Charge neutrality and boundary conditions in the classical Coulomb lattice gas

1981 J. Phys. A: Math. Gen. 14 L257

(http://iopscience.iop.org/0305-4470/14/7/007)

J. Phys. A: Math. Gen. **14** (1981) L257–L261. Printed in Great Britain

LETTER TO THE EDITOR

Charge neutrality and boundary conditions in the classical Coulomb lattice gas

E R Smith

Mathematics Department, University of Melbourne, Parkville, Victoria 3052, Australia

Received 6 May 1981

Abstract. Exact equivalences between the two-dimensional classical Coulomb lattice gas, the discrete Gaussian solid on solid model and the Villain plane rotator model are explored for finite lattices. The energy of the Coulomb system is written in terms of solutions to the lattice Poisson equation with Dirichlet, Neumann or periodic boundary conditions. The role of charge neutrality conditions on the Coulomb system is clarified.

The two-dimensional classical Coulomb lattice gas (CG) is known to be equivalent to the discrete Gaussian solid on solid model (DG) and the Villain plane rotator model (VPR) (Berezinskii 1971, Kosterlitz and Thouless 1973, Villain 1975, Chui and Weeks 1976, Knops 1977, José *et al* 1977, Kadanoff 1978). The equivalences have been used in simulation studies of one model on a finite lattice to predict properties of the other models (e.g. Shugard *et al* 1978, 1980). A precise theory of the role of charge neutrality in CG is lacking and this letter presents some clarifying results for finite systems. Note that in CG, the charge on a lattice site is equal to an elementary charge times any integer.

Consider a finite lattice $\Lambda \subset Z^2$. The configurations of CG are sets of integers $\{q(\boldsymbol{n});\, \boldsymbol{n} \in \Lambda,\, q(\boldsymbol{n}) \in Z\}$. The energy of a configuration may be written

$$E = \tfrac{1}{2}Q^2 \sum_{\boldsymbol{n}\in\Lambda} q(\boldsymbol{n})\phi(\boldsymbol{n}; C) \tag{1}$$

where $\phi(\boldsymbol{n}; C)$ is the solution of the lattice Poisson equation

$$D^2\phi(\boldsymbol{n}; C) = -q(\boldsymbol{n}) \tag{2}$$

on Λ with some specified boundary condition C. The operator D^2 is the two-dimensional symmetric difference analogue of the Laplacian. The partition function in boundary conditions C is then

$$Z_{\mathrm{CG}}(Q^2; \Lambda; C) = \sum_{\{q(\boldsymbol{n})\}} \exp\left(-\tfrac{1}{2}Q^2 \sum_{\boldsymbol{n}\in\Lambda} q(\boldsymbol{n})\phi(\boldsymbol{n}; C)\right). \tag{3}$$

Only those sets $\{q(\boldsymbol{n})\}$ for which a solution to (2) exists are included in the sum. Three boundary conditions are considered.

(i) D (Dirichlet). Let $\Lambda = L_N = [1, N]^2$, $L_N^* = [0, N+1]^2$, $\partial L_N^* = L_N^* \backslash L_N$. For $\{q(\boldsymbol{n}): \boldsymbol{n} \in L_N\}$, solve (2) on L_N such that $\phi(\boldsymbol{n}; D) = 0$ if $\boldsymbol{n} \in \partial L_N^*$.

(ii) Ne (Neumann). For $\{q(\boldsymbol{n}): \boldsymbol{n} \in L_N\}$, solve (2) on L_N such that $\phi(1, n; Ne) - \phi(0, n; Ne) = \phi(N+1, n; Ne) - \phi(N, n; Ne) = \phi(n, 1; Ne) - \phi(n, 0; Ne) = \phi(n, N+1; Ne) - \phi(n, N; Ne) = 0$, $1 \leq n \leq N$.

0305-4470/81/070257+05\$01.50

(iii) P (Periodic). Let $\Lambda=\Lambda_N=[-N, N]^2$. For $\{q(\boldsymbol{n}): \boldsymbol{n}\in\Lambda_N\}$, extend periodically with period $(2N+1)$ to $\{q(\boldsymbol{n}): \boldsymbol{n}\in Z^2\}$. Solve (2) on $\Lambda=Z^2$ with $\phi(\boldsymbol{n}+(2N+1)\boldsymbol{m}; P)=\phi(\boldsymbol{n}; P)$ for $\boldsymbol{n}, \boldsymbol{m}\in Z^2$.

Consider the boundary conditions for D. Define $f_k(n)=(2/(N+1))^{1/2}\sin[\pi kn/(N+1)]$ and $F_{\boldsymbol{k}}(\boldsymbol{n})=f_{k_1}(n_1)f_{k_2}(n_2)$. Then for all $\{q(\boldsymbol{n}): \boldsymbol{n}\in L_N\}$

$$\phi(\boldsymbol{n}; D)=\sum_{\boldsymbol{n}'\in L_N}\sum_{\boldsymbol{k}\in L_N}\frac{F_{\boldsymbol{k}}(\boldsymbol{n})F_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(\pi\boldsymbol{k}/(N+1))}q(\boldsymbol{n}') \tag{4}$$

with $\lambda(\boldsymbol{\xi})=4-2\cos\xi_1-2\cos\xi_2$. Thus

$$Z_{\mathrm{CG}}(Q^2; L_N; D)=\sum_{\{q(\boldsymbol{n})\}}\exp\left[-\tfrac{1}{2}Q^2\sum_{\boldsymbol{n},\boldsymbol{n}'\in L_N}q(\boldsymbol{n})\left(\sum_{\boldsymbol{k}\in L_N}\frac{F_{\boldsymbol{k}}(\boldsymbol{n})F_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(\pi\boldsymbol{k}/(N+1))}\right)q(\boldsymbol{n}')\right]. \tag{5}$$

Use of the Poisson summation formula gives

$$Z_{\mathrm{CG}}(Q^2; L_N; D)=Z_{\mathrm{SW}}(L_N; D)Z_{\mathrm{DG}}(\pi^2/Q^2; L_N^*; D).$$

Here

$$Z_{\mathrm{SW}}(L_N; D)=\prod_{\boldsymbol{k}\in L_N}(2\pi\lambda(\pi\boldsymbol{k}/(N+1))/Q^2)^{1/2}$$

is a spin wave partition function and

$$Z_{\mathrm{DG}}(K; L_N^*; D)=\sum_{\{m(\boldsymbol{n}):\boldsymbol{n}\in L_N^*\}}\exp\left(-K\sum_{\boldsymbol{n}\in L_N^*}\sum_{\boldsymbol{a}\in R(\boldsymbol{n})}[m(\boldsymbol{n})-m(\boldsymbol{n}+\boldsymbol{a})]^2\right). \tag{6}$$

In this equation $R(\boldsymbol{n})$ is that subset of $\{(\pm1, 0), (0, \pm1)\}$ such that $\boldsymbol{n}+\boldsymbol{a}\in L_N^*$ and $m(\boldsymbol{n})=0$ if $\boldsymbol{n}\in\partial L_N^*$. Thus $Z_{\mathrm{DG}}(K; L_N^*; D)$ is the partition function for a DG model on L_N^* with zero displacement at the edge sites. The standard transformation to the VPR model (e.g. José *et al* 1977) gives $Z_{\mathrm{DG}}(K; L_N^*; D)=Z_{\mathrm{VPR}}(V_{1/K}; L_{N+1}; D)$, the partition function for the VPR model on L_{N+1} with free boundaries and the nearest-neighbour potential

$$\exp(-V_{1/K}(\theta))=(\pi/2K)^{1/2}\sum_{l=-\infty}^{\infty}\exp\left(-\frac{1}{8K}(\theta-2\pi l)^2\right). \tag{7}$$

In their celebrated analysis of two-dimensional systems, Kosterlitz and Thouless (1973) assumed that only configurations with $q(\boldsymbol{n})=0, \pm1$ were important near the presumed critical point. The CG − DG equivalence for D boundary conditions gives

$$\langle q^2(\boldsymbol{n})\rangle_{\mathrm{CG}}=\frac{4}{Q^2}\left(1-\frac{\pi^2}{Q^2}\left\langle\left\{\sum_{\boldsymbol{a}\in R(\boldsymbol{n})}[m(\boldsymbol{n})-m(\boldsymbol{n}+\boldsymbol{a})]\right\}^2\right\rangle_{\mathrm{DG}}\right). \tag{8}$$

Defining $Q_N=\Sigma_{\boldsymbol{n}\in L_N}q(\boldsymbol{n})$, the result

$$\langle Q_N^2\rangle_{\mathrm{CG}}=\frac{4N}{Q^2}\left(1-\frac{\pi^2}{NQ^2}\left\langle\left[\sum_{n=1}^{N}m(1, n)+m(n, 1)+m(n, N)+m(N, n)\right]^2\right\rangle_{\mathrm{DG}}\right) \tag{9}$$

is obtained. Equations (8) and (9) give simple bounds for $\langle q^2(\boldsymbol{n})\rangle_{\mathrm{CG}}$ and $\langle Q_N^2\rangle_{\mathrm{CG}}$. Shugard *et al* (1978) give the estimate $K_R^{-1}\simeq2.92$ so that $\langle q^2(\boldsymbol{n})\rangle_{\mathrm{CG}}\lesssim0.13$ at the presumed critical point. This certainly suggests that only small values of $q(\boldsymbol{n})$ will contribute at the presumed critical point. This boundary condition requires no charge neutrality constraint but equation (9) shows that deviations from overall charge neutrality are governed by $\langle Q_N^2\rangle_{\mathrm{CG}}\leqslant4N/Q^2$ and that $N^{-2}\langle Q_N^2\rangle_{\mathrm{CG}}\to0$ as $N\to\infty$.

For the boundary conditions Ne, define $L'_N=[0,N-1]^2$, $g_k(n)=(2/N)^{1/2}\cos[\pi k(n-\frac{1}{2})/N]$ if $k\neq 0$, $g_0(n)=N^{-1/2}$ and $G_{\boldsymbol{k}}(\boldsymbol{n})=g_{k_1}(n_1)g_{k_2}(n_2)$ for $\boldsymbol{k}\in L'_N$. If and only if $Q_N=\Sigma_{\boldsymbol{n}\in L_N}q(\boldsymbol{n})=0$, equation (2) has a solution which is

$$\phi(\boldsymbol{n};Ne)=\sum_{\boldsymbol{n}'\in L_N}\sum_{\substack{\boldsymbol{k}\in L'_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}\frac{G_{\boldsymbol{k}}(\boldsymbol{n})G_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(\pi\boldsymbol{k}/N)}q(\boldsymbol{n}') \tag{10}$$

plus an arbitrary constant. The partition function is

$$Z_{\mathrm{CG}}(Q^2;L_N;Ne)=\sum_{\{q(\boldsymbol{n})\}}\delta_{Q_N,0}\exp\left(-\tfrac{1}{2}Q^2\sum_{\boldsymbol{n},\boldsymbol{n}'\in L_N}q(\boldsymbol{n})\sum_{\substack{\boldsymbol{k}\in L'_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}\frac{G_{\boldsymbol{k}}(\boldsymbol{n})G_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(\pi\boldsymbol{k}/N)}q(\boldsymbol{n}')\right). \tag{11}$$

Use of the Poisson summation formula gives

$$Z_{\mathrm{CG}}(Q^2;L_N;Ne)=Z_{\mathrm{SW}}(L_N;Ne)Z_{\mathrm{DG}}(\pi^2/Q^2;L_N;Ne).$$

Here

$$Z_{\mathrm{SW}}(L_N;Ne)=N^{-1}\prod_{\substack{\boldsymbol{k}\in L'_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}[2\pi\lambda(\pi\boldsymbol{k}/N)/Q^2]^{1/2}$$

is another spin wave partition function while

$$Z_{\mathrm{DG}}(K;L_N;Ne)=\sum_{\{m(\boldsymbol{n})\}}\delta_{m(1,1),0}\exp\left(-K\sum_{\boldsymbol{n}\in L_N}\sum_{\boldsymbol{a}\in S(\boldsymbol{n})}[m(\boldsymbol{n})-m(\boldsymbol{n}+\boldsymbol{a})]^2\right). \tag{12}$$

In equation (12) the sum over $\boldsymbol{a}\in S(\boldsymbol{n})$ is over those $\boldsymbol{a}(=(\pm1,0),(0,\pm1))$ for which $\boldsymbol{n}+\boldsymbol{a}\in L_N$. This is the partition function for a DG model on L_N with free edges and the displacement at one site (chosen as (1, 1), in a corner) fixed and zero. For these boundary conditions, equation (8) holds but with $R(\boldsymbol{n})$ replaced by $S(\boldsymbol{n})$ and the CG and DG expectations with D of equation (8) replaced by expectations with Ne, as long as $\boldsymbol{n}$ is not on an edge of L_N. Further transformation gives $Z_{\mathrm{DG}}(K;L_N;Ne)=Z_{\mathrm{VPR}}(V_{1/K};L_{N+1};Ne)$ the partition function for a VPR model with nearest-neighbour potential $V_{1/K}(\theta)$ and with the rotors on the edge of L_{N+1} fixed at $\theta(\boldsymbol{n})=0$.

For the boundary conditions P, define $h_k(n)=(2N+1)^{-1/2}\exp(2\pi ikn/2N+1)$ and $H_{\boldsymbol{k}}(\boldsymbol{n})=h_{k_1}(n_1)h_{k_2}(n_2)$. If and only if $Q_N=\Sigma_{\boldsymbol{n}\in\Lambda_N}q(\boldsymbol{n})=0$, then equation (2) has a solution which is

$$\phi(\boldsymbol{n},P)=\sum_{\boldsymbol{n}'\in\Lambda_n}\sum_{\substack{\boldsymbol{k}\in\Lambda_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}\frac{H^*_{\boldsymbol{k}}(\boldsymbol{n})H_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(2\pi\boldsymbol{k}/(2N+1))}q(\boldsymbol{n}') \tag{13}$$

plus an arbitrary constant. Thus the partition function may be written

$$Z_{\mathrm{CG}}(Q^2;\Lambda_N;P)=\sum_{\{q(\boldsymbol{n})\}}\delta_{Q_N,0}\exp\left(-\tfrac{1}{2}Q^2\sum_{\boldsymbol{n},\boldsymbol{n}'\in\Lambda_N}q(\boldsymbol{n})\sum_{\substack{\boldsymbol{k}\in\Lambda_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}\frac{H^*_{\boldsymbol{k}}(\boldsymbol{n})H_{\boldsymbol{k}}(\boldsymbol{n}')}{\lambda(2\pi\boldsymbol{k}/(2N+1))}q(\boldsymbol{n}')\right). \tag{14}$$

Transformation to the DG model gives

$$Z_{\mathrm{CG}}(Q^2;\Lambda_N;P)=Z_{\mathrm{SW}}(\Lambda_N;P)Z_{\mathrm{DG}}(\pi^2/Q^2;\Lambda_N;P).$$

Here

$$Z_{\mathrm{SW}}(\Lambda_N;P)=(2N+1)^{-1}\prod_{\substack{\boldsymbol{k}\in\Lambda_N\\ \boldsymbol{k}\neq\boldsymbol{0}}}\{2\pi\lambda[2\pi\boldsymbol{k}/(2N+1)]/Q^2\}^{1/2}$$

is a further spin wave partition function and

$$Z_{\mathrm{DG}}(K;\Lambda_N;P)=\sum_{\{m(\boldsymbol{n})\}}\delta_{m(\mathbf{0}),0}\exp\Big(-K\sum_{\boldsymbol{n}\in\Lambda_N}\sum_{\boldsymbol{a}\in T}[m(\boldsymbol{n})-m(\boldsymbol{n}+\boldsymbol{a})]^2\Big) \tag{15}$$

is the partition function for a DG model in periodic boundary conditions with one site (chosen as $\mathbf{0}$) having fixed zero displacement. For $\boldsymbol{a}\in T$, $\boldsymbol{n}+\boldsymbol{a}$ is a nearest neighbour of $\boldsymbol{n}$ defined periodically. For these boundary conditions, equation (8) holds for all $\boldsymbol{n}$ if T replaces $R(\boldsymbol{n})$ and the expectations are taken with the P boundary condition. Transformation of this DG model to a VPR model must be carried out with some care to give $Z_{\mathrm{DG}}(K;\Lambda_N;P)=Z_{\mathrm{VPR}}(V_{1/K};\Lambda_N;P)$, where

$$\begin{aligned}
Z_{\mathrm{VPR}}&(V_K;\Lambda_N;P)\\
&=\int_{-\pi}^{\pi}\frac{\mathrm{d}\phi_1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\phi_2}{2\pi}\Big(\prod_{\boldsymbol{n}\in\Lambda_N}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta(\boldsymbol{n})}{2\pi}\Big)\\
&\times\exp\Big(-\sum_{\substack{\boldsymbol{n}\in\Lambda_N\\ n_1\neq 0}}V_K(\theta(n_1,n_2)-\theta(n_1+1,n_2))\\
&-\sum_{\substack{\boldsymbol{n}\in\Lambda_N\\ n_2\neq 0}}V_K(\theta(n_1,n_2)-\theta(n_1,n_2+1))-\sum_{n_2=-N}^{N}V_K(\theta(0,n_2)-\theta(1,n_2)+\phi_1)\\
&-\sum_{n_1=-N}^{N}V_K(\theta(n_1,0)-\theta(n_1,1)+\phi_2)\Big).
\end{aligned} \tag{16}$$

This is the partition function for a VPR model in periodic boundary conditions on Λ_N in which the usual interactions between rotors at (n_1, n_2), (n_1+1, n_2) and at (n_1, n_2), (n_1, n_2+1) are replaced by three-rotor interactions of the pair of rotors and a third rotor as shown. This means that while periodic boundary conditions apply, the model is not translationally invariant.

Chui and Weeks (1976) consider a periodic DG partition function which on Λ_N may be written

$$Z_{\mathrm{DG}}(K;\Lambda_N;\nu^2)=\sum_{\{m(\boldsymbol{n})\}}\exp\Big(-K\sum_{\boldsymbol{n}\in\Lambda_N}\sum_{\boldsymbol{a}\in T}[m(\boldsymbol{n})-m(\boldsymbol{n}+\boldsymbol{a})]^2-\nu^2\sum_{\boldsymbol{n}\in\Lambda_N}m^2(\boldsymbol{n})\Big). \tag{17}$$

They give arguments connecting this partition function in the limit $\nu\to 0$ to that for a CG system with periodic boundary conditions and an exact charge neutrality constraint. A connection with this work is made by the relation

$$\lim_{\nu\to 0}\Big[Z_{\mathrm{DG}}(K;\Lambda_N;\nu^2)-\frac{\sqrt{\pi}}{(2N+1)\nu}Z_{\mathrm{DG}}(K;\Lambda_N;P)\Big]=0. \tag{18}$$

In the transformation of $Z_{\mathrm{DG}}(K;\Lambda_N;\nu^2)$ to a CG partition function, the divergence as $\nu\to 0$ displayed by equation (18) appears in the spin wave partition function and $Z_{\mathrm{DG}}(K;\Lambda_N;P)$ transforms to $Z_{\mathrm{CG}}(\pi^2/K;\Lambda_N;P)$.

The author thanks D B Abraham for several enlightening discussions.

References

Berezinskii V L 1971 *Sov. Phys.-JETP* **32** 493–500
Chui S T and Weeks J D 1976 *Phys. Rev.* B **14** 4978–82
José J V, Kadanoff L P, Kirkpatrick S and Nelson D R 1977 *Phys. Rev.* B **16** 1217–41
Kadanoff L P 1978 *J. Phys. A: Math. Gen.* **11** 1399–417
Knops H J F 1977 *Phys. Rev. Lett.* **39** 766–9
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181–206
Shugard W J, Weeks J D and Gilmer G H 1978 *Phys. Rev. Lett.* **41** 1399–402
—— 1980 *Phys. Rev.* B **21** 5309–11
Villain J 1975 *J. Physique* **36** 581–7