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EXACT SOLUTION OF A TWO-DIMENSIONAL MODEL FOR HYDROGEN-BONDED CRYSTALS

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A model of two-dimensional hydrogen-bonded crystals satisfying the ice rule is presented and solved exactly in the presence of an external electric field. The transfer-matrix method is used. The model includes, for special values of the parameters, the ice problem, the Rys F model of an antiferroelectric, and the Slater KDP model of a ferroelectric.

Recently, Lieb solved the two-dimensional "ice" problem.[1] We report here a generalization of his results. We consider a hydrogen-bonded $N\times N$ square lattice with periodic boundary conditions, and allow the hydrogen atoms to sit off center in either of two positions. We then impose the "ice rule" that exactly two hydrogen atoms are near each site.[2] We represent a hydrogen atom near a site by an arrow directed along the bond, toward the site. Then energies are assigned to the various site configurations. The six configurations for a site, consistent with the ice rule, and the respective energy assignments of our model, are shown in Fig. 1. We then apply an external electric field E in the vertical direction, giving an energy $-E$ to each up arrow, $+E$ to each down arrow, and zero to the horizontal arrows.

$\delta=\epsilon=0$ is the ice problem,[3-5] previously solved by Lieb[1]; $\delta=0$ is the Rys F model of an antiferroelectric[6]; and $\epsilon=+\frac{1}{2}\delta$ is the Slater KDP model of a ferroelectric.[7]

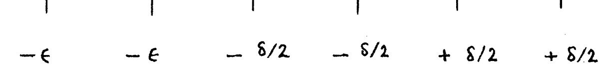

FIG. 1. Allowed configurations and energy assignments.

We first set $E=0$ and construct a transfer matrix A, whose elements are between two successive rows of vertical arrows, and are given by

$$\{\text{matrix element of } A \text{ between rows 1 and 2}\}$$
$$=A(1,2)$$
$$=\sum\exp\{-1/T[\text{energy of the intervening sites}]\}.$$

The summation is over all ways of placing the intervening row of horizontal arrows. Note that if n is the number of down arrows in row 1, $A(1,2)=0$ unless row 2 also has n down arrows. Thus A conserves n.

Let $y=1-2n/N$, and $\Lambda(y)$ be the largest eigenvalue of A for given y. The partition function Z is given by

$$Z=\max_y\{\exp[EyN^2/T][\Lambda(y)]^N\}. \tag{1}$$

We find that the eigenvector of A corresponding to the maximum eigenvalue for given y, $\Lambda(y)$, is identical to the eigenvector of the anisotropic chain of spin-spin interactions with minimum energy for given y. The spin-spin problem has been discussed by Yang and Yang.[8] In their notation the Hamiltonian is

$$H(\Delta)=-\tfrac{1}{2}\sum\{\sigma_x\sigma_x'+\sigma_y\sigma_y'+\Delta\sigma_z\sigma_z'\}. \tag{2}$$

Δ measures the anisotropy, and we find the correspondence

$$2\Delta=e^{-\delta/T}+e^{+\delta/T}-e^{2\epsilon/T}. \tag{3}$$

The transformation

$$\delta\to\delta'=-\delta \tag{4}$$

leaves Δ invariant, as it should. From now on we may restrict ourselves to $\delta\geqslant 0$, or if $\eta=e^{\delta/T}$, then $\eta\geqslant 1$.

The eigenvalue $\Lambda(y)$ is the sum of two terms,

$$\Lambda(y)=\Lambda_R(y)+\Lambda_L(y). \tag{5}$$

For $\Delta\leqslant 1$, the two terms may be written

$$\Lambda_R(y)=e^{N\delta/2T}\prod_{j=1}^{n}\left\{\frac{2\Delta-e^{\delta/T}-\exp(ik_j)}{e^{\delta/T}-\exp(ik_j)}\right\}, \tag{6}$$

$$\Lambda_L(y)=\Lambda_R(y) \text{ with } \delta\to-\delta. \tag{7}$$

The k_j's are as given in Yang and Yang; they become distributed with a density $\rho(k)$ in the limit $N\to\infty$. The free energy per site F, with applied field, is

$$F=\min_y\{-Ey-(T/N)\ln[\max(\Lambda_R(y),\Lambda_L(y))]\}. \tag{8}$$

In the limit $N\to\infty$,

$$\frac{\ln\Lambda_R(y)}{N}=\left(\frac{1+|y|}{4}\right)\frac{\delta}{T}+\frac{1}{2}\int\rho(k)dk\ln\left[\frac{(2\Delta-e^{\delta/T})^2-2(2\Delta-e^{\delta/T})\cos k+1}{2(\cosh\delta-\cos k)}\right]. \tag{9}$$

We then find that for $\Delta\leqslant 1$, $\Lambda_R(y)\geqslant\Lambda_L(y)$.

The singularities in the thermodynamic functions occur in y at $y=0$, $\Delta<1$; and in T at $\Delta=-1$, $y=0$ and $\Delta=+1$, all y.

The author would like to thank Professor C. N. Yang for drawing his attention to E. H. Lieb's solution of the ice problem.

Note added in proof.—We recently received a preprint from E. H. Lieb, treating the Rys F model in a similar way with similar results.

[1]E. H. Lieb, Phys. Rev. Letters 18, 692 (1967).

[2]J. F. Nagle, J. Math. Phys. 7, 1482, 1492 (1966).

[3]L. Onsager and M. Dupuis, Rendiconti della Scuola Internazionale di Fisica (Enrico Fermi), X Corso, "Termodinamica dei Processi Irreversibili" (Società Italiàna di Fisica, Bologna, 1960), p. 294.

[4]L. Pauling, J. Am. Chem. Soc. 57, 2680 (1935).

[5]W. F. Giaque and J. W. Stout, J. Am. Chem. Soc. 58, 1144 (1936).

[6]F. Rys, Helv. Phys. Acta 36, 537 (1963).

[7]J. C. Slater, J. Chem. Phys. 9, 16 (1941).

[8]C. N. Yang and C. P. Yang, Phys. Rev. 147, 303 (1966); 150, 321, 327 (1966); 151, 258 (1966).

UNIVERSAL INSTABILITY OF A RESISTIVE PLASMA COLUMN*

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The stability of a collision-dominated, weakly ionized plasma column confined in a magnetic field has been considered by a number of authors,[1-3] and their results have been substantiated by experimental observations of instabilities in positive column-type discharges. These instabilities are caused by differential mobility of the charged particles in the applied or self-generated equilibrium electric fields. Our concern here is with a more prevalent universal mode, related to some previously derived drift modes, that also grows via differential drifts but sets in when the column is somewhat more highly ionized. Thus the model applies to such low-temperature laboratory plasmas as those generated by a differentially pumped hollow-cathode discharge.

We have carried out an analysis for such a