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 $-1/\bar{\nabla}\cdot\nabla$ and $1/(\bar{\nabla}\cdot\nabla)^2$ 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 $-1/\bar{\nabla}\cdot\nabla$ and $1/(\bar{\nabla}\cdot\nabla)^2$ where $\bar{\nabla}\cdot\nabla$ is the lattice laplacian defined on a triangular lattice of spacing 1 by

$$\bar{\nabla}\cdot\nabla f(\boldsymbol{x})=\tfrac{2}{3}\sum_{\boldsymbol{i}}[f(\boldsymbol{x}+\boldsymbol{i})-f(\boldsymbol{x})]\,, \tag{1}$$

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,

$$-\bar{\nabla}\cdot\nabla v_2(\boldsymbol{x})=\frac{2}{\sqrt{3}}\,\delta_{\boldsymbol{x},\boldsymbol{0}}\,,$$

$$(\bar{\nabla}\cdot\nabla)^2 v_4(\boldsymbol{x})=\frac{2}{\sqrt{3}}\,\delta_{\boldsymbol{x},\boldsymbol{0}}\,. \tag{2}$$

Then the right-hand side becomes a Dirac δ-function in the continuum limit and v_2, v_4 tend, for $|\boldsymbol{x}|\to\infty$, to the solutions of $-\partial^2 v_2=\delta(\boldsymbol{x})$, $\partial^4 v_4=\delta(\boldsymbol{x})$.

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

$$v_2'(\boldsymbol{x})=\frac{2}{\sqrt{3}}\int\frac{\mathrm{d}^2k^{(i)}}{(2\pi)^2}\,\frac{\exp(\mathrm{i}k^{(i)}x^{(i)})-1}{\bar{\boldsymbol{K}}\cdot\boldsymbol{K}}\,,$$

$$v_4'(x)=\frac{2}{\sqrt{3}}\int\frac{\mathrm{d}^2k^{(i)}}{(2\pi)^2}\,\frac{\exp(\mathrm{i}k^{(i)}x^{(i)})}{(\bar{\boldsymbol{K}}\cdot\boldsymbol{K})^2}\,, \tag{3}$$

with

$$\bar{\boldsymbol{K}}\cdot\boldsymbol{K}\equiv 4-\tfrac{4}{3}[\cos k^{(1)}+\cos k^{(2)}+\cos(k^{(1)}+k^{(2)})]\,.$$

Here $x^{(i)}$ are the components of $\boldsymbol{x}$ in the basis $(1,0)$, $(-\frac{1}{2},\frac{1}{2}\sqrt{3})$, 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

$$v_2'(n,n)\equiv\int_0^{2\pi}\frac{\mathrm{d}p}{2\pi}\int_0^{\pi}\frac{\mathrm{d}q}{\pi}\times\frac{\cos(2pn)-1}{4-\frac{4}{3}[2\cos p\cos q+\cos(2p)]}\,,$$

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$$v_4'(n,n)=\int_0^{2\pi}\frac{dp}{2\pi}\int_0^{\pi}\frac{dq}{\pi}$$

$$\times\frac{\cos(2pn)-1}{\{4-\frac{4}{3}[2\cos p\cos q+\cos(2p)]\}^2}\,.$$

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

$$v_2'(n,0)=\frac{1}{2\pi}\int_0^{\pi/2}dp\,\frac{\cos(2np)-1}{\sin p}\frac{1}{s_z}\,, \tag{4}$$

$$v_4''(n,0)=\frac{1}{16\pi}\Bigg(n^2+\int_0^{\pi/2}dp\,[\cos(2np)-1$$

$$+2n^2\sin^2p]\,\frac{1}{\sin^3p}\frac{1}{s_z}$$

$$-4z\frac{\partial}{\partial z}\int_0^{\pi/2}dp\,[\cos(2np)-1]\,\frac{1}{\sin^3p}\frac{1}{s_z}\Bigg)\,, \tag{5}$$

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

$$s_z=\sqrt{1-z\sin^2p}\,. \tag{6}$$

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_4, a second subtraction has been performed, to arrive at the finite expression

$$v_4''(\boldsymbol{x})\equiv v_4'(\boldsymbol{x})+\tfrac{1}{2}\boldsymbol{x}^2v_2(\boldsymbol{0})\,, \tag{7}$$

which vanishes at $\boldsymbol{x}=\boldsymbol{0}$, and $\boldsymbol{x}=(1,0)$.

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

$$\int_0^{\pi/2}dp\,\sin^\alpha p\,\frac{1}{s_z^{2\rho}}$$

$$=B((1+\alpha)/2,\tfrac{1}{2})F((1+\alpha)/2,\rho,1+\alpha/2,z)\,. \tag{8}$$

Observe that F can also be rewritten as

$$F=(1-z)^{-\rho}F(\tfrac{1}{2},\rho,1+\alpha/2,z/(z-1)) \tag{9a}$$

or as

$$F=(1-z)^{-(1+\alpha)/2}(1+\alpha/2-\rho,\rho,$$

$$1+\alpha/2,z/(z-1))\,, \tag{9b}$$

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,

$$F(\tfrac{1}{2},\tfrac{1}{2},\tfrac{3}{2},z)=z^{-1}\,\mathrm{arsin}\,z\,. \tag{10}$$

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

$$(t^2-1)\frac{d}{dt}P_\nu^\mu(t)$$

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

$$-\mu tP_\nu^\mu(t)\,,$$

which imply that the functions

$$f(\lambda,w)=F(\tfrac{1}{2},\tfrac{1}{2},\lambda,w)$$

satisfy

$$f(\lambda,w)=(\lambda-\tfrac{3}{2})^{-2}[(\lambda-2)(\lambda-1)$$

$$+(\lambda-1)(1-w)\partial_w]f(\lambda-1,w)\,. \tag{11}$$

Using this and (10), I can calculate successively $F(\frac{1}{2},\frac{1}{2},1+\alpha/2,z)$ 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 $\rho=1/2$,

$$B((1+\alpha)/2,\tfrac{1}{2})F((1+\alpha)/2,\tfrac{1}{2},1+\alpha/2,z)$$

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

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

$$-\bar{\nabla}\cdot\nabla v_2'(n,-m)=\frac{2}{\sqrt{3}}\delta_{x,0}$$

to calculate the remaining $v_2'(n,-m)$ by solving the equation for $v_2'(n,-m-1)$ successively for $n=0,\ldots,n=n_{\max}$; $m=0,\ldots,n-1$. The result is shown in table 1, in the case of v_4'', I use $-\bar{\nabla}\cdot\nabla v_4''(n,-m)=v_2'(n,-m)$ to do likewise; see again table 1.

Table 1
Subtracted triangular lattice Green functions $v'_2(\boldsymbol{x})$, $v''_4(\boldsymbol{x})$, continuum normalization ($\boldsymbol{x}=(x^{(1)}-x^{(2)}/2, \sqrt{3}\,x^{(2)}/2)$).

$x^{(1)}$	$-x^{(2)}$	$v'_2(\boldsymbol{x})$	$v''_4(\boldsymbol{x})$
0	1	$-1/2\sqrt{3}$	0
0	2	$-4/\sqrt{3}+6/\pi$	$3/4\sqrt{3}-3/4\pi$
0	3	$-81/2\sqrt{3}+72/\pi$	$9\sqrt{3}/2-45/2\pi$
0	4	$-464/\sqrt{3}+840/\pi$	$73\sqrt{3}-393/\pi$
0	5	$-11249/2\sqrt{3}+10200/\pi$	$2299\sqrt{3}/2-12495/2\pi$
0	6	$-70308/\sqrt{3}+637614/5\pi$	$70857\sqrt{3}/4-385515/4\pi$
0	7	$-1792225/2\sqrt{3}+8126832/5\pi$	$268619\sqrt{3}-7308231/5\pi$
1	1	$1/\sqrt{3}-3/\pi$	$3/8\pi$
1	2	$15/2\sqrt{3}-15/\pi$	$-\sqrt{3}/2+33/8\pi$
1	3	$105/\sqrt{3}-192/\pi$	$-25\sqrt{3}/2+285/4\pi$
1	4	$2671/2\sqrt{3}-2424/\pi$	$-459\sqrt{3}/2+5019/4\pi$
1	5	$17177/\sqrt{3}-155787/5\pi$	$-7619\sqrt{3}/2+165909/8\pi$
1	6	$445535/2\sqrt{3}-2020287/5\pi$	$-60355\sqrt{3}+2627439/8\pi$
1	7	$2912113/\sqrt{3}-184869672/35\pi$	$-930987\sqrt{3}+50658909/10\pi$
2	2	$-24/\sqrt{3}+42/\pi$	$3\sqrt{3}/2-21/4\pi$
2	3	$-369/2\sqrt{3}+333/\pi$	$47\sqrt{3}/2-981/8\pi$
2	4	$-2996/\sqrt{3}+27162/5\pi$	$2125\sqrt{3}/4-11529/4\pi$
2	5	$-84225/2\sqrt{3}+381909/5\pi$	$9744\sqrt{3}-2120331/40\pi$
2	6	$-584152/\sqrt{3}+37083642/35\pi$	$330411\sqrt{3}/2-17978619/20\pi$
2	7	$-16031265/2\sqrt{3}+508856151/35\pi$	$2672097\sqrt{3}-4071177399/280\pi$
3	3	$657/\sqrt{3}-5967/5\pi$	$-81\sqrt{3}+3591/8\pi$
3	4	$10303/2\sqrt{3}-46728/5\pi$	$-962\sqrt{3}+104931/20\pi$
3	5	$89377/\sqrt{3}-5673984/35\pi$	$-21090\sqrt{3}+573879/5\pi$
3	6	$2657151/2\sqrt{3}-84341997/35\pi$	$-386100\sqrt{3}+117652995/56\pi$
3	7	$19372089/\sqrt{3}-245959593/7\pi$	$-13283079\sqrt{3}/2+10119001143/280\pi$
4	4	$-19168/\sqrt{3}+1216776/35\pi$	$3510\sqrt{3}-19083/\pi$
4	5	$-304065/2\sqrt{3}+9651408/35\pi$	$37374\sqrt{3}-28468317/140\pi$
4	6	$-2738196/\sqrt{3}+173828766/35\pi$	$3228261\sqrt{3}/4-614814927/140\pi$
4	7	$-84370065/2\sqrt{3}+2678031408/35\pi$	$29506005\sqrt{3}/2-2247753873/28\pi$
5	5	$579249/\sqrt{3}-36772521/35\pi$	$-140499\sqrt{3}+30581547/40\pi$
5	6	$9255951/2\sqrt{3}-293797737/35\pi$	$-2821497\sqrt{3}/2+2149414101/280\pi$
5	7	$85379241/\sqrt{3}-8517344832/55\pi$	$-60376353\sqrt{3}/2+22997230047/140\pi$
6	6	$-17895384/\sqrt{3}+12496574106/385$	$10801755\sqrt{3}/2-822871899/28\pi$
6	7	$-287386737/2\sqrt{3}+14334701607/55$	$104550807\sqrt{3}/2-876109787451/3080\pi$
7	7	$561273441/\sqrt{3}-5095277250087/5005\pi$	$-202592070\sqrt{3}+61733513181/56\pi$

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

$$v'_2(\boldsymbol{x}) = -\frac{1}{2\pi}\ln(|\boldsymbol{x}|2\sqrt{3}\,e^{\gamma}) , \qquad (12a)$$

$$v''_4(\boldsymbol{x}) = \frac{1}{8\pi}\,[\,|\boldsymbol{x}|^2\ln(|\boldsymbol{x}|\;2\sqrt{3}\,e^{\gamma-1}) - \tfrac{1}{2}\ln(|\boldsymbol{x}|2\sqrt{3}\,e^{\gamma-1/6})\,] . \qquad (12b)$$

These expressions are reliable as soon as $|\boldsymbol{x}|$ 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 $\sqrt{2}$.

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