EXACT INTERACTION ENERGIES OF VORTICES AND DISCLINATIONS
ON A TRIANGULAR LATTICE AND THEIR ASYMPTOTIC LIMITS

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Vortex and defect models of superfluid and melting transitions in two dimensions require the knowledge of the interaction potentials \(-1/\vec{V} \cdot \vec{v}\) and \(1/(\vec{V} \cdot \vec{v})^2\) and their asymptotic forms (to determine the natural core energies). I present an exact evaluation of these potentials on a triangular lattice.

Many recent discussions of the superfluid and the melting transition in two dimensions are based on simple \(XY\) and roughening type models formulated on square or triangular lattices. In the spirit of Kosterlitz and Thouless, the transitions can be understood in terms of pair separation processes [1]. While the universal aspects of these transitions depend only on the long-range part of the potential and thus are independent of the lattice structure, the detailed understanding of the lattice models themselves requires the knowledge of the Green functions \(-1/\vec{V} \cdot \vec{v}\) and \(1/(\vec{V} \cdot \vec{v})^2\) where \(\vec{V} \cdot \vec{v}\) is the lattice laplacian defined on a triangular lattice of spacing 1 by

\[
\vec{V} \cdot \vec{v}(x) = \frac{1}{3} \sum_i \left[ f(x+i) - f(x) \right],
\]

with \(x\) being the lattice sites and \(i\) the links to the 6 nearest neighbours. Our normalization is such as to reproduce the ordinary laplacian in the continuum limit. In the same spirit we shall define the Green functions as follows,

\[
\int -\vec{V} \cdot \vec{v}/2 = \frac{2}{3} \delta_{x,y},
\]

\[
(\vec{V} \cdot \vec{v})/2 = \frac{2}{3} \delta_{x,y}.
\]

Then the right-hand side becomes a Dirac \(\delta\)-function

in the continuum limit and \(v_2, v_4\) tend, for \(|x| \to \infty\), to the solutions of \(-\partial^2 v_2 = \delta(x), \partial^4 v_4 = \delta(x)\).

After a Fourier transformation, \(v_2, v_4\) are given by the integrals

\[
v_2(x) = \frac{2}{\sqrt{3}} \int \frac{d^2 k^{(i)} \exp(ik^{(i)}x^{(i)})}{(2\pi)^2 K \cdot K},
\]

\[
v_4(x) = \frac{2}{\sqrt{3}} \int \frac{d^2 k^{(i)} \exp(ik^{(i)}x^{(i)})}{(2\pi)^2 (K \cdot K)^2},
\]

with

\[
K \cdot K = 4 - \frac{4}{3} \left[ \cos k^{(1)} + \cos k^{(2)} + \cos(k^{(1)} + k^{(2)}) \right].
\]

Here \(x^{(i)}\) are the components of \(x\) in the basis \((1, 0), (-1/2, 1/\sqrt{3}), (1/2, 1/\sqrt{3})\), and \(k^{(i)}\) those in the reciprocal basis \((1, 1/\sqrt{3}), (0, 2/\sqrt{3})\). A subtraction has been performed at the origin to remove the leading infrared singularity.

A direct integration of (1) is possible along the diagonal direction \((x^{(1)}, x^{(2)}) = (n, n)\) where the momentum variables can be changed to \(p = (k^{(1)} + k^{(2)})/2, q = (k^{(1)} - k^{(2)})/2\) so that

\[
v_2(n, n) = \int_0^{2\pi} \frac{dp}{2\pi} \int_0^{\pi} \frac{dq}{\pi} \cos(2pn) \frac{1}{4 - \frac{4}{3} [2 \cos p \cos q + \cos(2p)]},
\]

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\]
\[ v_z'(n, n) = \int_0^{2\pi} \int_0^{\pi} dp \, dq \cos(2\pi n) \frac{1}{\sqrt{4 - \frac{4}{3} [2 \cos p \cos q + \cos(2p)]}}. \]

Notice that \( v(n, n) = v(n, 0) = v(0, n) \), due to the sixfold symmetry. Integrating out \( q \) gives the formulas

\[ v_z'(n, 0) = \frac{1}{2\pi} \int_0^{\pi/2} dp \frac{\cos(2np) - 1}{\sin p} - \frac{1}{s_z}, \quad (4) \]

\[ v_z''(n, 0) = \frac{1}{16\pi} \left( n^2 + \int_0^{\pi/2} dp \frac{\cos(2np) - 1}{\sin^3 p} \frac{1}{s_z} + 2n^2 \sin^2 p \right) - 4z \frac{\partial}{\partial z} \left( \int_0^{\pi/2} dp \frac{\cos(2np) - 1}{\sin^3 p} \frac{1}{s_z} \right), \quad (5) \]

to be evaluated at \( z = 0 \), where I have found it convenient to introduce the abbreviation

\[ s_z = \sqrt{1 - z \sin^2 p}. \quad (6) \]

The introduction of the variable \( z \) has the advantage that for \( z = 0 \), the Green functions reduce to the known square lattice results [2]. This has proven useful for a cross check in all our formulas.

In \( v_0 \), a second subtraction has been performed, to arrive at the finite expression

\[ v_z''(x) = v_z'(x) + \frac{1}{2} x^2 v_2(0), \quad (7) \]

which vanishes at \( x = 0 \), and \( z = (1, 0) \).

I now expand \( \cos(2np) \) in powers of \( \sin^2 p \) and use the well-known integral formula \( B \) is the beta function, \( F \) the hypergeometric function

\[ \int_0^{\pi/2} dp \sin^np \frac{1}{s_z^p} = B((1 + \alpha)/2, \frac{1}{2}) F((1 + \alpha)/2, \rho, 1 + \alpha/2, z). \quad (8) \]

Observe that \( F \) can also be rewritten as

\[ F = (1 - z)^{-\alpha} F \left( \frac{1}{2}, \rho, 1 + \alpha/2, z/(z - 1) \right) \quad (9a) \]

or as

\[ F = (1 - z)^{-(1 + \alpha)/2} (1 + \alpha/2 - \rho, \rho, 1 + \alpha/2, z/(z - 1)), \quad (9b) \]

the latter being useful for the later calculation of the asymptotic limits.

Using (8) one sees that the calculation of (4) and (5) reduces to finite sums of hypergeometric functions \( F(\frac{1}{2}, \frac{1}{2}, 1 + \alpha/2, z) \) for \( \alpha = 1, 3, 5, \ldots \). The first of these is well known,

\[ F(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, z) = z^{-1} \arcsin z. \quad (10) \]

The higher ones are obtained from the recursion relation for Legendre functions,

\[ \frac{d}{dt} P_\nu(t) \]

\[ = (\nu + \mu)(\nu - \mu + 1)(t^2 - 1)^{1/2} P_{\nu - 1}(t) - \mu P_\nu(t), \]

which imply that the functions

\[ f(\lambda, w) = F(\frac{1}{2}, \frac{1}{2}, \lambda, w) \]

satisfy

\[ f(\lambda, w) = (\lambda - \frac{1}{2})^{-2} [ (\lambda - 2)(\lambda - 1) + (\lambda - 1)(1 - w) \partial_w ] f(\lambda, w). \quad (11) \]

Using this and (10), I can calculate successively \( F(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, 1 + \alpha/2, z) \) with \( \alpha = 1, 3, \ldots \). There is an exceptional case, \( \alpha = -1 \). This, however, occurs only in the last term in (5) and, there, only its derivative is needed. So I use the original expression for the integral (8) at \( \rho = 1/2 \),

\[ B((1 + \alpha)/2, \frac{1}{2}) F((1 + \alpha)/2, \frac{1}{2}, 1 + \alpha/2, z) \]

and find its derivative at \( \alpha = -1 \) to be \( F(1, \frac{1}{2}, \frac{3}{2}, z) = (1 - z)^{1/2} \).

In this way I have calculated \( v_{2,4}(n, 0) \) up to \( n = 14 \).

After setting \( v(i, 0) = v(0, -i) \) and \( v(i, 1) = v(i - 1, -1) \) for all \( i \) one can use the laplacian equation

\[ -\nabla \cdot \nabla v_z'(n, -m) = \frac{2}{\sqrt{3}} \delta_{n,0} \]

to calculate the remaining \( v_z'(n, -m) \) by solving the equation for \( v_z'(n, -m - 1) \) successively for \( n = 0, \ldots, n = n_{\text{max}}, m = 0, \ldots, n - 1 \). The result is shown in table 1, in the case of \( v_z'' \), I use \( -\nabla \cdot \nabla v_z''(n, -m) = v_z''(n, -m) \) to do likewise; see again table 1.
Table 1
Subtracted triangular lattice Green functions \(v_2'(x), v_4'(x)\), continuum normalization \((x = (x^{(1)} - x^{(2)}/2, \sqrt{3}x^{(2)}/2))\).

<table>
<thead>
<tr>
<th>(x^{(1)})</th>
<th>(-x^{(2)})</th>
<th>(v_2'(x))</th>
<th>(v_4'(x))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>(-1/2\sqrt{3})</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>(-4/\sqrt{3}+6/\pi)</td>
<td>3/4, (\sqrt{3}/4\pi)</td>
</tr>
<tr>
<td>0</td>
<td>3</td>
<td>(-81/2, \sqrt{3}+72/\pi)</td>
<td>9/\sqrt{3}/2 - 45/2\pi</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>(-464/3+840/\pi)</td>
<td>73, (\sqrt{3}/393)</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
<td>(-11249/2, \sqrt{3}+10200/\pi)</td>
<td>2299, (\sqrt{3}/2 - 12495/2\pi)</td>
</tr>
<tr>
<td>0</td>
<td>6</td>
<td>(-70308/\sqrt{3}+637614/5\pi)</td>
<td>70857, (\sqrt{3}/4 - 385515/4\pi)</td>
</tr>
<tr>
<td>0</td>
<td>7</td>
<td>(-1792225/2, \sqrt{3}+8126832/5\pi)</td>
<td>268619, (\sqrt{3}/7308231/5\pi)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>(1/, \sqrt{3} - 3/\pi)</td>
<td>3/8\pi</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>(15/2, \sqrt{3} - 15/\pi)</td>
<td>(-\sqrt{3}/2 + 33/8\pi)</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>(105/2, \sqrt{3} - 192/\pi)</td>
<td>(-25/\sqrt{3}+285/4\pi)</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>(2671/2, \sqrt{3} - 2424/\pi)</td>
<td>(-459, \sqrt{3}/2 + 5019/4\pi)</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>(17177/3, \sqrt{3} - 155787/5\pi)</td>
<td>(-7619, \sqrt{3}/2 + 165909/8\pi)</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>(445355/2, \sqrt{3} - 2020287/5\pi)</td>
<td>(-60355\sqrt{3}/3 + 262743/9\pi)</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
<td>(2912113/\sqrt{3} - 184869672/35\pi)</td>
<td>(-930987, 3 + 50658909/10\pi)</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>(-24/3 + 42/\pi)</td>
<td>(3/\sqrt{3}/2 - 21/4\pi)</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>(-369/2, \sqrt{3} + 333/\pi)</td>
<td>(47/\sqrt{3}/2 - 981/8\pi)</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>(-2996/\sqrt{3} + 27162/\pi)</td>
<td>(2125, 3/4 - 11529/4\pi)</td>
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<tr>
<td>2</td>
<td>5</td>
<td>(-84225/2, \sqrt{3} + 381909/5\pi)</td>
<td>(9744, 3/4 - 2102331/40\pi)</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>(-584152/\sqrt{3} + 37083642/35\pi)</td>
<td>(330411, 3/4 - 17978619/20\pi)</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>(-16031265/2, \sqrt{3} + 508856151/35\pi)</td>
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</tr>
<tr>
<td>3</td>
<td>3</td>
<td>(657/\sqrt{3} - 3967/\pi)</td>
<td>(-81, \sqrt{3} + 3591/8\pi)</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>(10305/2, \sqrt{3} - 46728/\pi)</td>
<td>(-962, \sqrt{3} + 104931/20\pi)</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>(89377/3, \sqrt{3} - 3673984/35\pi)</td>
<td>(-21090, \sqrt{3} + 573879/5\pi)</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>(2657151/2, \sqrt{3} - 84341997/35\pi)</td>
<td>(-386100, \sqrt{3} + 117652995/56\pi)</td>
</tr>
<tr>
<td>3</td>
<td>7</td>
<td>(19372089/\sqrt{3} - 245959939/7\pi)</td>
<td>(-13283079, \sqrt{3}/2 + 10119001143/280\pi)</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>(-19168/3 + 1216776/35\pi)</td>
<td>(3510, \sqrt{3} - 19083/\pi)</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>(-304065/2, \sqrt{3} - 9651408/35\pi)</td>
<td>(37374, \sqrt{3} - 28468317/140\pi)</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>(-2738196/\sqrt{3} - 173828766/35\pi)</td>
<td>(3228261, 3/4 - 6148194927/140\pi)</td>
</tr>
<tr>
<td>4</td>
<td>7</td>
<td>(-84370065/2, \sqrt{3} - 2678031408/35\pi)</td>
<td>(29506005, \sqrt{3}/2 - 2247753873/280\pi)</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>(579249/\sqrt{3} - 36772521/35\pi)</td>
<td>(-140499, \sqrt{3} + 30581547/40\pi)</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>(9255951/2, \sqrt{3} - 293797737/35\pi)</td>
<td>(-2821497, \sqrt{3}/2 + 2149441014/280\pi)</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
<td>(85379241/3 - 8517344832/55\pi)</td>
<td>(-60376353, \sqrt{3}/2 + 22997230047/140\pi)</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>(-17893584/\sqrt{3} + 124965746108/35\pi)</td>
<td>(10801755, \sqrt{3}/2 - 822871899/28\pi)</td>
</tr>
<tr>
<td>6</td>
<td>7</td>
<td>(-287386737/2, \sqrt{3} + 14334701607/55\pi)</td>
<td>(104550807, \sqrt{3}/2 - 876109787451/3080\pi)</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>(561273441/\sqrt{3} - 5095277250087/5005\pi)</td>
<td>(-202592070, \sqrt{3} + 61733513181/56\pi)</td>
</tr>
</tbody>
</table>

For most practical calculations it is sufficient to use the large \(|x|\) formulas. For these I find after some lengthy manipulations [2], using formula (9b)

\[
v_2'(x) = -\frac{1}{2\pi} \ln(|x|2\sqrt{3} \varepsilon^2), \tag{12a}
\]

\[
v_4'(x) = \frac{1}{8\pi} \left[ |x|^{2} \varepsilon^{2} \right] \ln(|x|2\sqrt{3} \varepsilon^{-1/6})
- \frac{1}{2} \ln(|x|2\sqrt{3} \varepsilon^{-1/6}) \right]. \tag{12b}
\]

These expressions are reliable as soon as \(|x|\) reaches beyond the nearest neighbor. Since my formulas (4), (5) give at \(z = 0\) the results for a square lattice, I can easily reproduce the potentials also in that case and find agreement with available lists [2,3].

For the asymptotic limits on a square lattice I find the same expressions as in (12), except with \(\sqrt{3}\) replaced by \(\sqrt{2}\).
References

  A.P. Young, Phys. Rev. B 19 (1979) 1855;
  K.J. Strandburg, Rev. Mod. Phys. 60 (1988) 161;
