{-2})\bigg|\varphi_k\bigg|^2+\varphi_k\rho_{-k}^{ext}\bigg]\end{aligned}$$

$$\Lambda_k^{-2}=\lambda_{qp}^{-2}+f_s\lambda_{TF}^{-2}\frac{k_x^2}{k_\gamma^2}, \tag{5}$$

the minimization with respect to θ_k becomes trivial. Then the remaining effective action for the electric field leads to an anisotropic screening length λ. Screening length in the y direction is $\lambda_y=\sqrt{\epsilon(\lambda_{qp}^{-1})}\lambda_{qp}$ and is due to the interaction of the electric field with quasiparticles excited over the gap. On the other hand, screening in the x direction is now determined by both quasiparticles and phasons leading to screening length $\lambda_x=\lambda_{TF}$.[12] This is again a manifestation of the fact that only the phason mode along the x direction couples to the electric field.[13]

IV. STRONG FIELDS

As we have just seen, electric fields in the x direction (along the chains) are screened at the short lengths, $\sim\lambda_{TF}$, at all temperatures. In contrast to that, the E_y component of the field can penetrate far enough into the bulk since its screening is determined by thermally excited quasiparticles, the concentration of which is exponentially decreased at low temperatures. However in strong electric fields the situation changes: Δ can no longer be considered constant and it may be energetically favorable for the system to expel the electric field from the sample by spatial variation of the magnitude of the gap.[14] First, it's obvious that in the limit $E_y\rightarrow\infty$ the state of the system is metallic. A simple argument for this is that in competition between condensate energy $-n(\epsilon_F)\Delta^2/2$ [here $n(\epsilon_F)=N_\perp/\pi v_F$ is density of states at the Fermi level, $N_\perp$ is the density of chains in the plane perpendicular to the chains] and electrostatic energy $ED/8\pi$ the latter always wins in the limit of strong fields: the gap vanishes giving rise to screening. Thus in the region of strong fields there is a thin layer near the edge of the sample in which the state is metallic. The electric field in this layer is screened at the distance $\sim\lambda_{TF}$. However, taking into account that actually the continuous model used here is not applicable at such small distances, one should substitute λ_{TF} for interchain distance. This corresponds to a metallic layer with the thickness of as small as a single interchain distance. However, in the bulk the electric field is absent and the DW state is restored.

Thus we establish that there must exist a critical value of E_y for which a transition occurs from DW to some other phase. As the field is increased from small values, two possibilities may occur: Δ can jump to a smooth configuration (type I) or a configuration with topological defects[8] (type II). The latter means that the ground state is characterized by the presence of vortices—centers the in-plane circulation of the phase of the order parameter around which is nonzero. These two possibilities correspond to the two types of superconductors in a magnetic field. An ordinary isotropic superconductor can be distinguished between these two types by the evaluation of the Ginsburg-Landau parameter $\kappa=\lambda/\xi$. Values $\kappa<1/\sqrt{2}$ and $\kappa>1/\sqrt{2}$ correspond to type I and type II, respectively. In our case, this simple argument is not applicable since DW materials are usually highly anisotropic. Indeed, usually along the x direction one has $\lambda_x\ll\xi_x$ whereas along the y direction either $\lambda_y\ll\xi_y$ and $\lambda_y\gg\xi_y$ can hold depending on temperature: λ_y exponentially increases with decreasing temperature (see below for a more detailed discussion). Instead we shall use a more physical argument to decide between type I and type II. Namely, we shall evaluate the critical field for these two cases. Then we can argue that the system will make a transition to the state for which the critical field is lower.

A. Type I

The critical field for this case can be obtained by equating condensate and electrostatic free energy densities:

$$\frac{ED}{4\pi}=\frac{1}{2}n(\epsilon_F)\Delta_0^2,$$

$$D_c^I=\frac{\Delta_0}{2e\lambda_{TF}}\sim\frac{d_0}{\xi_x\lambda_{TF}}. \tag{6}$$

Here we have introduced $d_0=v_F/2e$—a parameter with the dimensionality of the electric dipole moment (see below). We use the value of the dielectric constant $\epsilon\sim 1$ because the metallic breakdown will occur in a thin layer near the boundary with the thickness $\sim\lambda_{TF}\ll\xi_y$—polarization will not develop at such small scales.

B. Type II—vortices

First of all let us clarify what a vortex is in a DW system. As was mentioned above the phase θ of the complex order parameter $\Delta=|\Delta|\exp(i\theta)$ is the degeneracy parameter of the state with broken translational symmetry. The order parameter, as a function of coordinates, should be univalued. This implies that, as we travel along a closed contour, the phase of the order parameter can get an increment $2n\pi$ where n is integer called *winding number*. The corresponding texture of the order parameter is called *n-times quantized vortex*. Let us now consider a singly quantized vortex located at $\vec{r}=0$

$$\Delta(\vec{r})=|\Delta(r)|\exp(i\phi), \tag{7}$$

where ϕ is azimuthal angle in the x-y plane. The absolute value of the gap is assumed to be constant everywhere except regions of the size ξ (correlation length) near the vortex centers. This assumption constitutes the so-called London approximation. From Eq. (7) we can calculate induced charge density (per chain) using Eq. (2),

$$e\rho=\frac{e}{\pi}\,\frac{\sin\phi}{r}. \tag{8}$$

We see that it falls off as $1/r$—it is highly nonlocal. However the *screening* makes the fall-off *exponential*. To see how this happens we make the following substitution in Eq. (5) in order to take vortex degrees of freedom into account:[8] $(\vec{\nabla}\theta)_k\to i\vec{k}\theta_k^{phason}+(i\vec{k}\times\hat{z}/k^2)n_k$, where $n(r)=2\pi\Sigma n_i\delta(r-r_i)$ is vorticity and n_i is the winding number of a vortex at r_i. Minimizing the free energy functional with respect to θ_k^{phason} we get an effective action:

$$F_{inhom}+F_{el}=\int\frac{d^2\vec{k}}{(2\pi)^2}\left[\frac{K\gamma^2}{2k_\gamma^2}\left|n_k-\frac{ieJk_y}{K}\varphi_k\right|^2 -\frac{1}{8\pi}(\epsilon k^2+\lambda_{tf}^{-2})\left|\varphi_k\right|^2+\varphi_k\rho_{-k}^{ext}\right]. \tag{9}$$

Electric potential produced by vortices is obtained by the minimization of Eq. (9) with respect to φ_k and is given by

$$\varphi_k=\frac{4\pi ie\gamma^2J}{\epsilon k^2+\Lambda_k^{-2}}\,\frac{k_y}{k_\gamma^2}n_k. \tag{10}$$

C. Single vortex

Now $n(r)=2\pi\delta(r)$ and the electrostatic potential produced by a single vortex is given by the Fourier transform of Eq. (10). It is hard to obtain an analytical expression in the general case, but one can get an idea of what this potential looks like from the consideration of the purely isotropic case: $\gamma=1$, $\Lambda_k=\Lambda=$const. With this simplification the potential is given by

$$\phi(\vec{r})=-2e\gamma^2J\sin\theta f(r),$$

$$f(r)=\int dk\frac{J_1(kr)}{\epsilon k^2+\Lambda^{-2}} =\begin{cases}\dfrac{r}{2\epsilon}\ln\dfrac{\epsilon^{1/2}\Lambda}{r} & r\ll\epsilon^{1/2}\Lambda,\\[2mm] \dfrac{\Lambda^2}{r}, & r\gg\epsilon^{1/2}\Lambda.\end{cases} \tag{11}$$

Here, J_1 is the first Bessel function. The effect of huge actual anisotropy in Λ can be taken into account qualitatively in the following way. First of all we may notice that there still will be two characteristic regions: $r\ll\epsilon^{1/2}\Lambda(\theta)$ and $r\gg\epsilon^{1/2}\Lambda(\theta)$ where $\Lambda(\theta)$ is now an angle-dependent crossover scale (which is, of course, extremely anisotropic). Then we may also notice that in the large-r region $f(r)$ is still angle independent: it is given by $f(r)\approx\Lambda_{av}^2/r$ where Λ_{av} is some "average" screening length. An important point here is that the *total charge density* in the large-r region falls off *exponentially*: one can check that by taking the Laplacian of $\varphi(\vec{r})$. But the above-mentioned extreme anisotropy comes to play in the small-r region—the core of a vortex is highly anisotropic and hard to analyze.

Some of the vortex properties, however, allow an exact description. From Eq. (10) it can be inferred that the total charge of a vortex is zero, but there is a nonzero electric dipole moment directed along y,

$$d_y=2\pi\epsilon eJ\lambda_{qp}^2=d_0\frac{\epsilon f_s}{2(1-f_s)}. \tag{12}$$

Here, $d_0=v_F/2e$. d_y is exponentially increased as $T\to 0$. It should be noted that this expression was derived for a vortex in the bulk; it is expected that for vortices near boundary (the case which is relevant for vortices produced by external fields—see below) the induced dipole moment is reduced.

D. Critical field

Now we estimate the critical field at which an appearance of a single vortex becomes energetically favorable. In order to do that we substitute Eq. (10) (with $n_k=2\pi$) back into Eq. (9):

$$F_{eff}=\int d^2\vec{k}\,\frac{K\gamma^2}{2k_\gamma^2}\left(\frac{\epsilon k^2+\lambda_{TF}^{-2}}{\epsilon k^2+\Lambda_k^{-2}}\right)-d_yE_y^{ext} \tag{13}$$

$$=\frac{\pi K\gamma}{2}\,\frac{\lambda_{qp}}{\lambda_{TF}}\ln\frac{W}{\epsilon^{1/2}\lambda_{qp}}-d_yE_y^{ext}. \tag{14}$$

Here, W is the size of the system in the y direction. From Eq. (14) and Eq. (12) we obtain the critical field:

$$D_c^{II}=\frac{\gamma d_0}{4\lambda_{qp}\lambda_{TF}}\log\frac{W}{\epsilon^{1/2}\lambda_{qp}}. \tag{15}$$

Comparing this expression with its superconducting analog one may call d_0 a ''quantum of electric dipole moment.'' The dependence of the critical field on temperature is given by $\lambda_{qp}^{-2}=\lambda_{TF}^{-2}\sqrt{2\pi\Delta_0/T}\,\exp(-\Delta_0/T)$. So the critical field for the vortex mixed state can be significantly lowered by increasing the screening length in the y direction as $T\to 0$. As we do so, an interesting situation can occur: D_c^{II} can be made smaller than D_c^{I} signaling a temperature-driven transition between type-I-like and type-II-like ground states. A more intuitive explanation of this transition is obvious: one can, in principle, evaluate $\kappa_x=\lambda_x/\xi_x$ and $\kappa_y=\lambda_y/\xi_y$. Usually one has $\kappa_x\ll 1$ while κ_y is exponentially temperature dependent. One can argue then that the type of the ground state is determined by the geometric mean of the two kappas: $\kappa=\sqrt{\kappa_x\kappa_y}$. This ''mean'' Ginsburg-Landau parameter κ is also temperature dependent. This raises a possibility of a Type-I/Type-II temperature-driven transition as some critical value $\kappa_c\sim 1$ is passed by κ in a temperature sweep.

E. Screening properties

From the physical point of view the reason why the appearance of vortices becomes favorable at high fields is that vortices can screen external electric fields. In order to show this we first introduce a ''dense limit approximation'' [8] in which the average distance between vortices is assumed to be much less than the characteristic length of the external electric field variation. Then one can take the vorticity $n(\vec{r})$ to be a continuous function rather than the sum of δ functions. The minimization of the effective energy, Eq. (9), with respect to n_k becomes trivial: $n_k=d_0^{-1}E_k^y$ and leaves us with the effective free energy which describes the screening with the screening length $\lambda=\lambda_{TF}$. In fact this contradicts to the above made dense limit approximation; nevertheless the conclusion about screening remains valid if we assume that the screening length is rather equal to the average inter-vortex distance: $\lambda=n^{-1/2}$. But now the screening length becomes coordinate dependent leading to a nonexponential screening. Indeed, the Poisson equation $\varphi''-\lambda^{-2}\varphi=0$ in this case reads as $\varphi''+d_0^{-1}\varphi\varphi'=0$. Its solution is

$$\varphi(y)=\frac{2d_0}{y+2d_0\varphi(0)^{-1}}. \tag{16}$$

At distances $\sim\lambda_{qp}$, however, the exponential screening due to quasiparticles comes into play. So in the bulk the DW state is restored. Thus the electric-field-induced transition to a vortex state is a *surface effect*. Therefore it is unlikely to be detected in any transport measurements.[15] On the other hand the best way to observe such a transition would be to measure directly the screening length. It would be expected that the screening length is $\sim\lambda_{qp}$ for field below critical whereas for fields above critical it collapses to some small value. Such experiments are currently underway.[16]

V. THERMALLY-EXCITED VORTICES

An alternative to the production of vortices in DW systems by applying a transverse electric field at low temperature is their thermal activation in the temperature region near T_c. We have already calculated the energy required to produce a singly quantized vortex in the absence of external electric field [Eq. (14)]—this energy is given by[18]

$$E_a=\frac{\pi K\gamma}{2}\frac{\lambda_{qp}}{\lambda_{TF}}\ln\frac{W}{\epsilon^{1/2}\lambda_{qp}}. \tag{17}$$

At low temperature this energy is big, but as we get closer to the transition point E_a it decreases rapidly because of decreasing rigidity K (it is proportional to the condensate density). Moreover, K is renormalized to smaller values in the vicinity of critical point by the fluctuations of the order parameter. The description of the dynamics of thermally excited vortices in external transverse electric fields is beyond the scope of this article and will be reported elsewhere; however a simple picture can be outlined here. The key point is that there is a gas of thermally activated vortices at some finite temperature. We shall restrict ourselves to only two kinds of vortices, namely those with winding numbers $n_i=\pm 1$ and dipole momenta $d_y=\pm|d_y|$, respectively. It is assumed that the excitation of vortices with higher winding numbers is suppressed to be their bigger energies. Then applying a transverse electric field one would be able to polarize the vortex gas. The dielectric constant of the vortex gas in the case of *weak fields* is

$$\epsilon=\frac{4\pi n d_y^2}{T}. \tag{18}$$

Here, n is the density of vortices. n also enters the expression for the correlation length in the gas of vortex dipoles. Thus one would be able to extract n from experiments concerned with the response of DW materials to transverse electric fields. Such experiments are currently underway.[16]

VI. CONCLUSIONS

We have performed an extensive analysis of vortices in highly anisotropic quasi-one-dimensional DW systems. This work builds a more detailed and correct picture of the structure and dynamics of vortices as compared to Ref. 8, and also predicts several unique properties of such vortices never encountered before with the case of their superconducting counterparts. Among those are the possibility of a temperature-controlled phase transition between type-I-like and type-II-like phases; the nonexponential screening of strong electric fields by vortices at comparably large scales as opposed to the incorrect conclusion about short range exponential screening drawn in Ref. 8; *temperature controlled ''flux quantum'' of a vortex—its dipole moment*. We would like to point out that the exploration of the dynamics of topological defects in DW systems is a relatively new and actively developing area of condensed matter physics with many surprises and, possibly, some connections to other branches of physics (see, e.g., a recent paper[17] and references therein).

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[9] The coefficients in the equation are given as follows:[10] $K = N_\perp v_F f_s/2\pi$, $N_\perp$ is the density of chains in the plane perpendicular to chains, $f_s(T) \approx 7\zeta(3)|\Delta|^2/4\pi^2 T_c^2$ for $T \approx T_c$ and $f_s(T) \approx 1 - \sqrt{2\pi\Delta_0/T}\exp(-\Delta_0/T)$ for $T \ll T_c$ is the dimensionless condensate density ρ_s/ρ_0, $\Delta_0 = 1.7T_c$ is the gap at $T=0$; $\gamma^2 = \xi_y^2/\xi_x^2$ is the anisotropy parameter, ξ_x and ξ_y are correlation lengths in the x and y directions, respectively.

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[11] Here $J = N_\perp f_s/\pi$; $\lambda_{qp}^{-2} = (1-f_s)\lambda_{TF}^{-2}$ is inverse squared screening length due to quasiparticles excited over the gap, $\lambda_{TF}^{-2} = 8N_\perp e^2/v_F$ is inverse squared Thomas-Fermi screening length in the metallic state.[8] See the main text for the discussion of ϵ.

[12] This conclusion is true for the case of *weak pinning* which is a common situation in usual DW materials; see M. V. Feigelman in *Charge Density Waves in Solids*, edited by L. P. Gorkov and G. Gruner (North-Holland, New York, 1989).

[13] The polarization contribution to the screening in the x direction is omitted because $\epsilon(\lambda_{TF}^{-1}) \approx 1$.

[14] The variation of the phase of the order parameter cannot screen the electric field in the y direction.

[15] This is true for *field-induced*, vortices. However, there are expected to be the so-called *commensuration vortices*, in the bulk which can, in dirty systems, contribute to conductivity due to the phenomenon of spectral flow.[17]

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[18] This is the energy of a vortex per unit length. For a vortex in a single plane one should multiply this expression by interplane distance.