Energy of infinite vortex lattices

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An expression is derived for the energy density of a lattice of point vortices (or other logarithmic objects) having an arbitrary number of vortices of arbitrary strengths in an arbitrary unit cell. The result is expressed in the form of a rapidly convergent series well suited for numerical evaluation. The effects of separately changing the shape and dimensions of the unit cell are shown for simple cases, and the energy of the triangular lattice is calculated as a function of slip displacement.

I. INTRODUCTION

We consider the problem of finding the energy of an infinite number of classical point particles confined to a planar lattice and interacting pair wise with a logarithmic potential. These particles will be viewed as vortices in an Eulerian fluid; they are also equivalent to rectilinear line charges, line currents, or screw dislocations. Our objective is to find the relative energy of different configurations of J vortices having strengths $\Gamma_1, \Gamma_2, \ldots, \Gamma_J$ in a unit cell defined by the lengths L_1 and L_2 of its sides and the angle ϕ between them.

If the sum of the vorticity strengths is not zero in the unit cell the system is stationary only in a coordinate frame rotating with angular velocity Ω,

$$\Omega = \frac{\Gamma}{2L_1L_2\sin\phi}, \quad \Gamma \equiv \sum_{j=1}^{J} \Gamma_j .$$

We consider the lattice only in such a frame or, equivalently, in a nonrotating frame with an imposed background solid-body rotation of the opposite sign. $-\Omega r$. Similarly, an opposite uniform background charge or current would be needed for line charges or currents. Such constant background fields play no role in the lattice properties, and serve merely to cancel formal[1] singularities that occur at zero wave number. Of course, these background fields must be explicitly included to study the global properties of finite[2] systems.

The task of deriving lattice sums for Coulomb interactions has a long history.[3] Our purpose here is to obtain the most efficient lattice sum for a general two-dimensional lattice and our method based on results by Glasser,[4] who considered the particular case of a rectangular unit cell ($\phi = 90°$). In addition to obtaining a rapidly convergent lattice summation, we obtain an expression for the energy density of a vortex lattice that is invariant to physically equivalent designations of the unit cell, which are not necessarily primitive cells. By means of this expression it becomes easy to compare the energy of *all possible* lattices containing the same mixture of vortex species.

II. LATTICE ENERGY

The total energy due to mutual vortex interaction is

$$E_T = -\frac{d}{4\pi}\sum_i \sum_j{}' \Gamma_i \Gamma_j \ln|\mathbf{r}_i - \mathbf{r}_j| , \tag{1}$$

where d is the fluid density (mass per unit area) and the double sum omits $i = j$. For an infinite lattice E_T is unbounded, even in the presence of a background. However this unboundedness is easily avoided by considering the energy per vortex E, which is finite:

$$E = \lim_{M\to\infty} \frac{4\pi}{dJM} E_T , \tag{2}$$

where M is the number of unit cells. It is convenient to subdivide the sum over all vortices into sums over the J vortex species in all unit cells,

$$\sum_j = \sum_{j_1} \sum_{j_2} + \cdots + \sum_{j_J} \tag{3}$$

and to note that

$$\sum_{j_\alpha} \sum_{j_b}{}' \Gamma_\alpha \Gamma_\beta \ln|\mathbf{r}_{j_\alpha} - \mathbf{r}_{j_\beta}| = M\Gamma_\alpha\Gamma_\beta \sum_n{}' \ln|\mathbf{r}_\alpha^0 - \mathbf{r}_\beta^0 + \mathbf{L}_n| . \tag{4}$$

The sum in the above equation is over all integers $n_1, n_2 = 0, \pm 1, \pm 2, \ldots,$ except if $\alpha = \beta$, in which case $n_1 = n_2 = 0$ must be omitted. The vortex positions are $\mathbf{r}_\alpha^0$, $\alpha = 1, \ldots, J$ in a reference unit cell and

$$\mathbf{L}_n = L_1 n_1 \mathbf{e}_1 + L_2 n_2 \mathbf{e}_2 \tag{5}$$

is a generic lattice vector ($\mathbf{e}_1 \cdot \mathbf{e}_2 = \cos\phi$). Using Eqs. (3) and (4) in Eq. (2) gives

$$E=-\overline{\Gamma}^2\sum_n{}'\ln|\mathbf{L}_n|-\frac{2}{J}\sum_{\substack{\alpha=1\\ \alpha<\beta}}^{J-1}\sum_{\beta=2}^{J}\Gamma_\alpha\Gamma_\beta\sum_n\ln|\mathbf{r}^0_{\alpha\beta}+\mathbf{L}_n| \,, \tag{6}$$

where

$$\overline{\Gamma^2}\equiv\frac{1}{J}\sum_{\alpha=1}^{J}\Gamma^2_\alpha \tag{7}$$

and

$$\mathbf{r}^0_{\alpha\beta}=\mathbf{r}^0_\alpha-\mathbf{r}^0_\beta \,.$$

III. LATTICE SUM

To evaluate the lattice sums in Eq. (6) express the Fourier transform of the logarithm function using box normalization,

$$-\ln|\mathbf{x}|=\lim_{\mu\to 0}\frac{2\pi}{s_1 s_2}\sum_k\frac{\exp(i\mathbf{k}\cdot\mathbf{x})}{k^2+\mu^2}, \quad \mathbf{k}=2\pi\left[\frac{n_1}{s_1},\frac{n_2}{s_2}\right] \,, \tag{8}$$

in the limit where s_1 and s_2 become infinite. A nonzero "mass" parameter μ changes the logarithm function into a short-ranged one, and is a fundamental parameter for understanding the effect of the background. To perform the lattice sum it is convenient to employ the so-called reciprocal-lattice vectors $\mathbf{g}$ defined by

$$\mathbf{g}=\frac{2\pi}{\sin\phi}\left[\frac{m_1}{L_1}\mathbf{v}_1+\frac{m_2}{L_2}\mathbf{v}_2\right], \quad \mathbf{v}_i\cdot\mathbf{e}_j=\delta_{ij}\sin\phi \,. \tag{9}$$

Then,

$$-\sum_n\ln|\mathbf{x}+\mathbf{L}_n|=V(x)+c_\infty \,, \tag{10}$$

where

$$V(x)=\frac{2\pi}{L_1L_2\sin\phi}\sum_{\mathbf{g}(\neq 0)}\frac{e^{i\mathbf{g}\cdot\mathbf{x}}}{g^2} \,, \tag{11}$$

$$c_\infty=\lim_{\mu\to 0}\frac{2\pi}{\mu^2 L_1 L_2\sin\phi} \,. \tag{12}$$

The divergent constant c_∞ corresponds to the $\mathbf{g}=\mathbf{0}$ component ($m_1=m_2=0$); the effect of the background is to cancel this divergent constant.

To apply Glasser's method one first writes Eq. (11) in a more explicit form,

$$V(x)=\frac{\rho\sin\phi}{2\pi}\sum_{m_1,m_2(\neq 0)}\frac{e^{2\pi i(m_1y_1+m_2y_2)}}{m_1^2+m_2^2\rho^2-2m_1m_2\rho\cos\phi} \,, \tag{13}$$

where $y_1=(x_1\sin\phi-x_2\cos\phi)/L_1\sin\phi$ and $y_2=x_2/L_2\sin\phi$. The same sequence of transformations of Ref. 4 then leads to

$$V(x)=(\sin\phi/\rho\pi)\sum_{k=1}^{\infty}\cos(kz_2/\sin\phi)/k^2 -\tfrac{1}{2}\ln\prod_{s=-\infty}^{\infty}h(s,z_1,z_2) \,, \tag{14}$$

where

$$h(s,z_1,z_2)=1-2e^{-|z_2+2\pi s\sin\phi|/\rho}\cos\left[z_1+\frac{2\pi s}{\rho}\cos\phi\right] +e^{-2|z_2+2\pi s\sin\phi|/\rho} \,, \tag{15}$$

with $z_i\equiv 2\pi x_i/L_i$ and $\rho\equiv L_1/L_2$.

In terms of these new variables a lattice translation $\mathbf{x}\to\mathbf{x}+\mathbf{L}_n$ becomes $z_1\to z_1+2\pi n_1+2\pi n_2\cos\phi/\rho$ and $z_2\to z_2+2\pi n_2\sin\phi$. It is easy to verify that Eq. (14) is invariant under lattice translations, consistent with Eq. (10). The first summation of Eq. (14) can be performed, giving the more efficient representation,[5]

$$(\sin\phi/\pi)\sum_{k=1}^{\infty}\cos(kz_2/\sin\phi)/k^2 =|z_2|(|z_2|/\sin\phi-2\pi)/4\pi+\pi(\sin\phi)/6 \,, \tag{16}$$

valid for $|z_2|\leq 2\pi\sin\phi$. The consequent loss of translational invariance in the $\mathbf{e}_2$ direction causes no difficulty in numerical evaluations.

The expression for $V(x)$ given by Eqs. (14)–(16) converges quite rapidly. In practice, the evaluation of the infinite product of terms $h(s,z_1,z_2)$ reduces to the multiplication of about four to eight terms because, for large integers s, $h(s,z_1,z_2)$ is dominated by unity plus terms proportional to $\exp(-s)$, which have a very fast decay. This product expansion is almost identical to the expansion for the Jacobi Θ functions; for the special case of $\phi=90°$ studied by Glasser, it reduces to them. Finally, an expression is needed for the first term of Eq. (6), which is the energy of identical vortices on a primitive lattice, a result derived also by Tkachenko.[6] This term is equivalent to the following limit:

$$\sum_n{}'\ln|\mathbf{L}_n|=\lim_{x\to 0}\left[\sum_n\ln|\mathbf{x}+\mathbf{L}_n|-\ln|\mathbf{x}|\right] \,. \tag{17}$$

Performing this limit on Eq. (14) gives

$$-\sum_n{}'\ln|\mathbf{L}_n|=\frac{\pi}{6\rho}\sin\phi-\ln(2\pi/L_1)-\ln\prod_{s=1}^{\infty}\{1-2e^{-2\pi s|\sin\phi|/\rho}\cos[2\pi s(\cos\phi)/\rho]+e^{-4\pi s|\sin\phi|/\rho}\} \,. \tag{18}$$

Now we scale the energy to obtain equal energies for physically equivalent lattices. This is simply done by noting that E in Eq. (6) is the energy per vortex. Hence, scaling the lengths L_1 and L_2 by a constant α gives the correct normalized energy and renders a constant vortex density. This causes no changes to the ratio L_1/L_2, but in Eq. (18) the dimensional constant L_1 enters alone. We choose the density to be unity, i.e.,

$$\frac{J}{\alpha^2 L_1 L_2 \sin\phi} \equiv 1 \ . \tag{19}$$

Solving for α and multiplying L_1 in Eq. (18) by α then gives

$$\ln(2\pi/\alpha L_1) = \ln\left[2\pi\left[\frac{\sin\phi}{J\rho}\right]^{1/2}\right] , \tag{20}$$

which removes all dimensional constants from Eq. (6), except for the Γ_α, whose dimensions are trivial to remove.

The final result for the energy density is

$$E = \overline{\Gamma}^2\left\{\frac{1}{\rho}\frac{\pi}{6}\sin\phi - \ln\left[2\pi\left[\frac{\sin\phi}{J\rho}\right]^{1/2}\right] - \ln\prod_{s=1}^{\infty} h(s,0,0)\right\}$$
$$+\frac{2}{J}\sum_{\substack{i=1\\ i<j}}^{J}\Gamma_i\Gamma_j\left\{\frac{1}{\rho}\left[\frac{|z_{2,ij}|}{4\pi}\left[\frac{|z_{2,ij}|}{\sin\phi}-2\pi\right]+\frac{\pi}{6}\sin\phi\right]-\tfrac{1}{2}\ln\prod_{s=-\infty}^{\infty} h(s,z_{1,ij},z_{2,ij})\right\} , \tag{21}$$

where $z_{1,ij} = 2\pi(\mathbf{r}_i^0 - \mathbf{r}_j^0)\cdot\hat{x}/L_1$, $z_{2,ij} = 2\pi(\mathbf{r}_i^0 - \mathbf{r}_j^0)\cdot\hat{y}/L_2$, and $h(s,z_1,z_2)$ is defined in Eq. (15). This expression for E gives the relative energy density of lattices containing fixed ratios of vortex species having fixed strengths. To compare the energies of lattices which do not have the same mixtures of vortices requires assumptions or physical information about the vortex self-energies.

What makes Eq. (21) useful for numerical evaluation is the fast convergence of the function $h(s,z_1,z_2)$. Some applications, not discussed here, require calculating the partial derivatives of E, for which it is convenient to change the unit-cell variables ρ and ϕ to $\sigma = 2\pi(\sin\phi)/\rho$ and $\chi = 2\pi(\cos\phi)/\rho$.

IV. EXAMPLES

The foregoing results will now be applied to some simple examples. First, consider the change of lattice energy density induced by varying the angle ϕ between the lattice generators while holding fixed the lengths of the unit cell and the relative positions of the vortices. Three cases will be considered: (a) one vortex per unit cell with $L_1 = L_2$; (b) two vortices per unit cell, also with $L_1 = L_2$; and finally (c) two vortices per unit cell with $L_1 = L_2/\sqrt{3}$. The results as calculated from Eq. (21) are shown in Fig. 1. The triangular lattice occurs for (a) when $\phi = 60°$ and $120°$ and for (c) when $\phi = 90°$. The

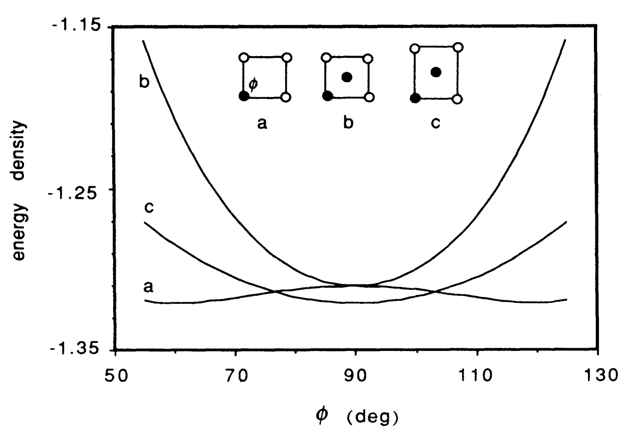

FIG. 1. Effect of varying the angle ϕ between the unit-cell generators for fixed unit-cell lengths. The different unit cells are illustrated for $\phi = 90°$. (a) One vortex per unit cell with $L_1 = L_2$. (b) Two vortices at positions (0,0) and (0.5,0.5) with respect to the unit-cell lengths, $L_1 = L_2$. (c) Two vortices at positions (0,0) and $(0,\sqrt{3}/2)$ in a unit cell with $L_1 = L_2/\sqrt{3} = 1$. The energy density is the energy per vortex in units of $d\Gamma^2/4\pi$, where d is the fluid density and Γ is the unit of circulation.

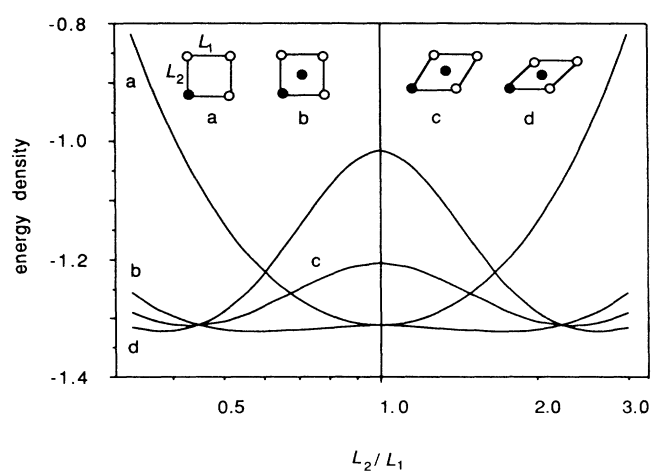

FIG. 2. Effect of changing the aspect ratio L_2/L_1 for fixed angle ϕ. The various unit cells are illustrated for $L_2/L_1 = 1$, with the vortices associated with the unit cell indicated by solid circles. (a) One vortex with $\phi = 90°$. (b) Two vortices with $\phi = 90°$. (c) Two vortices with $\phi = 60°$. (d) Two vortices with $\phi = 45°$.

square lattice occurs for both (a) and (b) at $\phi=90°$. The energy densities of the triangular and square lattices are $-1.321\,117\,428\,4$ and $-1.310\,532\,925\,9$, respectively. (Earlier evaluations of the energies of these simple lattices are equivalent within constants.[6,2]) Although curve (b) has a minimum at $\phi=90°$ this is a constrained minimum and does not result in a stable lattice; indeed, it joins curve (a) which leads to the absolute minimum.

Next, the angle ϕ is constrained and the ratio of unit-cell lengths L_2/L_1 is varied. These results are shown in Fig. 2, where the various cases are (a) one vortex and (b) two vortices per unit cell with $\phi=90°$, (c) two vortices with $\phi=60°$, and (d) two vortices with $\phi=45°$. Only curve (b) achieves the triangular lattice. This occurs at $L_2/L_1=\sqrt{3}$ and $1/\sqrt{3}$. Note that the horizontal scale is logarithmic, to illustrate the symmetry around $L_2/L_1=1$. It appears that curve (d) may also reach the low energy of the triangular lattice. In fact, it does not, nor is the minimum it does reach an unconstrained minimum of the lattice. Also despite appearances, curves (b), (c), and (d) do not mutually intersect.

Finally, the slip strength of the triangular vortex lattice is calculated for displacements along one of the principal axis directions. That is, the energy density is evaluated as a function of a rigid displacement, through one lattice spacing, of a number n of lattice rows with respect to the same number of fixed rows. The pattern repeats, of course, to infinity. During this displacement the unit-cell dimensions and angle are held fixed so, in particular, there is no change in volume. Figure 3 shows the results for various n, as labeled. Obviously, the maximum occurs for a displacement halfway between equilibrium positions and is largest for alternating single rows ($n=1$). This energy is just that of a rectangular lattice with $L_2/L_1=(\sqrt{3}/2)^{\pm 1}=(0.866)^{\pm 1}$, which can be verified by comparing the maximum in Fig. 3 with curve (a) in Fig. 2 at that ratio. The curves are approximately related to each other by

$$n_j[E_j(d)-E_t]\approx n_k[E_k(d)-E_t]\ , \tag{22}$$

where E_t is the triangular lattice energy density (given above) and d is the displacement. Future publications will treat other applications, especially those that involve seeking minima of the energy density in the presence of additional dynamics, mixtures of vortex strengths, and the unconstrained space of lattice variables.[7]

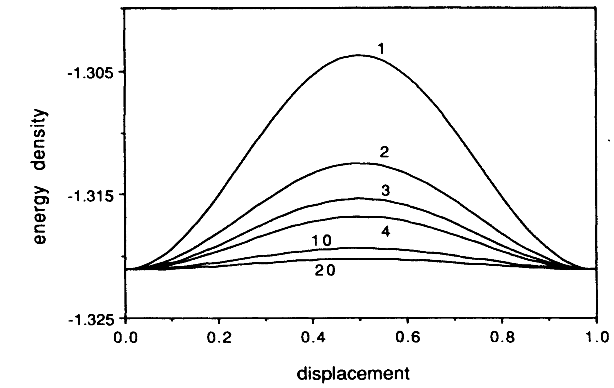

FIG. 3. Slip strength of triangular vortex lattice for the rigid displacement of n rows of vortices with respect to n stationary rows in each unit cell. The curves are labeled by n and the range of displacement is one lattice spacing along a principal axis.

V. CONCLUSION

Lattices of nonneutral vortices, like charges, have a long-range interaction which leads to a formal singularity when the lattice energy is calculated as the $N\rightarrow\infty$ limit of a finite system. By the same method as used for charges, this singularity can be removed by adding a neutralizing background. For vortices, this background is taken to be uniform, with the result that there is no phenomenon of screening. Also, like charges, the field for each vortex leads to a formal singularity in the self-energy in the limit of vanishing core size. This singularity, too, is irrelevant, except that it prevents, in the absence of further assumptions or physical information, a comparison of the lattice energies of vortex systems containing different mixtures of vortex strengths.

The energy density of the general vortex lattice (arbitrary unit cell and arbitrary number, magnitudes and signs of strengths of vortices per unit cell) is given by Eq. (21), which has the virtue of being easily evaluated numerically, in the sense of rapid convergence of its infinite products. This expression provides a new, practical tool for studying a wide range of vortex lattice problems.

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