We show how to calculate semi-analytically the dense vortex state in strong type-II superconducting nanostructures. For the specific case of a strip, we find vortex lattice solutions which also incorporate surface superconductivity. We calculate the energy cost to displace individual vortex rows parallel to the surfaces and find that this energy oscillates with the magnetic field. Remarkably, we also find that, at a critical field $H^*$ below $H_{c2}$, this “shear” energy becomes strictly zero for the surface rows due to an unexpected mismatch with the bulk lattice.

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Despite increased technological interest in the transport properties of the vortex lattice state (VLS) \[1\] in type-II superconducting nanostructures, the theoretical understanding of the interplay between the VLS and the interfaces is still mostly qualitative. While experiments are routinely done in nanostructures with various interface geometries \[2-3\] and explore all values of magnetic field $H$ and temperature $T$, the order parameter, $\Psi(x)$, has been almost exclusively calculated in only two regimes. (i) For fields above the upper critical field $H_{c2}$, which separates the VLS from the metallic phase, solutions of the Ginzburg-Landau differential equations revealed long ago the existence of a highly localized or-\[12\]ical simulations \[11\]. (ii) On the other extreme, $\Psi(x)$ has been calculated for values of $H$ just above the lower critical field $H_{c1}$, which separates the Meissner state from the VLS. The order parameter takes the form of a dilute VLS in which the inter-vortex distance, $a_0$, is large compared to the coherence length $\xi$ (typical size of the vortex cores). The properties of this dilute VLS in the presence of a surface parallel to $H$ were analyzed in the past \[3\] and numerous studies in thin films have been reported over the years \[2\].

The dilute VLS, which is correctly described in the London approximation where the vortex cores are ignored, only exists in a narrow range of $H$ above $H_{c1}$ for strong type-II ($\kappa \gg 1$) superconductors \[4,6\]. Instead, a dense vortex state occupies most of the $H-T$ phase diagram down to $H \approx 0.3H_{c2}$. In this regime, the vortex cores fill most of the space, interact strongly among themselves, and, most importantly, interact directly with the interfaces. To the best of our knowledge, only numerical simulations for nanostructures such as thin films or slabs (placed parallel to $H$) \[10\] and strips (perpendicular to $H$) \[11\] have been reported in this regime. Our goal is to show that, for systems with simple geometries and simple orientations with respect to $H$, one can minimize semi-analytically the Ginzburg-Landau energy functional and obtain the full solution of the order parameter in the dense vortex regime. We illustrate the procedure for a disorder-free two-dimensional strip perpendicular to $H$.

The order parameter comprises, generically, both a dense vortex regime. We illustrate the procedure for a strip, we find vortex lattice solutions which also incorporate surface superconductivity. We calculate the energy cost to displace individual vortex lattice solutions which also incorporate surface superconductivity. We calculate the energy cost to displace individual vortex rows parallel to the surfaces and find that this energy oscillates with the magnetic field. Remarkably, we also find that, at a critical field $H^*$ below $H_{c2}$, this “shear” energy becomes strictly zero for the surface rows due to an unexpected mismatch with the bulk lattice.

At the mean-field level (excluding thermal fluctuations) \[5\] the order parameter can be obtained from minimization of the Ginzburg-Landau functional

$$G = G_n + \int d\mathbf{r} \left[ \alpha |\Psi(\mathbf{r})|^2 + \frac{\beta}{2} |\Psi(\mathbf{r})|^4 + \frac{1}{2m^*} |\Psi^*(\mathbf{r}) \left( -ih \nabla - \frac{e^*}{c} \mathbf{A}(\mathbf{r}) \right) |^2 \Psi(\mathbf{r}) + \left( \frac{\hbar(\mathbf{r}) - H^2}{8\pi} \right) \right],$$

where $G$ and $G_n$ are the Gibbs free energies of the superconducting and metallic states, respectively. The term $[-i\hbar \nabla - e^*/c \mathbf{A}(\mathbf{r})/c^2/2m^*$ is the kinetic energy operator for Cooper pairs of charge $e^* = 2e$ and mass $m^* = 2m$ in a vector potential $\mathbf{A}(\mathbf{r})$ associated with the magnetic induction $h(\mathbf{r})$. The parameters $\alpha$ and $\beta$ have the usual meaning \[3\].

If, for simplicity, we restrict ourselves to two dimensions, $\kappa$ becomes effectively infinite and $h(\mathbf{r}) = H$ \[3\]. In order to be able to find analytically the solutions which minimize Eq. 1 we first expand the order parameter as

$$\Psi(\mathbf{r}) = \sum_p \phi_p(\mathbf{r}),$$

where $\phi_p(\mathbf{r})$ are the normalized eigenfunctions of the kinetic energy operator. The geometry of the interfaces determines the appropriate gauge choice and quantum number $p$ (which is usually the linear or angular momentum); the microscopic details of the interfaces determine the boundary conditions for
the eigenfunctions $\Phi_k$. To obtain the order parameter in the dense vortex regime it is sufficient to consider an expansion of $\Psi(\mathbf{r})$ in the lowest band (LB). $n = 0$. The LB expansion allows us to write Eq. (1) as

$$G - G_n = \sum_{p} \alpha_p |C_p|^2 + \frac{\beta}{2} \sum_{p_1, p_2, p_3, p_4} C_{p_1}^* C_{p_2}^* C_{p_3} C_{p_4} \int \mathrm{d}r \Phi_{p_1}^* \Phi_{p_2}^* \Phi_{p_3} \Phi_{p_4}$$

where $N_c$ is the number of components, $\alpha_p = \alpha + \epsilon(p)$ is the condensation energy of the $p$ component, and the second term represents the “interaction” between Cooper pairs. The interfaces are responsible for the non-uniformity of the condensation energy through the kinetic energy, $\epsilon(p)$, of the Cooper pair. $-\alpha_p$ increases near interfaces with insulators, which favors surface superconductivity (see Fig. [5,4,12]), and shrinks near those with metals.

![FIG. 1. Cooper pair LB structure (in units of the cyclotron energy $h\omega_c/2$) in a $W = 16\xi$ strip for different values of $H$ (shifted for clarity). Notice the bending of the LB near the surfaces. Dashed lines represent $-\alpha$. As $H$ increases [from (a) to (e)] the number of components of the order parameter increases progressively. When $-\alpha$ lies below the LB in the center of the strip [panel (e)] only surface superconductivity survives.]

It is the $p$ dependence of $\alpha_p$ which, in principle, makes the minimization of Eq. (2) non-trivial. In order to accomplish this task one has to find: (i) the optimum $N_c$, (ii) the quantum numbers $\{p\}$, and (iii) the complex coefficients $C_p$. Some simple considerations (which are specific for each geometry) allow us to solve this problem analytically. As an illustration we calculate the order parameter in an isolated strip. The dimensions of this ideal strip are $L_y \to \infty$, $L_z \to 0$, and $W$, while $H$ is chosen in the $z$ direction. The appropriate LB eigenfunctions are (in the Landau gauge) $\Phi_k(\mathbf{r}) \propto e^{iky} \chi_k(x)$, where $k$ is the wavevector in the $y$ direction and $\chi_k(x)$ are nodeless functions which may be calculated numerically subjected to the boundary conditions of zero current on both surfaces. The integrals in Eq. (2) become

$$I(k_1, k_2, k_3, k_4) \equiv (L_y L_z)^{-1} \delta_{k_1 + k_2, k_3 + k_4} \int dx \chi_{k_1}(x) \chi_{k_2}(x) \chi_{k_3}(x) \chi_{k_4}(x)$$

and may also be calculated numerically.

To find the lowest energy configuration we minimize the Gibbs free energy in Eq. (2) for each possible $N_c$ separately (we will skip the trivial case $N_c = 1$, which is only relevant for very narrow strips with $W \approx \xi$).

One vortex row ($N_c = 2$): From the symmetry of the system one can consider the two components in a pair $(k, -k)$ with $k > 0$ [see, e.g., Fig. [1](e)]. The symmetry also tells us that we can choose $C_k = C_{-k}$. (Since the overall phase is irrelevant and the relative one only determines the position of the row in the $y$ direction, we consider both coefficients to be real and positive.) There are only two types of interaction terms: (i) $I(k, k, k, k) = I(-k, -k, -k, -k)$, which represent the interaction between Cooper pairs occupying the same state [in shorthand, $I(k)$], and (ii) $I(k, -k, -k, k) = I(k, -k, k, -k) = I(-k, -k, -k, k) = I(-k, -k, k, -k)$, which represent the interaction between Cooper pairs occupying different states [in shorthand, $I(k, -k)$]. The Gibbs free energy becomes

$$G - G_n = 2\alpha_k C_k^2 + \beta A_k C_k^4,$$

where $A_k = I(k) + 2I(k, -k)$. Straightforwardly one obtains the minimal values of the coefficients, $C_k = \sqrt{-\alpha_k/\beta A_k}$, and the minimum Gibbs free energy, $G - G_n = -\alpha_k^2/\beta A_k$, for any pair $(k, -k)$. Knowing the band structure and the interaction integrals, the minimum-energy pair, $(k, -k)$, can now be found, and $\Psi(\mathbf{r})$ takes the form of one centered vortex row as long as the two components overlap significantly. For $W \gg \xi$ and $H > H_{c2}$ the order parameter is always formed by two components which do not overlap and constitute the usual surface superconductivity on both sides of the strip [see Fig. [1](e)].

Two vortex rows ($N_c = 3$): In addition to the pair $(k, -k)$ with positive, real coefficients $C_k = C_{-k}$ a third component can be considered at $k = 0$ [see, e.g., Fig. [1](a)] with a complex coefficient $|C_0|e^{i\phi_0}$. The Gibbs free energy becomes

$$G - G_n = 2\alpha_k C_k^2 + |C_0|^2 + \beta \left(2A_k C_k^4 + I(0)|C_0|^4 + 4[2I(k, 0) + \cos (2\phi_0)I(k, 0, -k)]C_k^2|C_0|^2\right),$$

where a new type of interaction terms, $I(k, -k, 0, 0) = I(-k, -k, 0, 0) = I(0, 0, k, -k) = I(0, 0, -k, k)$, appear $[I(k, 0, -k)$ in shorthand]. The last term in Eq. (3) represents the “correlation” energy between rows and, regardless of the magnitude of the coefficients, the minimum energy is obtained for $\phi_0 = \pi/2$, i.e., when the two rows
are offset by half a row period, $a'_{0}/2$. Upon minimization one obtains

$$
\tilde{C}_k = \sqrt{\frac{\alpha_0 S_k - \alpha_k I(0)}{\beta I(0) A_k - 2S_k^2}}
$$

(6)

$$
|\tilde{C}_0| = \sqrt{\frac{2\alpha_0 S_k - \alpha_0 A_k}{\beta I(0) A_k - 2S_k^2}}
$$

(7)

$$
G - G_n = -\frac{2\alpha_2^2 I(0) - \alpha_0^2 A_k + 4\alpha_k \alpha_0 S_k}{2\beta I(0) A_k - 2S_k^2}
$$

(8)

for any trio $(-k, 0, k)$, where $S_k = 2I(k, 0) - I(k, 0, -k)$.

Three vortex rows ($N_c = 4$): The four components may correspond to pairs $(k_2, -k_2)$ and $(k_1, -k_1)$ with $k_2 > k_1 > 0$ [see Fig. 1(b)]. We assume $C_{k_2} = C_{-k_2}$ and $|C_{k_1}| = |C_{-k_1}|$. Once again two of the phases have been set to zero ($\phi_{k_2}$ and $\phi_{-k_2}$). The other two, $\phi_{k_1}$ and $\phi_{-k_1}$, must be chosen to minimize the energy. To make things analytically accessible we drop, for the moment, the weak correlation terms between vortex rows in the resulting Gibbs free energy:

$$
G - G_n = 2\alpha_k |C_{k_1}|^2 + 2\alpha_{k_2} |C_{k_2}|^2 + \beta(A_{k_1} |C_{k_1}|^4 + A_{k_2} |C_{k_2}|^4 + 4S_{k_1,k_2} |C_{k_1}|^2 |C_{k_2}|^2),
$$

where $S_{k_1,k_2} = I(k_1,k_2) + I(k_1,-k_2)$. Minimizing we obtain

$$
|\tilde{C}_{k_1}| = \sqrt{\frac{\alpha_{k_1} A_{k_2} - 2\alpha_{k_2} S_{k_1,k_2}}{\beta[4S_{k_1,k_2}^2 - A_k A_{k_2}]}}
$$

(10)

$$
\tilde{C}_{k_2} = \sqrt{\frac{\alpha_{k_2} A_{k_1} - 2\alpha_{k_1} S_{k_1,k_2}}{\beta[4S_{k_1,k_2}^2 - A_k A_{k_2}]}}
$$

(11)

$$
G - G_n = \frac{\alpha_2^2 A_{k_1} + \alpha_0^2 A_{k_2} - 4\alpha_k \alpha_0 S_{k_1,k_2}}{\beta[4S_{k_1,k_2}^2 - A_k A_{k_2}]}
$$

(12)

for any set of four components $(-k_2, -k_1, k_1, k_2)$. The correlation terms between adjacent rows, which ultimately determine the relative position between them, can be recast in the form

$$
\delta_{k_2,3k_1} 2\beta |C_{k_1}|^3 C_{k_2} I(-k_1, k_1, k_2) \times \left[ \cos (2\phi_{k_2} - \phi_{-k_1}) + \cos (2\phi_{k_2} - \phi_{-k_1}) \right].
$$

(13)

Notice that for $k_2 = 3k_1$, the sake of minimization, there are the same period $a_{0}'$. The minimum contribution of this term to the energy corresponds to $\phi_{k_1} = \phi_{-k_1} = \pi$, which sets the offset between adjacent rows to $a_{0}'/2$. The total energy can now be approximately obtained by subtracting the “lock-in” energy $4\beta |C_{k_1}|^3 C_{k_2} I(-k_1, k_1, k_2)$ from Eq. (12). If $k_2 \neq 3k_1$ the choice of phases is irrelevant since the period of adjacent rows is different and they cannot fall into place. The above choice of phases gives the worst relative position between non-adjacent rows, i.e., aligns non-adjacent vortices. However, the term that accounts for such correlation is proportional to $I(-k_2, -k_1, k_1, k_2)$ and can be safely dropped since the overlap of $\chi_{-k_2}$ and $\chi_{k_2}$ is negligible in the expected minimal solution.

For more than three vortex rows one adds more components [see panels (c) and (d) in Fig. 1] and follows similar considerations as for $N_c = 4$: (i) to neglect correlations between non-adjacent rows, (ii) to minimize without the correlation terms for adjacent rows, and (iii) to subtract the lock-in energy at the end. One can thus obtain analytical expressions for the $\tilde{C}_k$’s and $G - G_n$ for any number of rows from which the optimum set of quantum numbers $\{k\}$ can be found. We will only discuss the results in the following. Figure 2 shows the number of vortex rows for strip thicknesses $W = 12\xi$ and $W = 16\xi$ as a function of $H$. As expected, the number increases in a step-wise manner. Figure 3 shows several snapshots of $\epsilon(k)$ for the $W = 16\xi$ strip for some characteristic values of $H$. As long as $-\alpha$ or “chemical potential” for the Cooper pairs (dashed lines) remains above the LB in the center of the strip [panels (a) to (d)], the number of vortex rows increases with $H$. When $-\alpha$ lies below the LB in the center, i.e., when $H > H_{c2}$ [panel (e)], the Cooper pairs can only nucleate near the surfaces (surface superconductivity). For the narrower strip [Fig. 3(a)] the number of vortex rows that can be accommodated before the quenching of bulk superconductivity is logically smaller than for the wider one [Fig. 3(b)]. (To the numerical accuracy of our calculations all the rows forming the lattice disappear at $H = H_{c2}$ in the limit $W \rightarrow \infty$.) Peaks in the measured magnetization of thin films have already been associated with these type of transitions in the number of vortex rows.
dependent and proportional to the shear modulus $c_{66}$ of the vortex lattice. To calculate $E_s$ one compares the minimum energy with that obtained by switching the phases away from their optimum values so that vortices in adjacent rows become aligned with each other. Dashed lines in Fig. 3 correspond to $E_s$ for the surface rows. Whenever a new row is added to the strip, $E_s$ experiences a sudden jump. This is because the addition of a new row "squeezes" all the others against each other, increasing their shear energy. On qualitative arguments only one of the two possible lattice orientations is expected in this system. Although near the transition points the lattice is fairly distorted with $a'_0 \neq a_0$ ($a_0$ corresponds to the perfect triangular lattice), the expected orientation is still apparent in our results. The experimental value of the flow stress, which is proportional to $E_s$, has been reported in Refs. 3 although instead of having the VLS confined in strips they had it “trapped” in disordered free grooves etched in a dirty film. Oscillations in the flow stress were reported for the whole range of $H$ and they were attributed to dislocations that appear when the periodicities of the groove superlattice and the VLS did not match. This picture does not consider the possible overall distortion of the lattice. From our calculations we conclude that, since the whole lattice reconstructs abruptly at each row addition, dislocations need not be invoked to explain jumps in the flow stress. Note that the boundary conditions that mimic the groove interfaces are different from the ones used here, but, as long as the vortex-interface interaction is sufficiently strong, this basic conclusion holds.

Finally, the most remarkable result to emerge from our calculations is the fact that $E_s$ goes strictly to zero at a critical field $H^* \approx 0.73H_{c2}$ as $W \to \infty$. This is due to the fact that the surface rows become incommensurable with the bulk lattice at this critical field. Shaded areas in Fig. 3 correspond to the situation where lock-in takes place between the two surface vortex rows and the bulk lattice and, consequently, there is always a finite value of $E_s$ for such rows. For $H > H^*$ up to $H_{c2}$ the condensation energy near the surfaces always overcomes the lock-in energy. The surface rows prefer to have a shorter period than the bulk ones despite of the fact that lock-in is no longer possible. Figure 3 shows the order parameter for $H$ near $H_{c2}$ where the mismatch in period between surface rows and bulk lattice is apparent. This mismatch might reflect in a premature quenching of the flow stress measured in deeply etched NbGe grooves in experimental setups similar to those of Refs. 3. The deep etching would create the necessary spatial modulation of the condensation energy which triggers this phenomenon.

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[13] This is not a drastic simplification for strong type-II three-dimensional nanostructures in the dense vortex regime where, although the magnetization is finite, $h(r)$ is still basically uniform.

[14] Away from the interfaces the LB approximation is equivalent to the lowest Landau level approximation, but near the interfaces the LB expansion includes higher Landau levels.

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