One-Dimensional Chain of Anisotropic Spin-Spin Interactions. III. Applications

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The magnetization–versus–magnetic-field curve of the one-dimensional chain at $T=0$ is discussed. Also, the corresponding p-V diagram of the quantum lattice gas (q.l.g.) is discussed. The ground-state wave function for the case $\Delta>1$, in a q.l.g. of a finite number of particles on an infinite lattice is analyzed in detail, giving the "surface energy" near the ends. In the Appendix some general properties of the q.l.g. in one, two, or three dimensions are given.

1. MAGNETIC CHAIN

THE results of paper II[1] yield immediately information on the zero-temperature-magnetization–versus–magnetic-field problem. We have

$\mathfrak{N}=$ number of sites,

$y=$ spin per site $(=-1\rightarrow 1)$,

$\mathcal{H}=$ magnetic field in proper units.

The energy of the system in a magnetic field is

$$E=\mathfrak{N}[f(\Delta,y)z-\mathcal{H}y],\quad (z=2). \tag{1}$$

Thus minimization of E gives

$$2\frac{\partial f}{\partial y}=\mathcal{H}. \tag{2}$$

The susceptibility χ is defined by

$$\chi^{-1}=\frac{\partial\mathcal{H}}{\partial y}=2\frac{\partial^2 f}{\partial y^2}.$$

It was shown in paper II[1] that $f(\Delta,y)$, for fixed Δ, concaves upwards in y. *Thus $\mathcal{H}$ is monotonically increasing as y increases.* Numerical computations of the y-$\mathcal{H}$ curves can be made from the integral equations (II 9). Some general features of these curves can be obtained from (II 49), (II E17), (II 69), (II 70), (II 71), (II 66), and (II 68).

(a) For $\Delta=0$, $\mathcal{H}=\sin(\pi y/2)$. [See (II 71).] (3)

(b) (II 66), (II 68), (II 69), and (II 70) show that for $-1\leqq\Delta<1$,

$$y(\mathcal{H}=0)=0,$$

$$\chi^{-1}(\mathcal{H}=0)=\frac{\pi(\pi-\mu)\sin\mu}{2\mu}. \tag{4}$$

The susceptibility $\chi(\mathcal{H}=0)$ at $\Delta=-1$ is, according to this, $2/\pi^2$, a result conjectured by Griffiths[2], who had obtained (II 52a) but did not use the Wiener-Hopf method to solve it.

(c) Griffiths has shown[2] that at $\Delta=-1$, as $y\rightarrow 0+$, the derivative

$$\frac{d\chi^{-1}}{dy}\rightarrow-\infty. \tag{5}$$

We see now from (II E22) that for $4\mu(\pi-\mu)^{-1}\neq$ integer, as $y\rightarrow 0+$,

$$\frac{d^n\chi^{-1}}{dy^n}\rightarrow\text{finite}\quad\text{for}\quad n<\frac{4\mu}{\pi-\mu}$$
$$\rightarrow\pm\infty\quad\text{for}\quad n>\frac{4\mu}{\pi-\mu}. \tag{6}$$

For the lowest n for which $n>4\mu/(\pi-\mu)$, the sign $\pm$ should be the same as the sign of d_2 which is the same as that of $-\tan\pi\mu/(\pi-\mu)$.

(d) For all $\Delta\leqq 1$, (II 70) gives at $y=1$,

$$\mathcal{H}=1-\Delta,\quad\frac{\partial\mathcal{H}}{\partial y}=0,\quad\frac{\partial^2\mathcal{H}}{\partial y^2}=-\frac{\pi^2}{4}. \tag{7}$$

(e) For $\Delta<-1$, at $y=0$, by (II 49) and (II B5)

$$\mathcal{H}=2(\sinh\lambda)\sum_{-\infty}^{\infty}\frac{(-1)^n}{2\cosh n\lambda}$$
$$=\frac{\pi\sinh\lambda}{\lambda}\sum_{-\infty}^{\infty}\operatorname{sech}\frac{\pi^2}{2\lambda}(1+2n), \tag{8}$$

$$\frac{\partial\mathcal{H}}{\partial y}=0, \tag{9}$$

[1] C. N. Yang and C. P. Yang, Phys. Rev. **149**, 327 (1966).

[2] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).

$$\frac{\partial^2 \mathcal{H}}{\partial y^2} = -4\pi^2 \mathcal{H}^{-2}(\sinh^3\lambda) \sum_{-\infty}^{\infty} \frac{(-1)^n n^2}{4 \cosh n\lambda}. \tag{10}$$

As $\lambda \to \infty$, (at $y=0$)

$$\mathcal{H} \to \sinh\lambda - \frac{2 \sinh\lambda}{\cosh\lambda} \to -\Delta - 2, \tag{11}$$

$$\frac{\partial^2 \mathcal{H}}{\partial y^2} \to 8\pi^2. \tag{12}$$

As $\lambda \to 0$, (at $y=0$)

$$\mathcal{H} \to 4\pi \exp(-\pi^2/2\lambda), \tag{13}$$

$$\frac{\partial^2 \mathcal{H}}{\partial y^2} \to \frac{2\pi^4}{\mathcal{H}}. \tag{14}$$

The fact that at $y=0$ and $\Delta < -1$, $\mathcal{H}$ is nonvanishing was already conjectured before. That $\partial\mathcal{H}/\partial y = 0$ at such a point is a new result.

Some of these results are illustrated in Fig. 1 and Table I.

We can also investigate the limit $\Delta \to -\infty$. In a straightforward way we obtain, from (II 7),

$$R(\alpha) = \tfrac{1}{2}(1+y) + O(\Delta^{-1}), \tag{15}$$

$$b = \pi(1-y)(1+y)^{-1} + O(\Delta^{-1}), \tag{16}$$

$$f(\Delta, y) = -\tfrac{1}{4}\Delta + \tfrac{1}{2}\Delta(1-y) - \frac{1+y}{2\pi} \sin\left(\pi \frac{1-y}{1+y}\right) + O(\Delta^{-1}). \tag{17}$$

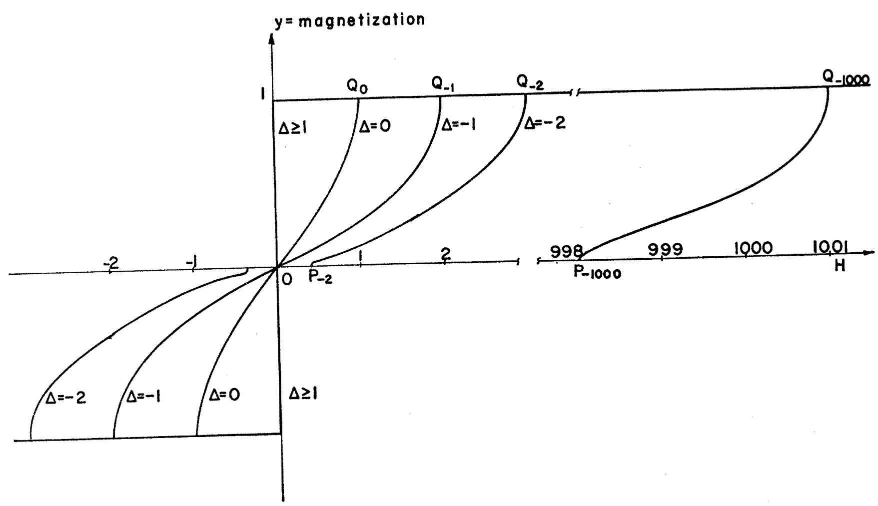

FIG. 1. Zero-temperature-magnetization – versus – $\mathcal{H}$ curves. For $\Delta=0$ the curve is sinusoidal. The $\Delta=-1$ curve is taken from Griffiths (Ref. 2). In general for $-1 \leq \Delta < 1$, the curve has a singularity in some derivative at $\mathcal{H}=0$. The order of the derivative becomes high as $\Delta \to 1$. For $\Delta < -1$, the curve has a horizontal part along the $\mathcal{H}$ axis. The tangents at P and Q are always vertical. The curvature at P_Δ approaches ∞ as $\Delta \to -1$. The curvature at Q is always the same. These properties are summarized in Table I. The curve for $\Delta=-2$ is approximate only. The curve for large negative Δ is shown by that for $\Delta=-1000$. See Eq. (18).

TABLE I. Values of $\mathcal{H}$ and its derivatives. $\Delta<1$.

		$\mathcal{H}$	$\frac{\partial \mathcal{H}}{\partial y}$	$\frac{\partial^2 \mathcal{H}}{\partial y^2}$
$y=1$		$1-\Delta$	0	$-\frac{\pi^2}{4}$
	$-1<\Delta<1$	0	$\frac{\pi(\pi-\mu)}{2\mu}\sin\mu$	(II E17) and (II E22)
	$\Delta=-1+0$	0	$\frac{\pi^2}{2}$	$-\infty$
$y=0$	$\Delta=-1$	0	$\frac{\pi^2}{2}$	$-\infty$ (Griffiths)
	$\Delta=-1-\frac{\lambda^2}{2}$, $\lambda \gtrsim 0$	$\approx 4\pi \exp\left(-\frac{\pi^2}{2\lambda}\right)$	0	$\approx \frac{\pi^3}{2}\exp\left(\frac{\pi^2}{2\lambda}\right)$
	$\Delta<-1$	(8)	0	(10)
	$\Delta\to-\infty$	$-2-\Delta$	0	$8\pi^2$

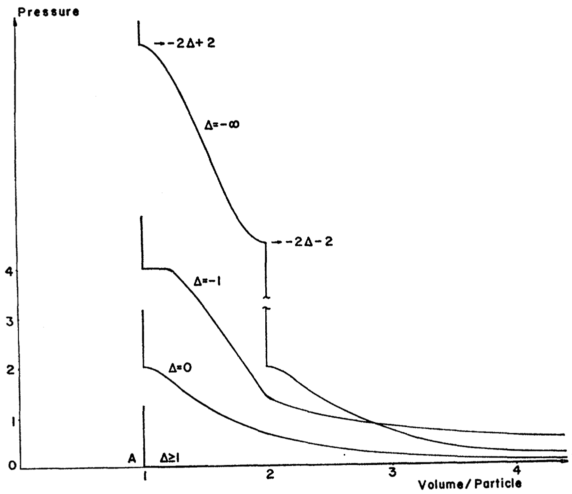

FIG. 2. Pressure-versus-volume/particle curves. For $\Delta>1$ point A represents a many-particle bound state at zero pressure. The $\Delta=0$ curve has no singularity at $v=\mathfrak{N}/m=2/(1-y)=2$, but other curves for $-1<\Delta<1$ have singularities in derivatives at this point. For $\Delta=-1$, the point $v=2$ has infinite second derivative. This curve is based on Griffiths' result (Ref. 2). For $\Delta<-1$, the curve has the same general shape as the $\Delta=-\infty$ curve except that the change in pressure occurring at the transition point $v=2$ is finite in size. All curves have zero slopes at $v=1+0$. All $\Delta<-1$ curves have zero slopes at $v=2\pm0$.

Thus

$$\lim_{\Delta\to\infty}(\mathfrak{H}+\Delta)=-\frac{d}{dy}\left[\frac{1+y}{\pi}\sin\left(\pi\frac{1-y}{1+y}\right)\right]. \qquad (18)$$

2. ONE-DIMENSIONAL QUANTUM LATTICE GAS

The quantum lattice gas (q.l.g.) was first discussed by Matsubara and Matsuda, and, Whitlock and Zilsel.[3] In the Appendix the same general properties of the quantum lattice gas are discussed. Applying these results we find the following:

(a) For $\Delta<1$, type (iii) $T=0$ isotherm obtains (Fig. 5). The isotherms are shown in Fig. 2. They are obtained from the corresponding isotherms in Fig. 1.

(b) For $\Delta\geqq 1$, type (i) $T=0$ isotherm obtains. The binding energy per particle in free space (i.e., in an infinite lattice) is, by (A21), $2\Delta'=2(\Delta-1)$.

For $\Delta>1$, one can in fact obtain the *exact* binding energy and the *exact* wave function for a system of m particles in an infinite lattice (i.e., $\mathfrak{N}=\infty$) by taking the wave function (I 7) and making all p's pure imaginary:

$$ip_j=\kappa_j. \qquad (19)$$

Assume for the time being that all κ's are real and unequal:

$$\kappa_1>\kappa_2>\kappa_2\cdots>\kappa_m. \qquad (20)$$

Also assume for the time being that there is only one term in the sum (I 7);

$$\psi=\exp[\kappa_1x_1+\kappa_2x_2+\cdots+\kappa_mx_m], \quad (x_1<x_2\cdots<x_m). \qquad (21)$$

Then the condition expressed by the equation just before (I 12) is

$$2\Delta e^{\kappa_j}-1-e^{\kappa_j+\kappa_l}=0 \quad \text{if} \quad j=l+1. \qquad (22)$$

By the method of construction explained in Fig. 3 one can find a chain of κ's satisfying (22), and satisfying the condition

$$\sum_1^m \kappa=0. \qquad (23)$$

Such a chain evidently gives a solution (21) with total momentum zero. The solution has no nodes. Hence it is the ground state.

The ground-state energy of the q.l.g. of m particles is thus

$$(E_{\text{q.l.g.}})_m=2\sum_1^m(1-\cosh\kappa_j).$$

By (22)

$$(E_{\text{q.l.g.}})_m=-2m(\Delta-1)+2\Delta-2e^{-\kappa_1}. \qquad (24)$$

Thus the average energy per particle is

$$-2(\Delta-1),$$

with an "end energy" for each end

$$\Delta-e^{-\kappa_1}>0.$$

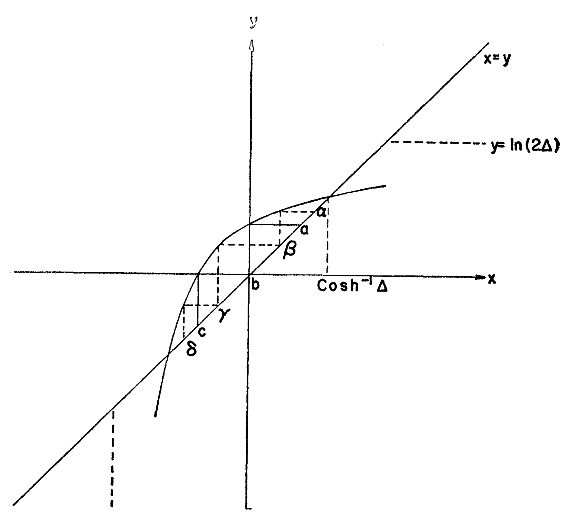

FIG. 3. Diagram construction of ground-state wave function of q.l.g. The curve is $2\Delta-e^y-e^{-x}=0$ (schematic). The points a, b, c have abscissas that are the κ values for three particles. The points α, β, γ, δ have abscissas that are those for four particles.

[3] The classical lattice gas was first discussed by T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952). The quantum lattice gas was first discussed in T. Matsubara and H. Matsuda, Progr. Theoret. Phys. (Kyoto) 16, 569 (1956); 17, 19 (1957). See also R. T. Whitlock and P. R. Zilsel, Phys. Rev. 131, 2409 (1963); P. R. Zilsel, Phys. Rev. Letters 15, 476 (1965).

For $m\to\infty$, this becomes

$$\Delta-[\Delta-(\Delta^2-1)^{1/2}]=(\Delta^2-1)^{1/2}. \tag{25}$$

The binding energy of the last particle is

$$+2(\Delta-1)+2e^{-(\kappa_1)m}-2e^{-(\kappa_1)m-1},$$

which increases with m and approaches $2(\Delta-1)$ as $m\to\infty$.

Writing $x_2-x_1=g_2$, $x_3-x_2=g_3$, $\cdots x_m-x_{m-1}=g_m$, we have

$$\psi=\exp[\kappa_2g_2+\kappa_3(g_3+g_2)+\kappa_4(g_4+g_3+g_2)+\cdots],$$

where

$$g_j\geqq 1.$$

Thus

$$\langle g_j\rangle=[1-\exp(2\textstyle\sum_j^m\kappa_l)]^{-1}. \tag{26}$$

Or

$$\langle g_2\rangle=[1-\exp(-2\kappa_1)]^{-1},$$
$$\langle g_3\rangle=[1-\exp(-2\kappa_1-2\kappa_2)]^{-1},$$
$$\text{etc.}$$

Thus the two end gaps are the longest. Successive inner gaps are successively shorter. For a very long chain,

$$\langle g_2\rangle-1=\frac{1}{e^{2\kappa_0}-1},\quad \langle g_3\rangle-1=\frac{1}{e^{4\kappa_0}-1},\ \text{etc.}, \tag{27}$$

where $\kappa_0=\cosh^{-1}\Delta$. Hence we have as $m\to\infty$,

$$[\text{excess length of chain over closest packing}]$$
$$=\frac{2}{e^{2\kappa_0}-1}+\frac{2}{e^{4\kappa_0}-1}+\cdots<\infty. \tag{28}$$

Thus the density of particles is 1, with an "end extension" equal to half of (28) at each end.

APPENDIX: QUANTUM LATTICE GAS (IN 3, 2, OR 1 DIMENSION)

A. Equivalence with Spin Problem

We consider a collection of bosons and replace

$$-\frac{\hbar^2}{2m}\nabla^2\to -\text{double difference}.$$

We write, i.e.,

$$\langle x|\text{kinetic energy}|\psi\rangle=-\langle x+1|\psi\rangle-\langle x-1|\psi\rangle+2\langle x|\psi\rangle. \tag{A1}$$

Further, we introduce an interaction energy -2Δ for nearest neighbors, $+\infty$ for the hard core. It is then easy to see that the problems of the quantum lattice gas and the spin problem in a magnetic field are kinematically the same. This leads to the construction of Table II. Notice that

$$H_{\text{sp}}=-\tfrac{1}{2}\sum\{\Delta\sigma_z\sigma_z'+\sigma_x\sigma_x'+\sigma_y\sigma_y'\}-\mathcal{H}\mathfrak{N}y. \tag{A2}$$

TABLE II. Correspondence between two problems. z = number of nearest neighbors per site. (A3) and (A4) are definitions. Then (A5) follows. (A6) is a definition. (A7) follows. (A8), (A9), and Eqs. (A10) and (A11) can then be derived. These relations are true for one-dimensional linear, two-dimensional square, or three-dimensional cubic lattices.

Quantum lattice gas	Spin in magnetic field $\mathcal{H}$	
Volume $(=V)$ or length $(=L)$	$=\mathfrak{N}$	(A3)
no. of atoms $(=m)$	$=$no. of down spins $[=m=\frac{1}{2}\mathfrak{N}(1-y)]$	(A4)
$H_{\text{q.l.g.}}-\left(\frac{1}{2}-\frac{\Delta}{4}\right)\mathfrak{N}z-z\mathfrak{N}y\left(\frac{\Delta}{2}-\frac{1}{2}\right)$	$=H_{\text{sp}}+\mathcal{H}\mathfrak{N}y$	(A5)
chem. potential $(=\mu)$	$=-2\mathcal{H}-z(\Delta-1)$	(A6)
$\exp(-\mu\mathfrak{N}/2T)$(grand partition function)$_{\text{q.l.g.}}$ where (G.P.F.) $=\text{Tr}\exp[(\mu m-H_{\text{q.l.g.}})/T]$	$=\exp\left[-\left(\frac{1}{2}-\frac{\Delta}{4}\right)\mathfrak{N}z/T\right]$[partition function]$_{\text{sp}}$ where (P.F.) $=[\text{Tr}\exp(-H_{\text{sp}}/T)]$	(A7)
pressure $(=\mathcal{P})$ $[\mathcal{P}=\mathfrak{N}^{-1}T\ln(\text{G.P.F.})]$	$=-\mathcal{H}-\frac{1}{4}z\Delta-\mathfrak{N}^{-1}\mathfrak{F}$ $[\mathfrak{F}=-T\ln(\text{P.F.})]$	(A8)
entropy $(=S)$	$=$entropy $(=S)$	(A9)

The two thermodynamical relations, for fixed $\mathfrak{N}$,

$$d\mathcal{P}=(S/\mathfrak{N})dT+(m/\mathfrak{N})d\mu, \tag{A10}$$

$$d\mathfrak{F}=-SdT-\mathfrak{N}yd\mathcal{H}\quad (y=\text{magnetization}) \tag{A11}$$

are derivable from each other.

B. Non-Nearest-Neighbor Interactions

The above discussions easily generalize to a case with non-nearest-neighbor interactions. We keep (A1) unchanged. Equation (A2) becomes

$$H_{\text{sp}}=-\tfrac{1}{2}\sum_{\text{n.n.}}(\sigma_x\sigma_x'+\sigma_y\sigma_y')-\tfrac{1}{2}\sum_i\Delta_i\sum_{\text{t.i.}}(\sigma_z\sigma_z'')-\mathcal{H}\mathfrak{N}y, \tag{A2'}$$

where n.n. means nearest neighbor, and t.i. means sum over all pairs of type i. Equations (A3)–(A11) remain valid with the replacement

$$z\Delta \to \sum z_i\Delta_i, \qquad \text{(A12)}$$

where z_i= number per site of neighbors of type i. (Notice that wherever z occurs without the factor Δ, it should not be replaced. That is, z remains equal to the number of nearest neighbors.)

C. Existence of Thermodynamical Limit

We shall only consider the case where the range of interaction is finite. It is then not difficult to prove rigorously that the thermodynamical limit exists for both the quantum lattice gas and the spin problem, and that the thermodynamical quantities satisfy (A3′)–(A11′), with the replacement (A12).

D. Some Properties of the Isotherms in the y-$\mathcal{H}$ Diagram

The isotherms in the y-$\mathcal{H}$ (magnetization-versus-field) diagram are of course symmetric with respect to the origin, i.e., they are invariant under

$$y \to -y,$$
$$\mathcal{H} \to -\mathcal{H}.$$

Furthermore, thermodynamic inequalities require that if $\mathcal{H}_1 > \mathcal{H}_2$, $y(\mathcal{H}_1) \geqq y(\mathcal{H}_2)$.

At $T=0$, the isotherm must reach $y=1$ at a finite $\mathcal{H}=\mathcal{H}_0$. To prove this we write (A2′) as

$$H_{\rm sp} = -\tfrac{1}{2}\sum_{\rm n.n.}(\sigma\cdot\sigma') - \tfrac{1}{2}\sum_i \Delta_i' \sum_{\rm t.i.}(\sigma_z\sigma_z'') - \mathcal{H}\mathfrak{N}y.$$

Now for those Δ_i' which are $\geqq 0$, we write

$$-\tfrac{1}{2}\Delta_i'\sigma_z\sigma_z'' = -\tfrac{1}{2}\Delta_i' + \tfrac{1}{2}\Delta_i'(1-\sigma_z\sigma_z''), \qquad \text{(A13)}$$

and for those $\Delta_i' < 0$, we write

$$-\tfrac{1}{2}\Delta_i'\sigma_z\sigma_z'' = +\tfrac{1}{2}\Delta_i'[1-\sigma_z-\sigma_z''] - \tfrac{1}{2}\Delta_i'(1-\sigma_z)(1-\sigma_z''). \qquad \text{(A14)}$$

The last terms of (A13) and (A14) are both positive operators. Thus

$$H_{\rm sp} = -\tfrac{1}{2}\sum_{\rm n.n.}(\sigma\cdot\sigma') - \tfrac{1}{2}\sum|\Delta_i'|\sum_{\rm t.i.}1 - \tfrac{1}{2}\Big(\sum_{\Delta'<0}\Delta_i' z_i\Big) \times \Big(\sum\sigma_z\Big) - \mathcal{H}\mathfrak{N}y + \text{(positive operator)}$$
$$= \text{constant} - \tfrac{1}{2}\sum_{\rm n.n.}(\sigma\cdot\sigma') - \tfrac{1}{2}\Big(\sum_{\Delta'<0}\Delta_i' z_i\Big)\mathfrak{N}y - \mathcal{H}\mathfrak{N}y + \text{(positive operator)}.$$

Now the positive operator and $-\tfrac{1}{2}\sum_{\rm n.n.}(\sigma\cdot\sigma')$ both attain their minima for the state with all spins up ($y=1$). Thus

$$E_{\rm sp} - E_{\rm sp}(y=1) \geqq \Big[\tfrac{1}{2}\Big(\sum_{\Delta'<0}\Delta_i' z_i\Big) + \mathcal{H}\Big]\mathfrak{N}(1-y).$$

Thus

$$\text{for } \mathcal{H} > -\tfrac{1}{2}\sum_{\Delta'<0}\Delta' z, \quad y=1. \qquad \text{(A15)}$$

We recall that

$$\Delta' = \Delta - 1 \quad \text{for nearest neighbors},$$
$$\Delta' = \Delta \quad \text{for other interactions}. \qquad \text{(A16)}$$

E. Isotherms in $\mathcal{P}$-density and y-$\mathcal{H}$ Diagrams

The isotherms are related because by (A10) and (A6), at constant T,

$$d\mathcal{P} = \frac{-m}{\mathfrak{N}} 2d\mathcal{H} = -(1-y)d\mathcal{H}.$$

Furthermore, as $\mathcal{H} \to +\infty$, $\mu \to -\infty$ and $\mathcal{P} \to 0$. The relationship is illustrated in Fig. 4.

From general principles,

$$\mathfrak{N}^{-1}[E_{\rm q.l.g.} - TS + \mathcal{P}\mathfrak{N} - \mu m] = 0.$$

Thus by (A6) and (A12)

$$\mathfrak{N}^{-1}[E_{\rm q.l.g.} - TS] = \mathfrak{N}^{-1}[\mu m - \mathcal{P}\mathfrak{N}] = \mu\tfrac{1}{2}(1-y) - \mathcal{P}$$
$$= \big(-\mathcal{H} + \tfrac{1}{2}z - \tfrac{1}{2}\sum z_i\Delta_i\big)(1-y) - \mathcal{P}. \qquad \text{(A17)}$$

z= number of nearest neighbors. The geometrical meaning of (A17) is illustrated in Fig. 4 and in its caption.

F. $T=0$ Isotherm

The $T=0$ isotherm has, according to (A15), a point γ at which $y=1$ and $\mathcal{H}=\mathcal{H}_\gamma$, to the left of which $y<1$. Further,

$$\mathcal{H}_\gamma \leqq -\tfrac{1}{2}\sum_{\Delta'<0}\Delta' z. \qquad \text{(A18)}$$

Clearly,

$$0 \leqq \mathcal{H}_\gamma. \qquad \text{(A19)}$$

Applying (A17) to γ we have the important relation

$$\mathcal{H}_\gamma + \tfrac{1}{2}\sum_{\rm all}\Delta' z = -\tfrac{1}{2}E_{\rm q.l.g.}/m$$
$$= \tfrac{1}{2}\,\text{(binding energy per particle for an infinitely large number of particles in \textit{free} space in the q.l.g.)}$$
$$\geqq 0. \qquad \text{(A20)}$$

We are now in a position to discuss the four different types of $T=0$ isotherm behavior near γ, illustrated in Fig. 5.

(i) $\mathcal{H}_\gamma = 0$. If all $\Delta' \geqq 0$, (i.e., if the nearest-neighbor interaction Δ is $\geqq 1$, and no interaction is repulsive)

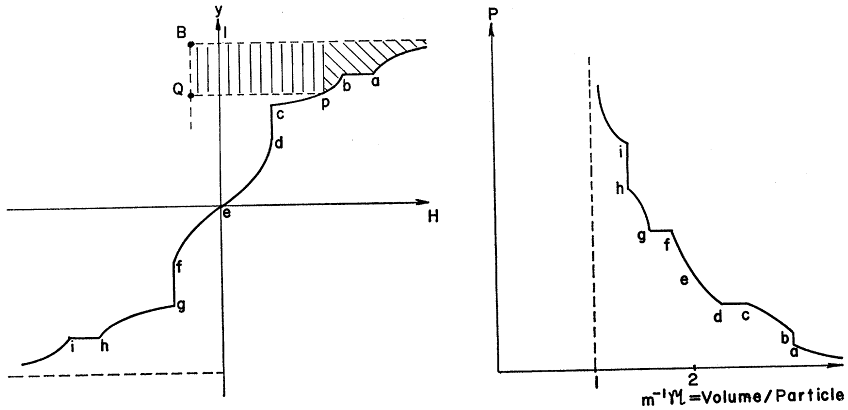

FIG. 4. Corresponding isotherms for any T (schematic). For a point P, the pressure $\mathcal{P}$ for the q.l.g. is equal to the diagonally hatched area. The free energy per particle $m^{-1}[E_{\mathrm{q.l.g.}}-TS]$ for the q.l.g. is equal to the sum of the two hatched areas divided by $-\frac{1}{2}(BQ)$. B is the point $y=1$, $\mathcal{H}=-\frac{1}{2}(\sum_i z_i\Delta_i)+\frac{1}{2}z$. The chemical potential μ for the q.l.g. is $-2(QP)$. A horizontal part of the isotherm in the left diagram corresponds to a vertical part of the isotherm in the right diagram, and vice versa.

(A18) and (A19) show that this case obtains. Notice that $H_\gamma=0$ implies that

$$\text{the binding energy per particle}=+\sum \Delta' z. \qquad (21)$$

(ii) $0<\mathcal{H}_\gamma$, and there is a vertical stretch γG. The point G represents a pressure-free q.l.g. system at a finite density. Thus it represents a "fluid" resembling He^4 liquid at $T=0$, or a crystal. It has a nonvanishing binding energy. Thus the distance $B\gamma>0$.

(iii) $0<\mathcal{H}_\gamma$, there is no vertical stretch going down from γ, and $B\gamma=0$. This is the case if some $\Delta'<0$, and all $\Delta'\leqq 0$, (e.g., if the nearest-neighbor interaction $\Delta<1$, and no other interaction is attractive) because then (A18) and (A20) lead to $\mathcal{H}_\gamma=\mathcal{H}_B$.

(iv) Same as (iii), but $B\gamma>0$. This case obtains if the q.l.g. forms "molecules" that repel each other.

G. Off-Diagonal Long-Range Order

The concept of off-diagonal long-range order (ODLRO) has been introduced[4] in the discussion of superfluidity. The same concept is also applicable in the quantum lattice gas. Because of the simplicity of the q.l.g. one hopes that the absence or presence of ODLRO can be investigated more readily. For the special case where there is only nearest-neighbor interaction with strength $\Delta_1=1$ [see (A2′)] one can in fact explicitly compute at $T=0$ the ODLRO for the 1-, 2-, or 3-dimensional lattice: The Hamiltonian is

$$H=\sum\left(-\tfrac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'\right). \qquad \text{(A22)}$$

Each term in the sum attains its minimum value when the wave function is symmetrical with respect to the two spins in question. Thus a wave function totally symmetrical with respect to *all* spins, if it exists, must represent the ground state. For a cyclic lattice of $\mathfrak{N}$ sites in 1, 2, or 3 dimensions, with m down spins and $(\mathfrak{N}-m)$ up spins, such a wave function exists and is a state in which all the $\mathfrak{N}![m!(\mathfrak{N}-m)!]^{-1}$ different spin arrangements have the same weight. For this state $\langle a_j^\dagger a_j\rangle=$ average number of down spins at site j

$$=m\mathfrak{N}^{-1}, \qquad \text{(A23)}$$

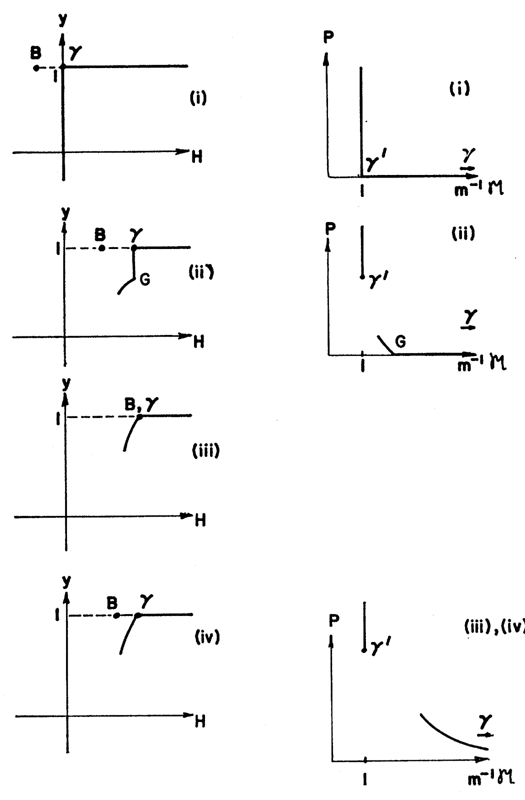

FIG. 5. $T=0$ isotherms (schematic). The point B is given by $y=1$, $\mathcal{H}=-\frac{1}{2}\sum\Delta' z$. B never lies to the right of γ and $2(B\gamma)$ = (binding energy per particle for an infinitely large number of particles in *free* space in the q.l.g. problem) $\geqq 0$. The point γ' is the point that corresponds to γ for $y=-1$. Notice that by the construction method of Fig. 4, one concludes that γ' has a *finite pressure* $\mathcal{P}$. Thus at $T=0$, a quantum lattice gas can always be squeezed to a fully packed density by a *finite* pressure.

[4] C. N. Yang, Rev. Mod. Phys. 34, 694 (1962); J. Math. Phys. 4, 418 (1963).

where a_j represents the annihilation operator at site j. In spin language a_j flips a down spin up, or

$$a_j=[\tfrac{1}{2}(\sigma_x+i\sigma_y)]_j. \quad \text{(A24)}$$

We can also calculate $\langle a_j^\dagger a_i\rangle$, which is the probability that at site j the spin is up and at site i it is down:

$$\langle a_j^\dagger a_i\rangle=\frac{m(\mathfrak{N}-m)}{\mathfrak{N}(\mathfrak{N}-1)}. \quad \text{(A25)}$$

Equations (A23) and (A25) give the elements of the reduced density matrix ρ_1 in coordinate representation:

$$\langle j|\rho_1|j\rangle=m/\mathfrak{N},$$
$$\langle i|\rho_1|j\rangle=m(\mathfrak{N}-m)\mathfrak{N}^{-1}(\mathfrak{N}-1)^{-1}. \quad \text{(A26)}$$

ρ_1 is a cyclic matrix which is diagonal in the momentum (which is discrete) representation:

$$\langle k'|\rho_1|k\rangle=0 \quad \text{if} \quad k\neq k',$$
$$\langle k|\rho_1|k\rangle=m\mathfrak{N}^{-1}-m(\mathfrak{N}-m)\mathfrak{N}^{-1}(\mathfrak{N}-1)^{-1}$$
$$=m(m-1)\mathfrak{N}^{-1}(\mathfrak{N}-1)^{-1}\leq 1, \quad \text{(A27)}$$
$$\langle k|\rho_1|k\rangle=m\mathfrak{N}^{-1}+m(\mathfrak{N}-m)\mathfrak{N}^{-1}$$
$$=m\mathfrak{N}^{-1}(\mathfrak{N}-m+1) \quad \text{if} \quad k=0.$$

These equations show that there is condensation of particles in *one* "single-particle state" characterized by $k=0$. In other "single-particle states" ($k\neq 0$) the occupation number is $\leqq 1$. This is an explicit example where the speculation of Girardeau[5] does not hold. [Girardeau's speculation is that, e.g., $\sim(m)^{2/5}$ states are multiply occupied each with $\sim(m)^{3/5}$ particles.] We suspect that it also does not hold in a physical system.

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Nuclear-Magnetic-Resonance Study of Self-Diffusion in a Bounded Medium*

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The investigation of the effects of diffusion in a magnetic field gradient on the spin-echo experiment in nuclear magnetic resonance (NMR) is extended to small samples in which the diffusion is bounded, or restricted. From the point of view of NMR, bounded diffusion means that the spin dephasing time $T_2\gg t_x$, the average time for a molecule to diffuse once across a sample width a. A more realistic criterion is that a is small enough or that the diffusion coefficient D is large enough that the quantity $\gamma Ga^3/D$ is about equal to or less than 1, where G is a linear magnetic field gradient and γ is the nuclear gyromagnetic ratio. An effective self-diffusion coefficient $D'(t)=-12\ln[M(t,G)/M(t,0)]/\gamma^2G^2t^3$ is defined from the Hahn spin-echo experiment, where $t=2\tau$ is the time of the echo, and $M(t,G)$ is the echo amplitude. For infinite samples, $D'=D$, the true self-diffusion coefficient. However, when $t_x\ll T_2$, then $D'/D<1$ and D' depends on t. The measurement of D' is made by holding the times of an echo, $t=2\tau$, constant and varying G. Experimental data are presented on $D'(t)$ for four values of a and values of $\gamma Ga^3/D$ which range from being much greater than unity to less than unity. Results of the Carr-Purcell experiment are also presented and briefly discussed. A comparison of data from the spin-echo experiment is made with a theoretical calculation of $D'(t)$ which uses Torrey's modification of the Bloch equations and requires that boundary conditions be satisfied. Results are compared with the theory developed by Robertson. A universal curve for D'/D versus t/t_x is plotted, illustrating that D' is independent of G. It is shown that the reduced rate of decay of the echo envelope in the case of bounded diffusion is, in effect, a motional-narrowing phenomenon.

I. INTRODUCTION

THIS paper is concerned with the effect of diffusion in a *noninfinite* sample on the Hahn spin-echo experiment[1] and the Carr-Purcell experiment.[2] In previous studies[1–4] known to the authors the assumption has been made that the sample is infinite in size. For many experiments this assumption is perfectly valid; however, there exists a group of experiments for which the diffusion coefficient D is so large and/or the sample size a is so small that the infinite-sample assumption breaks down. In particular, two such experiments have motivated the present work. Measurements of the spin-lattice relaxation time T_1 and the spin dephasing time T_2 were made on small particles of liquid lithium[5] and on rapidly self-diffusing protons[6] in powdered NbH_x under

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