Spatial Variations of Spontaneous Magnetization in a Layered Ising Model

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The extrema of the position-dependent spontaneous magnetization in a periodically layered two-dimensional Ising model are calculated exactly. Their asymptotic behaviour for infinite width of the surrounding homogeneous sublayer is given. The perturbations caused by the neighbouring sublayers on this extremum in a very thick sublayer are shown to be decoupled. Thus the asymptotic decay of the magnetization far from a *single* layer-shaped inhomogeneity can be inferred from the quoted asymptotics of an extremum, and it is found to be $d^{-3/2}\exp(-d/\xi_1^<)$ where d is the distance to the inhomogeneity and $\xi_1^<$ the correlation length in the underlying homogeneous lattice. The connection of this decay law to the asymptotic decay of correlations is dicussed.

1. Introduction and Summary

It is the purpose of this paper to present exact calculations [1] on the position dependence of the spontaneous magnetization of a two-dimensional Ising model in which layer-shaped inhomogeneities are present. The interest in such layered Ising models arises from the fact that the critical behaviour of real crystalline magnets is heavily influenced by any disturbance of the full translational symmetry of the infinite homogenous lattice (e. g. point defects, dislocations, grain boundaries, finiteness of the sample). In the past, the phase transition in such layered lattices has been studied by many authors [2–7]. Correlations and spontaneous magnetization were already discussed by McCoy and Wu [3] and Au-Yang and McCoy [8], but without explicit calculation of the position dependence.

In this paper a particular case of a quadratic $S=1/2$ layered Ising model with nearest-neighbour interactions is considered. The period layer consists of two sublayers within which the exchange couplings are chosen to be position-independent (but generally direction-dependent, see Figure 2). This model contains grain boundaries and interfaces as special cases. — In Chapter 2 the "local spontaneous magnetization" of a layered lattice is expressed through the eigenvectors of the "layer transfer matrix". In Chapter 3 this matrix is diagonalized for the special lattice of Figure 2. Chapter 4 gives an expression for $m(l_0)$, the local magnetization in lattice chain l_0, in terms of a block Toeplitz determinant. In Chapter 5 the extrema of $m(l_0)$ are explicitly evaluated as limits of scalar Toeplitz determinants. Chapter 6 contains the calculation of the asymptotic behaviour of such an extremum if the width of the surrounding sublayer tends to infinity. Finally, on the basis of this asymptotics, the asymptotic decay of $m(l_0)$ far from a single layer-shaped inhomogeneity is given. Chapter 7 discusses the results of this work.

In the first of the appendices the transcendental equation defining the global critical temperature $\tilde{T}_c$ of the layered lattice is discussed. One finds the interesting possibility of $\tilde{T}_c$ getting zero if the two sublayers favour opposite types of order (ferromagnetic resp. antiferromagnetic) and have suitable sublayer widths (see Figure 7).

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2. Spontaneous Magnetization of a Layered Lattice

Much work [9, 10] on the spontaneous magnetization of two-dimensional Ising lattices is based on the formula

$$m = \lim_{|k'-k|\to\infty} \lim_{M,N\to\infty} \sqrt{\langle \sigma_{kl}\,\sigma_{k'l}\rangle_{MN}}\,, \qquad (2.1.)$$

where $\sigma_{kl} = \pm 1$ is an Ising spin at the lattice site (k, l) of an $M \times N$ square lattice, and $\langle\,\rangle_{MN}$ denotes the average over a canonical ensemble of such lattices. (2.1) has only recently [11] been proven to be correct for ferromagnetic couplings, but since the calculations in the present work can be done for an antiferromagnetic lattice as well, we shall use the form

$$m(l) = \lim_{|k'-k|\to\infty} \lim_{M,N\to\infty} \sqrt{|\langle \sigma_{kl}\,\sigma_{k'l}\rangle_{MN}|} \qquad (2.2)$$

for both cases (without proving that it has any meaning in the antiferromagnetic case). In a layered lattice with layers parallel to the k direction m will depend on l so we have written $m(l)$ in (2.2).

In the correlation function

$$\langle \sigma_{kl}\,\sigma_{k'l}\rangle_{MN} = \frac{\sum_{\{\sigma\}} \sigma_{kl}\,\sigma_{k'l} \exp\{-E_{MN}(\{\sigma\})/k_B T\}}{\sum_{\{\sigma\}} \exp\{-E_{MN}(\{\sigma\})/k_B T\}} \tag{2.3}$$

the Hamiltonian of the lattice is

$$E_{MN}(\{\sigma\}) = -\sum_{k=1}^{M}\sum_{l=1}^{N}(J_{kl}\,\sigma_{kl}\,\sigma_{k+1,l} + \bar{J}_{kl}\,\sigma_{kl}\,\sigma_{k,l+1}) \tag{2.4}$$

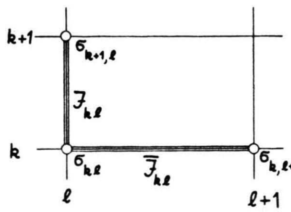

Fig. 1. Definition of the exchange couplings in (2.4).

(see Fig. 1), where cyclic boundary conditions have been applied in both lattice directions:

$$\sigma_{M+k,l} = \sigma_{k,l}, \quad \sigma_{k,N+l} = \sigma_{k,l}. \tag{2.5}$$

In (2.3) $\sum_{\{\sigma\}}$ means the sum over all lattice states $\{\sigma\} \equiv \{\sigma_{11}, \dots, \sigma_{MN}\}$. – The correlation function (2.3) can be conveniently evaluated by means of the transfer matrix

$$V_l = (V_l^{(2)})^{1/2}\, V_l^{(1)}\, (V_{l+1}^{(2)})^{1/2} \tag{2.6}$$

connecting lattice columns number l and $(l+1)$, and defined in terms of Boltzmann exponentials by

$$\left.\begin{aligned} \langle[\sigma]|V_l^{(1)}|[\sigma']\rangle &= \exp\sum_{k=1}^{M}\bar{K}_{kl}\,\sigma_k\,\sigma_k', \\ \langle[\sigma]|V_l^{(2)}|[\sigma']\rangle &= \delta_{[\sigma],[\sigma']}\exp\sum_{k=1}^{M}K_{kl}\,\sigma_k\,\sigma'_{k+1}. \end{aligned}\right\} \tag{2.7}$$

Here $[\sigma] \equiv \{\sigma_1, \dots, \sigma_M\}$ denotes the state of a single lattice column, and we use Dirac's notation to describe the corresponding state vector. In (2.7)

$$K_{kl} = J_{kl}/k_B T, \quad \bar{K}_{kl} = \bar{J}_{kl}/k_B T \tag{2.8}$$

are the "reduced" exchange couplings. With these definitions we have

$$\langle \sigma_{kl_0}\,\sigma_{k'l_0}\rangle_{MN} = \mathrm{Tr}\{\Sigma_{kk'}(\prod_{l=l_0}^{N}V_l)(\prod_{l=1}^{l_0-1}V_l)\}/\mathrm{Tr}\{\prod_{l=1}^{N}V_l\}, \tag{2.9}$$

where
$$\Sigma_{kk'} = \sum_{\{\sigma\}}|[\sigma]\rangle\,\sigma_k\,\sigma_{k'}\,\langle[\sigma]|. \tag{2.10}$$

[Since $V_l^{(2)}$, according to (2.7), is diagonal and thus commutes with $\Sigma_{kk'}$ we may use in (2.9) the form (2.6) of V_l instead of one of the forms $V_l = V_l^{(1)}\,V_{l+1}^{(2)}$ or $V_l = V_l^{(2)}\,V_l^{(1)}$. Note also the modification (3.20/21) used later in this work.]

In the following we consider a *periodically layered* lattice with period

$$n = N/\nu \quad (\nu \text{ integer}),$$

that means

$$\begin{aligned} J_{kl} &= J_l \equiv J_{l+pn}, \\ \bar{J}_{kl} &= \bar{J}_l \equiv \bar{J}_{l+pn} \end{aligned} \quad (l = 1, \dots, n; \quad p = 0, \dots, \nu-1) \tag{2.11}$$

for all k. For such a lattice it is convenient to introduce the "layer transfer matrix" $V_n(l_0)$ by

$$V_n(l_0) = \prod_{l=l_0}^{l_0+n-1} V_l. \tag{2.12}$$

The eigenvalues of $V_n(l_0)$ are $\Lambda_1, \Lambda_2, \dots$ with $|\Lambda_1| \geqq |\Lambda_2| \geqq \dots$, the corresponding right and left eigenvectors are $|\Lambda_1^R\rangle$, $|\Lambda_2^R\rangle, \dots$, resp., $\langle\Lambda_1^L|$, $\langle\Lambda_2^L|, \dots$. [For general l_0 the matrix $V_n(l_0)$ is not symmetric, hence we must distinguish between right and left eigenvectors.] Let g be the multiplicity of the eigenvalue of largest modulus, $\Lambda_{max} = \Lambda_1$, and let $|\Lambda_1^R\rangle, \dots, |\Lambda_g^R\rangle$, resp. $\langle\Lambda_1^L|, \dots, \langle\Lambda_g^L|$ be the corresponding right, resp., left eigenvectors. Using then the bi-orthonormality

$$\langle\Lambda_i^L|\Lambda_j^R\rangle = \delta_{ij} \tag{2.13}$$

and the bi-completeness

$$\sum_{i=1}^{2^M}|\Lambda_i^R\rangle\langle\Lambda_i^L| = \mathbf{1}, \tag{2.14}$$

it is easy to show that

$$\langle\sigma_{kl_0}\,\sigma_{k'l_0}\rangle_{MN} = (\sum_i \Lambda_i^\nu\langle\Lambda_i^L|\Sigma_{kk'}|\Lambda_i^R\rangle)/(\sum_i \Lambda_i^\nu) \tag{2.15}$$

and therefore

$$\lim_{M,N\to\infty}\langle\sigma_{kl_0}\,\sigma_{k'l_0}\rangle_{MN} = \lim_{M\to\infty}\frac{1}{g}\sum_{i=1}^{g}\langle\Lambda_i^L|\Sigma_{kk'}|\Lambda_i^R\rangle. \tag{2.16}$$

(Here the limit $N\to\infty$ is taken through $\nu\to\infty$ with n constant.)

Later in this work we shall use a representation of our matrices in terms of the Pauli matrices τ^x, τ^y, τ^z. In this representation the operator $\Sigma_{kk'}$ can be written as

$$\Sigma_{kk'} = \tau_k^x\,\tau_{k'}^x, \tag{2.17}$$

where τ_k^x is the direct product [(2.18b) of [10]] of τ^x with (2×2) unit matrices. Therefore in this representation we may write

$$m(l_0, T) = \lim_{|k'-k|\to\infty} \lim_{M\to\infty} \left\{ \left| \frac{1}{g} \sum_{i=1}^{g} \langle \Lambda_i^{\mathrm{L}} | \tau_k^x \tau_{k'}^x | \Lambda_i^R \rangle \right| \right\}^{1/2}. \tag{2.18}$$

Since the $\langle \Lambda_i^{\mathrm{L}}|$, $|\Lambda_i^{\mathrm{R}}\rangle$ are eigenvectors of $V_n(l_0)$ they depend on l_0, T, and M.

3. Diagonalization of the Layer Transfer Matrix

In this and the following chapter we shall take over as far as possible the many-fermion technique used by Schultz et al. [10] (hereafter referred to as SML) in the diagonalization of the transfer matrix V_l. One should note that our coupling constants $\overline{K}_l$, K_l correspond to K_1, K_2 in SML. – For the sake of convenience we shall abbreviate the frequently occurring circular and hyperbolic functions by special symbols:

$\mathrm{S}_x \equiv \sin x$	$\mathfrak{S}_x \equiv \sinh x$
$\mathrm{C}_x \equiv \cos x$	$\mathfrak{C}_x \equiv \cosh x$
$\mathrm{T}_x \equiv \tan x$	$\mathfrak{T}_x \equiv \tanh x$

(The abbreviation T_x should not be confused with the "local critical temperatures" $T_{\mathrm{c}1}$, $T_{\mathrm{c}2}$ defined later.)

The Pauli matrices used in the representation (2.17/18) are transformed to fermion operators by the Jordan-Wigner transformation SML (3.2/4):

$$\left.\begin{aligned} c_k &= (-1)^{N_{k-1}^{(\tau)}} \tau_k^-, \\ c_k^+ &= (-1)^{N_{k-1}^{(\tau)}} \tau_k^+, \end{aligned}\right\} \tag{3.1}$$

where

$$\tau_k^{\pm} = \tfrac{1}{2}(\tau_k^x \pm i\,\tau_k^y) \tag{3.2}$$

and

$$N_{k-1}^{(\tau)} = \sum_{j=1}^{k-1} \tau_j^+ \tau_j^-. \tag{3.3}$$

In terms of these fermion operators the factors of the transfer matrix V_l, (2.6/7), are given by SML (3.5/9):

$$\left.\begin{aligned} V_l^{(1)} &= (2\,\mathfrak{S}_{2\overline{K}_l})^{M/2} \exp\{-\overline{K}_l{}^* \sum_{k=1}^{M} (2\,c_k^+ c_k - 1)\}, \\ V_l^{(2)} &= \exp\{K_l [\sum_{k=1}^{M} (c_k^+ - c_k)(c_{k+1}^+ + c_{k+1}) \\ &\quad - P_{\mathrm{c}} (c_M^+ - c_M)(c_1^+ + c_1)]\}. \end{aligned}\right\} \tag{3.4}$$

The star in $\overline{K}_l{}^*$ denotes the familiar duality transform of $\overline{K}_l$ ([12], cf. Eqs. (14 – 20) of [9]):

$$\mathfrak{T}_{K^*} = e^{-2K} \Leftrightarrow \mathfrak{S}_{2K^*} \mathfrak{S}_{2K} = 1 \Leftrightarrow e^{-2K^*} = \mathfrak{T}_K. \tag{3.5}$$

In (3.4) we have defined the "c parity" P_{c} by

$$P_{\mathrm{c}} = (-1)^{N_M^{(\mathrm{c})}} \tag{3.6}$$

with $N_M^{(\mathrm{c})}$ defined analogously to (3.3):

$$N_M^{(\mathrm{c})} = \sum_{k=1}^{M} c_k^+ c_k.$$

For all l, V_l commutes with P_{c} as can be seen from (3.4) [cf. SML (3.11)]:

$$[P_{\mathrm{c}}, V_l] = 0. \tag{3.7}$$

Hence the layer transfer matrix $V_n(l_0)$ (being simply a product of different V_l's) also commutes with P_{c}:

$$[P_{\mathrm{c}}, V_n(l_0)] = 0. \tag{3.8}$$

Thus the eigenvectors of $V_n(l_0)$ can be classified according to their c parity, and we can, in analogy to SML, define two different operators $V_n^+(l_0)$ and $V_n^-(l_0)$ in the two subspaces with $P_{\mathrm{c}} = +1$, resp., $P_{\mathrm{c}} = -1$:

$$V_n^{\pm}(l_0) = \prod_{l=l_0}^{l_0+n-1} V_l^{\pm} \tag{3.9}$$

with $V_l^{\pm}$ given by SML (3.13). Therefore, $V_n^+(l_0)$ and $V_n^-(l_0)$ differ only in the anticyclic, resp., cyclic boundary condition

$$c_{M+1} = \mp c_1. \tag{3.10}$$

Like V_l we have for $V_n(l_0)$ the

Theorem 3.1: The set of eigenvectors of $V_n(l_0)$ consists of the "c-even" eigenvectors of $V_n^+(l_0)$ and the "c-odd" ones of $V_n^-(l_0)$.

Because of the $\overline{J}_{kl}$, J_{kl} being independent of k (*layered* lattice!) we can transform to running-wave fermion operators η_q by SML (3.16). Then $V_n^{\pm}(l_0)$ splits into a direct product of commuting factors, each belonging to fixed modulus of the wave number q:

$$V_n^{\pm}(l_0) = \prod_{l=1}^{n} (2\,\mathfrak{S}_{2\overline{K}_l})^{M/2} \underset{0\le q_\pm \le \pi}{\boxed{\otimes}} V_n^{q_\pm}(l_0). \tag{3.11}$$

The $q_{\pm}$ are two different sets of wave numbers corresponding to the two different boundary conditions (3.10) and are given by SML (3.17):

$$\begin{aligned} q_+ &= \pm \frac{2\pi}{M} (\mu + 1/2); \\ q_- &= \pm \frac{2\pi}{M} \mu, \pi; \end{aligned} \qquad \left(\mu = 0, \dots, \frac{M}{2} - 1\right) \tag{3.12}$$

where M is chosen to be even. The factor $V_n{}^q{}_\pm(l_0)$ is a product of the corresponding factors $V_l{}^q{}_\pm$ of V_l [see SML (3.19–21), denoted there by V_q]:

$$V_n{}^q{}_\pm(l_0) = \prod_{l=l_0}^{l_0+n-1} V_l{}^q{}_\pm . \qquad (3.13)$$

(In the following the subscript "$\pm$" of q will be suppressed until this distinction becomes essential.) Since the $V_n{}^q(l_0)$ all commute they can be diagonalized separately, and (like $V_l{}^q$) each $V_n{}^q(l_0)$ is a (4×4) matrix in the subspace spanned by

$$\{|\overset{q}{\text{vac}}\rangle_\eta, |q\rangle_\eta, |-q\rangle_\eta, |-q\,q\rangle_\eta\} . \qquad (3.14)$$

(Here $|-q\,q\rangle_\eta = \eta^+_{-q}\,\eta_q{}^+|\overset{q}{\text{vac}}\rangle_\eta = -|q, -q\rangle_\eta$, and similar.) Since the running-wave basis (3.14) is the same for all V_l [and for $V_n(l_0)$ too] the following result of SML on the $V_l{}^q$ can be taken over to the $V_n{}^q(l_0)$:

Theorem 3.2: $V_n{}^q(l_0)$ is diagonal with respect to $|q\rangle_\eta$ and $|-q\rangle_\eta$ with eigenvalues

$$\tilde\lambda_1 = \tilde\lambda_2 = \exp\left(2\,C_q \sum_{l=1}^{n} K_l\right).$$

In the subspace spanned by $\{|\overset{q}{\text{vac}}\rangle_\eta, |-q\,q\rangle_\eta\}$ $V_n{}^q(l_0)$ is represented by a (2×2) matrix

$$\exp\left(2\,C_q \sum_{l=1}^{n} K_l\right)\tilde M(l_0)$$

with

$$\tilde M(l_0) = \prod_{l=l_0}^{l_0+n-1} M_l .$$

Here $M_l = M_l(K_l, \bar K_l{}^*)$ is defined through the identification of $\exp(2\,C_q K_l) M_l$ with the corresponding (2×2) matrix of $V_l{}^q$ in the concerned subspace, see SML (3.27). Thus we are left with the diagonalization of the (2×2) matrix product

$$\tilde M(l_0) = \prod_{l=l_0}^{l_0+n-1} M_l . \qquad (3.15)$$

3.1. Eigenvalues

At this stage it is necessary to specialize (2.11) to a particular periodically layered lattice. We are interested in the behaviour of the magnetization near grain boundaries and interfaces. Thus we choose the couplings $\bar J_l$, J_l to be piecewise constant (Fig. 2):

$$(\bar J_l, J_l) = \begin{cases} (\bar J_1, J_1) & \text{for} \quad 0 \leqq l < n_1 \\ (\bar J_2, J_2) & \phantom{\text{for}} \quad n_1 \leqq l < n . \end{cases} \qquad (3.16)$$

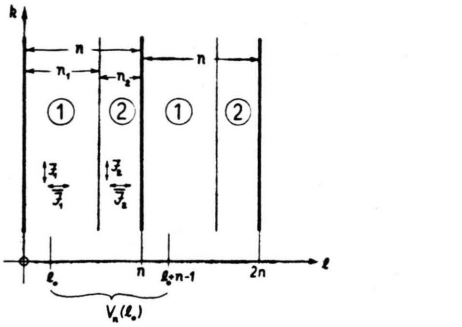

Fig. 2. The special layered lattice of (3.16). In each sublayer the exchange couplings are position-independent.

With this choice we get from (3.15):

$$\tilde M(l_0) = \begin{cases} \tilde M^{(1)}(l_0) = M_1{}^{(n_1-l_0)}\, M_2{}^{n_2}\, M_1{}^{l_0} \\ \qquad\qquad (0 \leqq l_0 < n_1) \\ \tilde M^{(2)}(l_0) = M_2{}^{(n-l_0)}\, M_1{}^{n_1}\, M_2{}^{(l_0-n_1)} \\ \qquad\qquad (n_1 \leqq l_0 < n) . \end{cases} \qquad (3.17)$$

It is sufficient to consider only one of these two cases since $\tilde M^{(2)}(l_0)$ and $\tilde M^{(1)}(l_0)$ are related by exchange of the parameters $(\bar J_1, J_1, n_1)$ with $(\bar J_2, J_2, n_2)$ and suitable renormalization of l_0. Therefore we shall confine ourselves to

$$0 \leqq l_0 < n_1 \qquad (3.18)$$

and suppress the superscript "(1)" whenever no confusion can arise.

The product (3.17) is most conveniently calculated by writing both M_1 and M_2 in their spectral representations

$$M_i = \sum_{j=3}^{4} |\mu_j{}^{(i)}\rangle\, \mu_j{}^{(i)}\, \langle\mu_j{}^{(i)}| \quad (i = 1, 2) . \qquad (3.19)$$

Thus we need the eigenvalues and eigenvectors of M_1, resp., M_2. Since M_l differs from the corresponding submatrix of $V_l{}^q$ by only a scalar factor

$$\exp(-2\,C_q K_l) ,$$

the eigenvalues μ of M_l are $\exp(-2\,C_q K_l)$ times the corresponding eigenvalues λ of $V_l{}^q$, and the eigenvectors $|\mu\rangle \equiv |\lambda\rangle$ are the same. In theorem 3.2 we have already identified $|q\rangle_\eta$ and $|-q\rangle_\eta$ to be the first, resp., second eigenvector of $V_n{}^q(l_0)$ (and, of course, also of each $V_l{}^q$). Therefore we shall denote the eigenvectors corresponding to the submatrix M_l by $|\lambda_3\rangle \equiv |\mu_3\rangle$, $|\lambda_4\rangle \equiv |\mu_4\rangle$, whence the sum $\sum_{j=3}^{4}$ in (3.19).

Since the transfer matrix V_l in (2.6) (and thus M_l) is not symmetric in the general case $J_l \neq J_{l+1}$

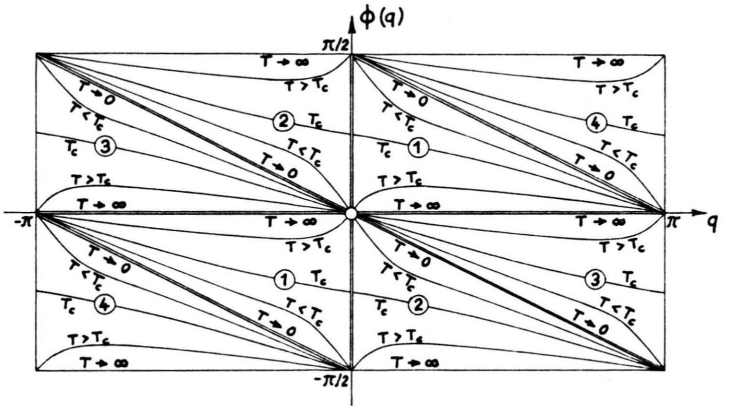

Fig. 3. Qualitative behaviour of the Bogoljubov angle $\varphi(q)$ in the "quadratic" lattice with $|\bar{J}|=|J|$. The numbers (1) to (4) refer to the various sign combinations of J and $\bar{J}$: (1) $J, \bar{J}>0$; (2) $J>0, \bar{J}<0$; (3) $J<0, \bar{J}>0$; (4) $J, \bar{J}<0$. In each case all curves contained in a triangle ◺ or ◹ belong to the same number.

we ought to distinguish between left and right eigenvectors in (3.19). To evade this complication (and to make use of the known results of SML on V_l) we alter the definition (2.6) into the symmetric form

$$V_l = (V_l^{(2)})^{1/2}\, V_l^{(1)}\, (V_l^{(2)})^{1/2}\,. \qquad (3.20)$$

This makes sense because, according to (2.7), $V_l^{(2)}$ is diagonal in that representation and therefore (3.20) has, in the product $\prod_l V_l$, the mere result of introducing the arithmetic mean

$$J_l^{\text{eff}} = (J_{l-1} + J_l)/2 \qquad (3.21)$$

instead of J_l. In our particular layered lattice (3.16) this comes into play only at the interfaces. [It should be noted that, owing to (3.21), our lattice is slightly different from that one treated in [5]].

With the "effective" mean couplings (3.21) introduced at the interfaces, we may thus use the symmetric definition (3.20) of the transfer matrix and take over the results of SML on the eigenvalues and eigenvectors of $M_l \triangleq \exp(-2\,\mathrm{C}_q K_l)\, V_l^q$. So we get for (3.19) (with $i=1, 2$ in the following)

$$M_i = |\lambda_3^{(i)}\rangle\, e^{\varepsilon_i}\, \langle\lambda_3^{(i)}| + |\lambda_4^{(i)}\rangle\, e^{-\varepsilon_i}\, \langle\lambda_4^{(i)}| \qquad (3.22)$$

with $\varepsilon_i(q)$ given by SML (3.29):

$$\mathfrak{C}_{\varepsilon_i} = \mathfrak{C}_{2K_i}\mathfrak{C}_{2\bar{K}_i^*} - \mathfrak{S}_{2K_i}\mathfrak{S}_{2\bar{K}_i^*}\,\mathrm{C}_q \qquad (3.23\text{ a})$$

$$\equiv (\mathfrak{C}_{2K_i}\mathfrak{C}_{2\bar{K}_i} - \mathfrak{S}_{2K_i}\mathrm{C}_q)/\mathfrak{S}_{2\bar{K}_i}\,,$$

$$\operatorname{Re}\varepsilon_i > 0\,. \qquad (3.23\text{ b})$$

[In the case $\bar{J}_i<0$, not considered by SML, $\varepsilon_i(q)$ is multiple-valued with a constant imaginary part of $(2\nu=1)\pi$, ν integer.] The $|\lambda_{3/4}^{(i)}\rangle$ are given by SML (3.30):

$$\left.\begin{aligned} |\lambda_3^{(i)}\rangle &= \mathrm{C}_{\varphi_i}\, \overset{q}{|\mathrm{vac}\rangle_\eta} + \mathrm{S}_{\varphi_i}\, |-q\, q\rangle_\eta\,, \\ |\lambda_4^{(i)}\rangle &= -\mathrm{S}_{\varphi_i}\, \overset{q}{|\mathrm{vac}\rangle_\eta} + \mathrm{C}_{\varphi_i}\, |-q\, q\rangle_\eta\,, \end{aligned}\right\} \qquad (3.24)$$

and the angle $\varphi_i(q)$ is defined by SML (3.32):

$$\cot 2\varphi_i = \frac{1}{\mathrm{S}_q}\,[\mathfrak{S}_{2K_i}\mathfrak{C}_{2\bar{K}_i} - (\mathfrak{C}_{2K_i} - 1)\,\mathrm{C}_q]^{-1} - \cot q\,, \qquad (3.25\text{ a})$$

$$\operatorname{sgn}\varphi_i = \operatorname{sgn}(q\,\bar{J}_i\, J_i) \quad \text{in} \quad -\pi < q \leqq \pi\,. \qquad (3.25\text{ b})$$

(This sign convention corresponds to the restriction $|\varphi_i| \leqq \pi/2$, see SML and [13].) The qualitative behaviour of $\varphi_i(q)$ is shown in Fig. 3 for various parameter combinations and all temperatures. Figure 4 gives the "critical" curves of $\varphi_i(q)$ at $T=T_c$ for different ratios $|J/\bar{J}|$.

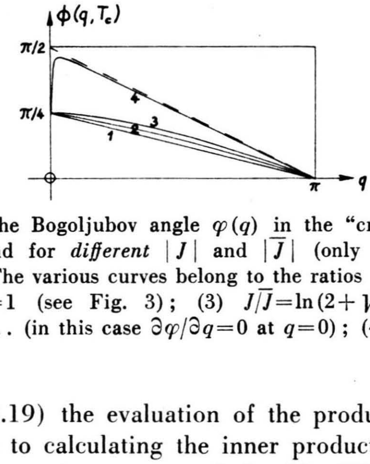

Fig. 4. The Bogoljubov angle $\varphi(q)$ in the "critical" case $T=T_c$ and for *different* $|J|$ and $|\bar{J}|$ (only $J>0$, $\bar{J}>0$ shown). The various curves belong to the ratios (1) $J/\bar{J}=0$; (2) $J/\bar{J}=1$ (see Fig. 3); (3) $J/\bar{J}=\ln(2+\sqrt{3})/\ln\sqrt{3}=2.39749\ldots$ (in this case $\partial\varphi/\partial q=0$ at $q=0$); (4) $J/\bar{J}\to\infty$.

With (3.19) the evaluation of the product (3.17) amounts to calculating the inner products between the various eigenvectors of the M_i. With (3.24) these are found to be

$$\left.\begin{aligned} \langle\lambda_3^{(1)}|\lambda_3^{(2)}\rangle &= \mathrm{C}_{\varphi_1-\varphi_2} = \langle\lambda_4^{(1)}|\lambda_4^{(2)}\rangle\,, \\ \langle\lambda_3^{(1)}|\lambda_4^{(2)}\rangle &= \mathrm{S}_{\varphi_1-\varphi_2} = -\langle\lambda_4^{(1)}|\lambda_3^{(2)}\rangle \end{aligned}\right\} \qquad (3.26)$$

whence we get in the basis $\{|\lambda_3^{(1)}\rangle, |\lambda_4^{(1)}\rangle\}$

$$\tilde{M}^{(1)}(l_0) \triangleq \begin{pmatrix} \tilde{A} & -e^{+(n_1-2l_0)\varepsilon_1}\tilde{D} \\ -e^{-(n_1-2l_0)\varepsilon_1}\tilde{D} & \tilde{B} \end{pmatrix} \qquad (3.27)$$

with

$$\left.\begin{array}{l}\tilde{A}\\ \tilde{B}\end{array}\right\} = e^{\pm n_1 \varepsilon_1}\left(\mathfrak{C}_{n_2 \varepsilon_2} \pm \mathfrak{S}_{n_2 \varepsilon_2} \mathrm{C}_{2(\varphi_1-\varphi_2)}\right), \qquad \tilde{D} = \mathfrak{S}_{n_2 \varepsilon_2} \mathrm{S}_{2(\varphi_1-\varphi_2)}\,. \tag{3.28}$$

Because $\det \tilde{M} = 1$, it is possible to write the eigenvalues as

$$\mu_{3/4} = e^{\pm \tilde{\varepsilon}(q)} \tag{3.29}$$

and therefore (using the invariance of $\operatorname{Tr} \tilde{M} = \mu_3 + \mu_4$ under similarity transformations)

$$\mathfrak{C}_{\tilde{\varepsilon}} = \frac{\tilde{A}+\tilde{B}}{2} = \mathfrak{C}_{n_1 \varepsilon_1} \mathfrak{C}_{n_2 \varepsilon_2} + \mathfrak{S}_{n_1 \varepsilon_1} \mathfrak{S}_{n_2 \varepsilon_2} \mathrm{C}_{2(\varphi_1-\varphi_2)} \tag{3.30 a}$$

with the additional convention

$$\operatorname{Re} \tilde{\varepsilon} > 0\,. \tag{3.30 b}$$

Equations (3.29/30) define the eigenvalues of $\tilde{M}(l_0)$ for all q values where

$$\mathrm{S}_{2(\varphi_1-\varphi_2)} \neq 0\,, \tag{3.31}$$

i. e. $\tilde{D} \neq 0$. If $\tilde{D} = 0$ the eigenvalues and eigenvectors can be taken directly from (3.27/28). (3.31) is certainly violated at $q = 0$ and $q = \pi$ (see Fig. 3) and, for special values of the exchange couplings and the temperature, at $q = \pm q_s$ with

$$\cos q_s = \left(\mathfrak{C}_{2\bar{K}_1} \mathfrak{S}_{2K_1} - \mathfrak{C}_{2\bar{K}_2} \mathfrak{S}_{2K_2}\right) / \left(\mathfrak{C}_{2K_1} - \mathfrak{C}_{2K_2}\right), \tag{3.32}$$

provided $|\cos q_s| \leq 1$.

From theorem 3.2 we have for the first and second eigenvalue of $V_n{}^q(l_0)$:

$$\tilde{\lambda}_1 = \tilde{\lambda}_2 = \exp\{2\,\mathrm{C}_q(n_1 K_1 + n_2 K_2)\}\,, \tag{3.33 a}$$

and from (3.29/30) the third and fourth eigenvalues follow as

$$\tilde{\lambda}_{3/4} = \exp\{2\,\mathrm{C}_q(n_1 K_1 + n_2 K_2)\}\, e^{\pm \tilde{\varepsilon}(q)}\,. \tag{3.33 b}$$

3.2. Eigenvectors

The third and fourth eigenvectors of $V_n{}^q(l_0)$ are the eigenvectors of $\tilde{M}(l_0)$ which can easily be deduced from (3.27) (for general l_0 left and right eigenvectors must be distinguished!):

$$\left.\begin{array}{l}
\langle \tilde{\lambda}_3{}^{\mathrm{L}}| = \mathrm{C}_{\tilde{\varphi}_{\mathrm{L}}} \langle \lambda_3{}^{(1)}| + \mathrm{S}_{\tilde{\varphi}_{\mathrm{L}}} \langle \lambda_4{}^{(1)}|\,; \\
\qquad |\tilde{\lambda}_3{}^{\mathrm{R}}\rangle = \mathrm{C}_{\tilde{\varphi}_{\mathrm{R}}} |\lambda_3{}^{(1)}\rangle + \mathrm{S}_{\tilde{\varphi}_{\mathrm{R}}} |\lambda_4{}^{(1)}\rangle\,; \\
\langle \tilde{\lambda}_4{}^{\mathrm{L}}| = -\mathrm{S}_{\tilde{\varphi}_{\mathrm{R}}} \langle \lambda_3{}^{(1)}| + \mathrm{C}_{\tilde{\varphi}_{\mathrm{R}}} \langle \lambda_4{}^{(1)}|\,; \\
\qquad |\tilde{\lambda}_4{}^{\mathrm{R}}\rangle = -\mathrm{S}_{\tilde{\varphi}_{\mathrm{L}}} |\lambda_3{}^{(1)}\rangle + \mathrm{C}_{\tilde{\varphi}_{\mathrm{L}}} |\lambda_4{}^{(1)}\rangle\,,
\end{array}\right\} \tag{3.34}$$

where the two angles $\tilde{\varphi}_{\mathrm{R}}(q)$, $\tilde{\varphi}_{\mathrm{L}}(q)$ are defined by

$$\left.\begin{array}{l}
\tan \tilde{\varphi}_{\mathrm{R}} = \dfrac{\tilde{A} - e^{\tilde{\varepsilon}}}{e^{(n_1-2l_0)\varepsilon_1} \tilde{D}} \equiv \dfrac{e^{-(n_1-2l_0)\varepsilon_1} \tilde{D}}{\tilde{B} - e^{\tilde{\varepsilon}}}\,, \\[2ex]
\tan \tilde{\varphi}_{\mathrm{L}} = \dfrac{e^{(n_1-2l_0)\varepsilon_1} \tilde{D}}{e^{-\tilde{\varepsilon}} - \tilde{A}} \equiv \dfrac{e^{-\tilde{\varepsilon}} - \tilde{B}}{e^{-(n_1-2l_0)\varepsilon_1} \tilde{D}}\,,
\end{array}\right\} \tag{3.35}$$

If we define the sum angles

$$\hat{\varphi}_{\mathrm{R}} = \tilde{\varphi}_{\mathrm{R}} + \varphi_1\,, \quad \hat{\varphi}_{\mathrm{L}} = \tilde{\varphi}_{\mathrm{L}} = \varphi_1\,, \tag{3.36}$$

we can relate our vectors (3.34), with the help of (3.24), to the running-wave basis $\{|\overset{q}{\mathrm{vac}}\rangle_\eta, |-q\,q\rangle_\eta\}$:

$$\left.\begin{array}{l}
\langle \tilde{\lambda}_3{}^{\mathrm{L}}| = \mathrm{C}_{\hat{\varphi}_{\mathrm{L}}}\, {}_\eta\langle \overset{q}{\mathrm{vac}}| + \mathrm{S}_{\hat{\varphi}_{\mathrm{L}}}\, {}_\eta\langle -q\,q|\,; \\
\qquad |\tilde{\lambda}_3{}^{\mathrm{R}}\rangle = \mathrm{C}_{\hat{\varphi}_{\mathrm{R}}} |\overset{q}{\mathrm{vac}}\rangle_\eta + \mathrm{S}_{\hat{\varphi}_{\mathrm{R}}} |-q\,q\rangle_\eta\,; \\
\langle \tilde{\lambda}_4{}^{\mathrm{L}}| = -\mathrm{S}_{\hat{\varphi}_{\mathrm{R}}}\, {}_\eta\langle \overset{q}{\mathrm{vac}}| + \mathrm{C}_{\hat{\varphi}_{\mathrm{R}}}\, {}_\eta\langle -q\,q|\,; \\
\qquad |\tilde{\lambda}_4{}^{\mathrm{R}}\rangle = -\mathrm{S}_{\hat{\varphi}_{\mathrm{L}}} |\overset{q}{\mathrm{vac}}\rangle_\eta + \mathrm{C}_{\hat{\varphi}_{\mathrm{L}}} |-q\,q\rangle_\eta\,.
\end{array}\right\} \tag{3.37}$$

The relation between the vectors (3.37) is shown in Figure 5.

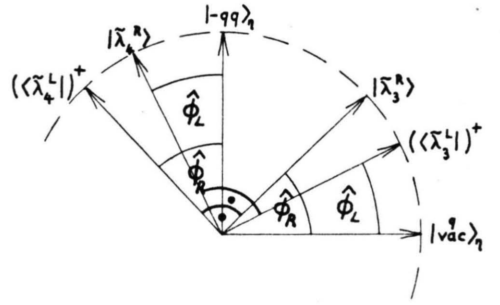

Fig. 5. The left and right eigenvectors (3.37) of $V_n{}^q(l_0)$.

In the special case $l_0 = n_1/2$ the matrix $\tilde{M}^{(1)}(l_0)$ is symmetric as can be seen from (3.17) and (3.27). [For $\tilde{M}^{(2)}(l_0)$ this occurs for $l_0 = n_1 + n_2/2$.] Then the two definitions (3.35) for $\tilde{\varphi}_{\mathrm{R}}$ and $\tilde{\varphi}_{\mathrm{L}}$ coincide, and there is only one common angle $\tilde{\varphi}(q)$:

$$\boxed{l_0 = n_1/2:} \quad \left.\begin{array}{l}\tilde{\varphi}_{\mathrm{R}}(q) \equiv \tilde{\varphi}_{\mathrm{L}}(q) \equiv \tilde{\varphi}(q)\,, \\ \hat{\varphi}_{\mathrm{R}}(q) \equiv \hat{\varphi}_{\mathrm{L}}(q) \equiv \hat{\varphi}(q)\,.\end{array}\right\} \tag{3.38}$$

Therefore the right and left eigenvectors become identical (as is to be expected for a symmetric matrix):

$$|\tilde{\lambda}_3{}^{\mathrm{R}}\rangle \equiv (\langle \tilde{\lambda}_3{}^{\mathrm{L}}|)^+, \quad |\tilde{\lambda}_4{}^{\mathrm{R}}\rangle \equiv (\langle \tilde{\lambda}_4{}^{\mathrm{L}}|)^+.$$

In this case there can be derived a more convenient equation for $\tilde{\varphi}$ not containing $\tilde{\varepsilon}$. For general l_0 one has from (3.35) [in analogy to SML (3.32 a)]:

$$\left.\begin{matrix}\cot 2\tilde{\varphi}_R \\ \cot 2\tilde{\varphi}_L\end{matrix}\right\} = \frac{1}{2\tilde{D}} \cdot \{(\tilde{B}-\tilde{A})\mathfrak{C}_{(n_1-2l_0)\varepsilon_1} \mp 2\,\mathfrak{S}_{\tilde{\varepsilon}}\mathfrak{C}_{(n_1-2l_0)\varepsilon_1}\} \quad (3.39)$$

and thus for $l_0 = n_1/2$:

$$\cot 2\tilde{\varphi} = \frac{\tilde{B}-\tilde{A}}{2\tilde{D}} = -\frac{\mathfrak{S}_{n_1\varepsilon_1}}{\mathfrak{T}_{n_2\varepsilon_2}\,S_{2(\varphi_1-\varphi_2)}} - \frac{\mathfrak{C}_{n_1\varepsilon_1}}{T_{2(\varphi_1-\varphi_2)}} \quad (3.40)$$

or

$$\cot 2\tilde{\varphi} = -(\operatorname{sgn}\bar{J}_1)^{n_1}\left\{\frac{\mathfrak{S}_{n_1\mathrm{Re}\,\varepsilon_1}}{\mathfrak{T}_{n_2\mathrm{Re}\,\varepsilon_2}\,S_{2(\varphi_1-\varphi_2)}} + \frac{\mathfrak{C}_{n_1\mathrm{Re}\,\varepsilon_1}}{T_{2(\varphi_1-\varphi_2)}}\right\}, \quad (3.40')$$

where $\mathrm{Re}\,\varepsilon_i$ is given by (3.23 a) with $\bar{K}_i$ replaced by $|\bar{K}_i|$. Since the $\tilde{\varphi}$ are given by (3.39/40) modulo $\pi/2$ only, there should be (to fix the eigenvectors uniquely) an additional condition like (3.25 b) which restricts the $\tilde{\varphi}$ to an interval of length π. Later, however, we shall see that both values of $\tilde{\varphi}$ given by (3.40) yield the same value of the spontaneous magnetization. So there is no need to fix an additional condition on $\tilde{\varphi}$ in this work.

3.3. Fermion Eigenstates

In the following we try to interpret (3.37), in analogy to SML (3.33), as a Bogoljubov transformation from the η fermions to new $\tilde{\xi}$ fermion states (which for general l_0, of course, have to be non-orthogonal [14]). Using the abbreviation

$$C_{RL} = \cos(\hat{\varphi}_R - \hat{\varphi}_L) \quad (3.41)$$

we therefore define the new operators

$$\left.\begin{aligned}\tilde{\xi}_q &= C_{RL}^{-1/2}\{\eta_q\,C_{\hat{\varphi}_R} + \eta_{-q}^+\,S_{\hat{\varphi}_R}\},\\ \tilde{\xi}_{-q}^{(+)} &= C_{RL}^{-1/2}\{-\eta_q\,S_{\hat{\varphi}_L} + \eta_{-q}^+\,C_{\hat{\varphi}_L}\}\end{aligned}\right\} \quad (3.42)$$

and the (renormalized) state vectors

$$\left.\begin{aligned}|\overset{q}{\mathrm{vac}}{}^R\rangle_\xi &= C_{RL}^{-1/2}\{C_{\hat{\varphi}_R}\,|\overset{q}{\mathrm{vac}}\rangle_\eta + S_{\hat{\varphi}_R}\,|-q\,q\rangle_\eta\},\\ |-q\,q^R\rangle_\xi &= C_{RL}^{-1/2}\{-S_{\hat{\varphi}_L}\,|\overset{q}{\mathrm{vac}}\rangle_\eta + C_{\hat{\varphi}_L}\,|-q\,q\rangle_\eta\},\\ |q\rangle_\xi &= |q\rangle_\eta,\\ |-q\rangle_\xi &= |-q\rangle_\eta\end{aligned}\right\} \quad (3.43)$$

and analogously for the left vectors. [It should be noted that these renormalized vectors satisfy the bi-orthonormality (2.13), and not the vectors (3.37).] It is easily seen that the operators (3.42) obey the usual fermion anticommutators

$$\{\tilde{\xi}_q, \tilde{\xi}_{q'}^{(+)}\} = \delta_{qq'}, \quad \{\tilde{\xi}_q\,\tilde{\xi}_{q'}\} = 0 \quad (3.44)$$

and that they create, resp., annihilate $\tilde{\xi}$ fermions in the states (3.43). Thus a (non-hermitian!) $\tilde{\xi}$-particle-number operator can be constructed too:

$$\mathfrak{N}_q = \tilde{\xi}_{-q}^{(+)}\,\tilde{\xi}_q + \tilde{\xi}_q^{(+)}\,\tilde{\xi}_{-q} \quad (3.45)$$

which counts the fermions in the states (3.43):

$$\left.\begin{aligned}\mathfrak{N}_q\,|\overset{q}{\mathrm{vac}}{}^R\rangle_\xi &= 0,\\ \mathfrak{N}_q\,|q\rangle_\xi &= 1\cdot|q\rangle_\xi,\\ \mathfrak{N}_q\,|-q\rangle_\xi &= 1\cdot|-q\rangle_\xi,\\ \mathfrak{N}_q\,|-q\,q^R\rangle_\xi &= 2\cdot|-q\,q^R\rangle_\xi.\end{aligned}\right\} \quad (3.46)$$

Comparison with the eigenvalues (3.33) of $V_n{}^q(l_0)$ leads to the following diagonal representation of $V_n{}^q(l_0)$:

$$V_n{}^q(l_0) = \exp\{2\,C_q(n_1 K_1 + n_2 K_2)\} \times \exp\{-\tilde{\varepsilon}(q)\,(\mathfrak{N}_q - 1)\} \quad (3.47)$$

which can be decomposed into two factors corresponding to $+q$ and $-q$:

$$\begin{aligned}V_n{}^q(l_0) &= \exp\{C_q(n_1 K_1 + n_2 K_2)\}\\ &\times \exp\{-\tilde{\varepsilon}(q)\,(\tilde{\xi}_q^{(+)}\,\tilde{\xi}_q - \tfrac{1}{2})\}\\ &\times \exp\{C_{-q}(n_1 K_1 + n_2 K_2)\}\\ &\times \exp\{-\tilde{\varepsilon}(-q)\,(\tilde{\xi}_{-q}^{(+)}\,\tilde{\xi}_{-q} - \tfrac{1}{2})\}.\end{aligned} \quad (3.48)$$

Our deduction of (3.48) is valid primarily for those values of q which fulfill (3.31), $S_{2(\varphi_1-\varphi_2)} \neq 0$. Nevertheless, it can easily be adapted to $q = 0$ and $q = \pi$ as well, which together give the two factors of (3.48) if we use $\cos(0) + \cos(\pi) = 0$ and define

$$\tilde{\varepsilon}(q) = 2\,n_1(\bar{K}_1{}^* \mp K_1) + 2\,n_2(\bar{K}_2{}^* \mp K_2) \quad \text{for } q = \{{}^0_\pi, \quad (3.49\text{ a})$$

$$\tilde{\xi}_q^{(+)} = \eta_q{}^+, \quad \tilde{\xi}_q = \eta_q \quad \text{for all } T \text{ and for } q = 0, \pi. \quad (3.49\text{ b})$$

(For $T < \tilde{T}_c$, where $\tilde{T}_c$ is the "global" critical temperature of the layered lattice [see Appendix A], the real part of one of the $\tilde{\varepsilon}(q)$ becomes negative according to (3.49 a), in contrast to the convention (3.30 b). Likewise (3.49 b) implies that $\hat{\varphi}_R = \hat{\varphi}_L = 0$ for $q = 0, \pi$ and for all T, in contradiction to (3.35). It can be shown [13], however, that (3.49) is equivalent to (3.30 b) and (3.35) in all respects, especially regarding the asymptotic degeneracy of the largest eigenvalue of $V_n(l_0)$.) In a similar manner (3.48) can be adapted to the exceptional values $q = \pm q_s$ [see (3.32)] if we define

$$\tilde{\varepsilon}(q_s) = n_1 \varepsilon_1(q_s) + \gamma_{q_s} n_2 \varepsilon_2(q_s) \quad (3.50\,\text{a})$$

with

$$\gamma_{q_s} = \cos 2(\varphi_1 - \varphi_2)|_{q_s} = \pm 1, \quad \text{and}$$

$$\tilde{\xi}^{(+)}_{q_s} = \xi^{+}_{q_s}(\varphi_1), \quad \tilde{\xi}_{q_s} = \xi_{q_s}(\varphi_1) \quad \text{for all } T. \quad (3.50\,\text{b})$$

The $\xi_q(\varphi_1)$ are given by (3.42) with $\tilde{\varphi}_R = \tilde{\varphi}_L = 0$ [or by SML (3.33) with $\varphi = \varphi_1$] and characterize the eigenvectors of the V_l belonging to the sublayer (1).

Since we now can write $V_n{}^q(l_0)$ in the form (3.48) for all q, we have [by the direct product (3.11)] also a diagonal representation of $V_n{}^{\pm}(l_0)$:

$$V_n{}^{\pm}(l_0) = [(2\,\mathfrak{S}_{2\bar{K}_1})^{n_1}(2\,\mathfrak{S}_{2\bar{K}_2})^{n_2}]^{M/2} \quad (3.51)$$

$$\cdot \exp\{-\sum_{-\pi<q_\pm\leq\pi} \tilde{\varepsilon}(q_\pm)(\tilde{\xi}^{(+)}_{q_\pm}\tilde{\xi}_{q_\pm} - \tfrac{1}{2})\},$$

where we have used $\sum_q \cos q = 0$. Thus the eigenvectors of $V_n{}^{\pm}(l_0)$ are simply the states of defined $\tilde{\xi}$-particle number. To get the eigenvectors of $V_n(l_0)$, however, we have to observe theorem 3.1, i.e. to consider the c-parity P_c of our vectors. Now (3.49 b) and (3.50 b) allow an extremely simple connection between P_c and the "$\tilde{\xi}$-parity"

$$P_{\tilde{\xi}} = (-1)^{\sum_q \tilde{\xi}_q{}^{(+)}\tilde{\xi}_q}. \quad (3.52)$$

For, like SML, we have $\sum_{k=1}^{M} c_k{}^+ c_k = \sum_q \eta_q{}^+ \eta_q$, i.e. $P_c = P_\eta$. Now (3.43) together with (3.49 b) and (3.50 b) leads to $P_\eta = P_{\tilde{\xi}}$, so we have

$$P_c = P_{\tilde{\xi}} \quad \text{for all } T. \quad (3.53)$$

Thus we can reformulate theorem 3.1 and get

Theorem 3.3: The set of eigenvectors of $V_n(l_0)$ consists of the "$\tilde{\xi}$-even" eigenvectors of $V_n{}^+(l_0)$ and of the "$\tilde{\xi}$-odd" ones of $V_n{}^-(l_0)$.

With this theorem we now can find the eigenvectors belonging to the largest eigenvalue of $V_n(l_0)$ which are needed in (2.18). According to theorem 3.3, the largest eigenvalue of $V_n(l_0)$ belongs to the $\tilde{\xi}$-vacuum

$$|\text{vac}^{\text{R}}\rangle_{\tilde{\xi}} = \prod_{0<q_+<\pi}^{q_+} \otimes |\text{vac}^{\text{R}}\rangle_{\xi} \quad (3.54)$$

(we have to choose q_+ here because the vacuum has even particle number) and has the value

$$\Lambda_{\max} = [(2\,\mathfrak{S}_{2\bar{K}_1})^{n_1}(2\,\mathfrak{S}_{2\bar{K}_2})^{n_2}]^{M/2} \exp\{\tfrac{1}{2}\sum_{-\pi<q_+\leq\pi} \tilde{\varepsilon}(q_+)\}. \quad (3.55)$$

At $T < \tilde{T}_c$, however, we can create a one-particle state which has, according to (3.49 a), an eigenvalue nearly equal to (3.55). In Appendix A we show that it is the $\tilde{q}_c = 0$ or $\tilde{q}_c = \pi$ fermion, according to

$$\cos \tilde{q}_c = \text{sgn}(n_1 J_1 + n_2 J_2), \quad (3.56)$$

whose "energy" $\tilde{\varepsilon}$ gets a negative real part at $T < \tilde{T}_c$ and thus makes the eigenvalue of the $|\tilde{q}_c\rangle_{\tilde{\xi}}$ state,

$$\Lambda_{(-)} = [(2\,\mathfrak{S}_{2\bar{K}_1})^{n_1}(2\,\mathfrak{S}_{2\bar{K}_2})^{n_2}]^{M/2} \quad (3.57)$$

$$\cdot \exp\tfrac{1}{2}\{\sum_{q_- \neq q_c} \tilde{\varepsilon}(q_-) - \tilde{\varepsilon}(\tilde{q}_c)\},$$

asymptotically degenerate with (3.55) (in the limit $M \to \infty$). It is this asymptotic degeneracy which causes the ordered state of our lattice [15]. All other eigenvalues of $V_n(l_0)$ differ from (3.55/57) by a factor $\exp \tilde{\varepsilon}(\tilde{q}_c)$ or more.

4. The Spontaneous Magnetization $m(l_0)$

In (2.18) the spontaneous magnetization is expressed in terms of the expectation values of $\tau_k{}^x \tau_{k'}{}^x$ in the states belonging to $\Lambda_{\max}$, i.e. the $\tilde{\xi}$-vacuum and the one-particle state $|\tilde{q}_c\rangle_{\tilde{\xi}}$, according to (3.55/57). To evaluate these expectation values we write the product $\tau_k{}^x \tau_{k'}{}^x$ in terms of the c's [see SML (4.7)]:

$$\tau_k{}^x \tau_{k'}{}^x = \prod_{j=k}^{k'-1} (i\, c_j{}^y)\, c^x_{j+1} \quad (4.1)$$

where [in analogy to (3.2)]

$$\left.\begin{matrix} c_j{}^x \\ i\, c_j{}^y \end{matrix}\right\} = c_j{}^+ \pm c_j. \quad (4.2)$$

In (4.1) we have assumed $k' > k$ without loss of generality. – By SML (3.16) and the inverse of (3.42) we can express the c's in terms of the $\tilde{\xi}$'s:

$$\left.\begin{matrix} c_j{}^x \\ i\, c_j{}^y \end{matrix}\right\} = M^{-1/2} \sum_{-\pi<q\leq\pi} \mathrm{C}_{\mathrm{RL}}^{-1/2}\{\tilde{\xi}_q{}^{(+)} e^{-i(qj \pm \hat{\varphi}_{\mathrm{R}} - \pi/4)} \quad (4.3)$$

$$\pm \tilde{\xi}_q\, e^{i(qj \pm \hat{\varphi}_{\mathrm{L}} - \pi/4)}\}.$$

Here we have used the antisymmetry of $\hat{\varphi}_{\mathrm{R}}$ and $\hat{\varphi}_{\mathrm{L}}$:

$$\hat{\varphi}_{\mathrm{R,L}}(-q) = -\hat{\varphi}_{\mathrm{R,L}}(q) \quad (4.4)$$

which can be seen from (3.35) and the following antisymmetry, resp., symmetry properties:

$$\varphi_i(-q) = -\varphi_i(q); \quad \varepsilon_i(-q) = +\varepsilon_i(q);$$
$$\tilde{\varepsilon}(-q) = +\tilde{\varepsilon}(q). \quad (i = 1, 2) \quad (4.5)$$

[These properties can be verified from the definitions (3.23, 25, 30).] Since by (4.2) the c^x, $i\, c^y$

are linear expressions of fermion operators, their anticommutators are c-numbers:

$$\{c_m^x, c_n^y\} = 0\,, \quad \{c_m^x, c_n^x\} = 2\,\delta_{mn} = \{c_m^y, c_n^y\}\,, \tag{4.6}$$

and we can apply Wick's theorem to (4.1). We then have to consider the products of all pairings of c's, a pairing being the corresponding ($\tilde{\xi}$-vacuum or $|\tilde{q}_c\rangle_\xi$) expectation value of the product of two c's. These expectation values in turn can be calculated conveniently with the help of (4.3). So we find in the ξ-vacuum state:

$$\left.\begin{aligned} \mathrm{XX}_{m-l} &:= {}_\xi\langle \mathrm{vac^L} \,|\, c_l^x\, c_m^x \,|\, \mathrm{vac^R}\rangle_\xi \\ \mathrm{YY}_{m-l} &:= {}_\xi\langle \mathrm{vac^L} \,|\, i\, c_l^y\, i\, c_m^y \,|\, \mathrm{vac^R}\rangle_\xi \end{aligned}\right\} = \pm \frac{1}{M} \sum_{-\pi<q\leq\pi} e^{-iq(m-l)} (1 \mp i\, \mathrm{T}_{\hat{\varphi}_\mathrm{R}-\hat{\varphi}_\mathrm{L}})\,, \tag{4.7}$$

$$\left.\begin{aligned} \mathrm{YX}_{m-l} &:= {}_\xi\langle \mathrm{vac^L} \,|\, i\, c_l^y\, c_m^x \,|\, \mathrm{vac^R}\rangle_\xi \\ \mathrm{XY}_{m-l} &:= {}_\xi\langle \mathrm{vac^L} \,|\, c_l^x\, i\, c_m^y \,|\, \mathrm{vac^R}\rangle_\xi \end{aligned}\right\} = \mp \frac{1}{M} \sum_{-\pi<q\leq\pi} e^{-iq(m-l)} \frac{e^{\mp i(\hat{\varphi}_\mathrm{R}+\hat{\varphi}_\mathrm{L})}}{\mathrm{C}_{\hat{\varphi}_\mathrm{R}-\hat{\varphi}_\mathrm{L}}} \tag{4.8}$$

These pairings differ from those in the $|\tilde{q}_c\rangle_\xi$ state by

$$\left.\begin{aligned} {}_\xi\langle \tilde{q}_c \,|\, c_l^x\, c_m^x \,|\, \tilde{q}_c\rangle_\xi - \mathrm{XX}_{m-l} \\ {}_\xi\langle \tilde{q}_c \,|\, i\, c_l^y\, i\, c_m^y \,|\, \tilde{q}_c\rangle_\xi - \mathrm{YY}_{m-l} \end{aligned}\right\} = \pm \frac{2\,i}{M}\, \mathrm{S}_{\tilde{q}_c(m-l)} = 0\,, \tag{4.9}$$

$$\left.\begin{aligned} {}_\xi\langle \tilde{q}_c \,|\, i\, c_l^y\, c_m^x \,|\, \tilde{q}_c\rangle_\xi - \mathrm{YX}_{m-l} \\ {}_\xi\langle \tilde{q}_c \,|\, c_l^x\, i\, c_m^y \,|\, \tilde{q}_c\rangle_\xi - \mathrm{XY}_{m-l} \end{aligned}\right\} = \pm \frac{2}{M}\, \mathrm{C}_{\tilde{q}_c(m-l)} = \pm \frac{2}{M} [\mathrm{sgn}(n_1 J_1 + n_2 J_2)]^{m-l}\,, \tag{4.10}$$

where (3.56) has been used.

Since the limit $M \to \infty$ in (2.18) has to be done before $|k-k'| \to \infty$, it is the limit of a finite sum of finite products of pairings. So one may carry out this limit already in the pairings (4.7 – 10). Because of $\Delta q = 2\,\pi/M$ [see (3.12)] we have to replace then

$$\frac{1}{M} \sum_{-\pi<q\leq\pi} \quad \text{by} \quad \frac{1}{2\,\pi} \int_{-\pi}^{\pi} \mathrm{d}q$$

and get for (4.7, 8):

$$\left.\begin{aligned} \mathrm{xx}_{m-l} &:= \lim_{M\to\infty} \mathrm{XX}_{m-l} \\ \mathrm{yy}_{m-l} &:= \lim_{M\to\infty} \mathrm{YY}_{m-l} \end{aligned}\right\} = \pm \int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\,\pi}\, e^{-iq(m-l)}\, (1 \mp i\, \mathrm{T}_{\hat{\varphi}_\mathrm{R}-\hat{\varphi}_\mathrm{L}})\,, \tag{4.11}$$

$$\left.\begin{aligned} \mathrm{yx}_{m-l} &:= \lim_{M\to\infty} \mathrm{YX}_{m-l} \\ \mathrm{xy}_{m-l} &:= \lim_{M\to\infty} \mathrm{XY}_{m-l} \end{aligned}\right\} = \mp \int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\,\pi}\, e^{-iq(m-l)}\, \frac{e^{\mp i(\hat{\varphi}_\mathrm{R}+\hat{\varphi}_\mathrm{L})}}{\mathrm{C}_{\hat{\varphi}_\mathrm{R}-\hat{\varphi}_\mathrm{L}}}\,. \tag{4.12}$$

The differences (4.9, 10) vanish in the limit $M \to \infty$, so we need only consider the $\tilde{\xi}$-vacuum expectation value in (2.18). [Cf. SML (4.19).]

To take into account in this expectation value all possible products of pairings with the correct signs, we use the fact that the sum of all these terms can be written as a Pfaffian or, more common, the square root of an antisymmetric determinant, the elements of which are the pairings [16]. Thus we get

$$\lim_{M\to\infty} ({}_\xi\langle \mathrm{vac^L} \,|\, \tau_k^x\, \tau_{k'}^x \,|\, \mathrm{vac^R}\rangle_\xi)^2 = \begin{vmatrix} a_0 & a_1 & \cdots & a_{k'-k-1} \\ a_{-1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1 \\ a_{-(k'-k-1)} & \cdots & a_{-1} & a_0 \end{vmatrix} \tag{4.13}$$

with the (2×2) submatrices

$$a_{l\neq 0} = \begin{pmatrix} \mathrm{yy}_l & \mathrm{yx}_{l+1} \\ \mathrm{xy}_{l-1} & \mathrm{xx}_l \end{pmatrix}, \quad a_0 = \begin{pmatrix} 0 & \mathrm{yx}_1 \\ \mathrm{xy}_{-1} & 0 \end{pmatrix}. \tag{4.14}$$

Here we have used certain symmetries of the pairings (4.11, 12) which in part follow from the anticommutators (4.6):

$$\mathrm{xy}_l + \mathrm{yx}_{-l} = 0\,, \quad \mathrm{xx}_l + \mathrm{xx}_{-l} = 2\,\delta_{l,0} = -(\mathrm{yy}_l + \mathrm{yy}_{-l})\,.$$

Directly from the definitions (4.11, 12) it can be seen that

$$(\mathrm{xy}_l)^* = -\mathrm{yx}_{-l}\,, \quad (\mathrm{xx}_l)^* = -\mathrm{yy}_{-l}\,,$$

i.e. xy_l and yx_l are *real*, and xx_l, yy_l satisfy the relation

$$\mathrm{xx}_l = (\mathrm{yy}_l)^* + 2\,\delta_{l,0}\,.$$

Then, from (2.18) and (4.13), the spontaneous magnetization in the l_0^{th} lattice column is given by

$$[m(l_0,T)]^4 = \lim_{|k'-k|\to\infty} \begin{vmatrix} a_0 & a_1 & \cdots & a_{k'-k-1} \\ a_{-1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1 \\ a_{-(k'-k-1)} & \cdots & a_{-1} & a_0 \end{vmatrix} \quad (4.15)$$

the limit of a (2×2)-block Toeplitz determinant.

Au-Yang and McCoy [8] have compiled the theorems on limits of block Toeplitz determinants known at that time. Since their determinant (3.1) of [8] [as well as ours, (4.15)] doesn't fit to the special conditions of these theorems the authors develop a procedure yielding after n steps a determinant with the required properties. ($n=n_1+n_2$ is the layer width.) Naturally this procedure is useful mainly for small n, and the authors treat explicitly the case $n=2$ only.

Meanwhile Widom [17] has published a general theorem on block Toeplitz determinants, but the application of this theorem to (4.15) must be deferred to later work. – So we use a different way to investigate the position dependence of m, evading the difficulties connected with block Toeplitz determinants but also renouncing the full knowledge of $m(l_0)$.

5. Extrema of $m(l_0)$

As stated in (3.38 – 40), for $l_0 = n_1/2$ things become much simpler. (For symmetry reasons,

$$m(l_0 = n_1/2) =: m_e^{(1)} \quad (5.1)$$

is the extremal value of the magnetization in the sublayer (1). For odd n_1, of course, $m_e^{(1)}$ is not the magnetization at a real lattice site. For large n_1, however, we can without large errors identify it with the real extremum.) Because of (3.38),

$$\hat{\varphi}_{\mathrm{R}}(q) \equiv \hat{\varphi}_{\mathrm{L}}(q) \equiv \hat{\varphi}(q)\,,$$

we get from (4.11)

$$\mathrm{xx}_l = -\mathrm{yy}_l = \delta_{l,0}\,. \quad (5.2)$$

Thus the diagonal elements in $a_{l\neq 0}$, (4.14), now vanish too, and (4.15) can be transformed by simultaneous interchange of rows and columns to the form

$$(m_e^{(1)})^4 = \lim_{r\to\infty} \begin{vmatrix} 0 & C_r \\ -C_r^{\mathrm{T}} & 0 \end{vmatrix} \quad (5.3)$$

with

$$C_r = \begin{pmatrix} yx_1 & yx_2 & \cdots & yx_r \\ yx_0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & yx_2 \\ yx_{-r+2} & \cdots & yx_0 & yx_1 \end{pmatrix}. \quad (5.4)$$

According to (4.12) the yx_l are given now by

$$\mathrm{yx}_l = -\int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\pi}\, e^{-iql}\, e^{-2i\hat{\varphi}(q)}\,. \quad (5.5)$$

If in (5.3) the sign of $-C_r^{\mathrm{T}}$ is reversed the determinant gets a factor $(-1)^r$, and if in addition the first r columns are interchanged with the last r ones another factor $(-1)^{r^2}$ results. Since $(-1)^{r+r^2} = +1$ for any r, we have

$$(m_e^{(1)})^4 = \lim_{r\to\infty} \begin{vmatrix} C_r & 0 \\ 0 & C_r^{\mathrm{T}} \end{vmatrix} = \lim_{r\to\infty} (\det C_r)^2 \quad (5.6)$$

or

$$(m_e^{(1)})^2 = \lim_{r\to\infty} |\det C_r|\,. \quad (5.7)$$

In contrast to (4.15), (5.7) is a simple (scalar) Toeplitz determinant which can be evaluated for $r\to\infty$ by the theorem of Szegö-Kac-Baxter [18] (SKB).

The transformation of the block Toeplitz determinant (4.15) to the scalar Toeplitz determinant (5.7) rests upon (3.38), i. e. the symmetry of $V_n(l_0)$. Thus for all l_0 that represent mirror lines of a periodically layered lattice we can calculate $m(l_0)$ simply by the SKB theorem. Cf. [3] (6.10 – 18) where a randomly layered but mirror symmetric lattice is considered. (The idea of a position dependent local magnetization in a periodically layered lattice seems to have appeared first in Chapter 6 of this paper.)

A sufficient condition for applicability of the SKB theorem to (5.7) is continuity of

$$f(q) := \hat{\varphi}(q) + q/2 = \tilde{\varphi}(q) + \varphi_1(q) + q/2 \quad (5.8)$$

in $-\pi \leqq q \leqq \pi$. A detailed investigation of (3.25) and (3.40) shows indeed [13] that for $T<\tilde{T}_c$ $f(q)$ is continuous and that for $T>\tilde{T}_c$ a jump at $q=\tilde{q}_c$ appears (cf. the analogon of $\varphi(q)+q/2$, Figure 3).

So we can use the SKB theorem to evaluate (5.7) for $T<\tilde{T}_c$ and get

$$m_e^{(1)} = \exp\left\{\frac{1}{2}\sum_{l=1}^{\infty} l\, k_l\, k_{-l}\right\} \tag{5.9 a}$$

$$= \exp\left\{-\frac{1}{4}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\int_{-\pi}^{\pi}\frac{d\bar{q}}{2\pi}\left(\frac{f(q)-f(\bar{q})}{\sin\frac{q-\bar{q}}{2}}\right)^2\right\} \tag{5.9 b}$$

where

$$k_l = -\frac{i}{\pi}\int_{-\pi}^{\pi} dq\, e^{-iql} f(q) \tag{5.10}$$

is the Fourier coefficient of $-2if(q)$. According to (3.17, 18) the same formula yields $m_e^{(2)}$ if in (5.8) we change $\varphi_1(q)$ into $\varphi_2(q)$ and interchange in the definition (3.40) of $\tilde{\varphi}(q)$ the quantities $(n_1, \varepsilon_1, \varphi_1)$ with $(n_2, \varepsilon_2, \varphi_2)$.

Of course (5.9) is not a very transparent result. But even without numerical work one can see [13] many limiting properties of $m_e^{(1)}$ from this formula:

$$\begin{array}{ll} n_1 \to 0: & m_e^{(1)} \to m_2 \\ n_2 \to 0: & m_e^{(1)} \to m_1 \\ n_1\varepsilon_1 \to \infty: & m_e^{(1)} \to m_1 \\ n_2\varepsilon_2 \to \infty,\ n_1 \to 0: & m_e^{(1)} \to m_2 \\ n_1 \to \infty: & m_e^{(1)} \to m_1 \\ (\bar{J}_1, J_1) \to (\bar{J}_2, J_2): & m_e^{(1)} \to m_1 = m_2 \\ T \to 0: & m_e^{(1)} \to m_1 = m_2 = 1\,, \end{array} \tag{5.11}$$

where m_1, resp., m_2 is the spontaneous magnetization of a homogeneous (1), resp., (2) lattice of infinite extent, as given by the Onsager-Yang [19] formula. In contrast to (5.11) the limit $T \to \tilde{T}_c$ cannot be investigated as easy, so we cannot verify the critical exponent $\beta = 1/8$ for the layered Ising lattice [cf. [8], (5.51)]. Nevertheless it can be seen from (5.9) and (3.40) that $m_e^{(1)} \to 0$ for $T \to \tilde{T}_c$ [13].

6. Asymptotics of $m(l_0)$

At the end of Chapt. 4 we abandoned the initial aim of calculating the full l_0 dependence of m. In this chapter we shall see that, nevertheless, one can deduce from the asymptotics of $m_e^{(1)}$ and $m_e^{(2)}$ for $n_1 \to \infty$ the asymptotic decay of m at large distances from a (1) – (2) interface. To that end we first discuss $m_e^{(1)}$ $(n_1 \to \infty)$.

6.1. $m_e^{(1)}$ for $n_1 \to \infty$

From (5.9 a) we have

$$\ln m_e^{(1)}(n_1) = \tfrac{1}{2}\sum_{l=1}^{\infty} l\, k_l(n_1)\, k_{-l}(n_1) \tag{6.1}$$

where $k_l(n_1)$ is given by (5.10) and (5.8) as the Fourier coefficient of the angle $\tilde{\varphi}(q, n_1) + \varphi_1(q) + q/2$. From the antisymmetry property (4.4) one finds

$$k_{-l}(n_1) = -k_l(n_1) \tag{6.2}$$

or

$$\ln m_e^{(1)}(n_1) = -\tfrac{1}{2}\sum_{l=1}^{\infty} l[k_l(n_1)]^2\,. \tag{6.3}$$

It is convenient to decompose $k_l(n_1)$ into an n_1-independent part and an n_1-dependent one, similar to (5.8):

$$k_l(n_1) = k_l^{(1)} + \varkappa_l(n_1) \tag{6.4}$$

with

$$k_l^{(1)} = -\frac{i}{\pi}\int_{-\pi}^{\pi} dq\, e^{-iql}[\varphi_1(q) + q/2]\,, \tag{6.5}$$

$$\begin{aligned} \varkappa_l(n_1) &= -\frac{i}{\pi}\int_{-\pi}^{\pi} dq\, e^{-iql}\tilde{\varphi}(q, n_1) \\ &= -\frac{2}{\pi}\int_{-0}^{\pi} dq \sin(ql)\,\tilde{\varphi}(q, n_1)\,, \end{aligned} \tag{6.6}$$

$k_l^{(1)}$ alone corresponds to an infinite homogeneous (1) lattice and was calculated already in [20], Eq. (75):

$$k_l^{(1)} = \frac{1}{2l}(\mathfrak{T}_{|\bar{K}_1|^*})^l\{(\mathfrak{T}_{K_1})^{-l} - (\mathfrak{T}_{K_1})^l\}\,. \tag{6.7}$$

According to (6.4) the sum (6.3) splits into three parts:

$$\ln m_e^{(1)}(n_1) = -\tfrac{1}{2}\sum_{l=1}^{\infty} l(k_l^{(1)})^2 - \sum_{l=1}^{\infty} l\, k_l^{(1)}\varkappa_l(n_1) - \tfrac{1}{2}\sum_{l=1}^{\infty} l[\varkappa_l(n_1)]^2\,, \tag{6.8}$$

the first of which yields $\ln m_1$. The second part is the first-order correction to $\ln m_1$ in the limit $n_1 \to \infty$ whereas the third part should be negligible, being a second-order correction.

To evaluate the asymptotics of $\ln m_e^{(1)}(n_1 \to \infty)$ we thus need the asymptotics of $\varkappa_l(n_1)$, i.e. the behaviour of $\tilde{\varphi}(q, n_1)$ for $n_1 \to \infty$. From (3.40) one may write

$$\tan 2\tilde{\varphi} = \frac{-2a(q)\exp\{-n_1|\mathrm{Re}\,\varepsilon_1|\}}{1 - \dfrac{\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1) - \mathfrak{T}_{n_2\varepsilon_2}\mathrm{C}_{2(\varphi_1-\varphi_2)}}{\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1) + \mathfrak{T}_{n_2\varepsilon_2}\mathrm{C}_{2(\varphi_1-\varphi_2)}}\exp\{-2n_1|\mathrm{Re}\,\varepsilon_1|\}} \tag{6.9}$$

with

$$a(q) = (\mathrm{sgn}\,\bar{J}_1)^{n_1}\mathfrak{T}_{n_2\varepsilon_2}\mathrm{S}_{2(\varphi_1-\varphi_2)}/\{\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1) + \mathfrak{T}_{n_2\varepsilon_2}\mathrm{C}_{2(\varphi_1-\varphi_2)}\}\,. \tag{6.10}$$

Now we define the *local critical temperature* T_{c1} of sublayer (1) to be the critical temperature of an infinite homogeneous (1) lattice, i. e. that temperature at which $\operatorname{Re} \varepsilon_1 = 0$ for a certain $q = q_{c1}$ given by

$$\cos q_{c1} = \operatorname{sgn} J_1 . \tag{6.11}$$

In the same way a temperature T_{c2}, the local T_c of sublayer (2), can be defined. Then for $T < T_{c1}$ there exists a *finite* $n_1 = N_1$ with

$$\exp\{-2 N_1 |\operatorname{Re} \varepsilon_1|\} \ll |\operatorname{sgn}(\operatorname{Re} \varepsilon_1) + \mathfrak{T}_{n_2 \varepsilon_2} \mathrm{C}_{2(\varphi_1 - \varphi_2)}| \tag{6.12}$$

for all q, whence for $n_1 \gtrsim N_1$ (6.9) has the asymptotic form

$$\tan 2 \tilde{\varphi} \sim -2\, \alpha(q) \exp\{-n_1 |\operatorname{Re} \varepsilon_1(q)|\} \tag{6.13}$$

uniformly in q. Because of $\alpha(q)$ being bounded there exists another finite $n_1 = \bar{N}_1$ so that $|\tan 2 \tilde{\varphi}| \ll 1$ for all q, whence for both $n_1 \gtrsim N_1$, $n_1 \gtrsim \bar{N}_1$ one has

$$\tilde{\varphi}(q, n_1) \sim -\alpha(q) \exp\{-n_1 |\operatorname{Re} \varepsilon_1(q)|\} \tag{6.14}$$

uniformly in q. With this expression we get from (6.6) an asymptotic formula for $\varkappa_l(n_1)$, using the method of Laplace [21]:

$$\varkappa_l(n_1) \sim \sqrt{\frac{2}{\pi}}\, \alpha_0' \frac{e^{-n_1 a}}{(b\, n_1)^{3/2}} (\operatorname{sgn} J_1)^l\, l\, e^{-l^2/(2 b n_1)} \tag{6.15}$$

for any fixed l and $n_1 \to \infty$. Here we have defined

$$\alpha_0' = \left.\frac{\partial \alpha(q)}{\partial q}\right|_{q_{c1}} = \tfrac{1}{2} (\operatorname{sgn} \bar{J}_1)^{n_1} \{(\mathfrak{C}_{2K_1} - \mathfrak{S}_{2|K_1|}\, \mathfrak{C}_{2\bar{K}_1})^{-1} - (\mathfrak{C}_{2K_2} - \mathfrak{S}_{2|K_2|}\, \mathfrak{C}_{2\bar{K}_2})^{-1}\}$$
$$\times [1 - \exp\{-2\gamma n_2 |2 K_2 \operatorname{sgn} J_1 + \ln \mathfrak{T}_{|\bar{K}_2|}|\}] \tag{6.16}$$

with

$$\gamma = \cos 2(\varphi_1 - \varphi_2)|_{q_{c1}} = \operatorname{sgn}[\bar{J}_1 \bar{J}_2 (T - T_{c1})]\, [\operatorname{sgn}(T - T_{c2})]^{(1 + \operatorname{sgn} J_1 J_2)/2} . \tag{6.17}$$

$a(T)$ and $b(T)$ are the first and second Taylor coefficients of $|\operatorname{Re} \varepsilon_1(q)|$ at $q = q_{c1}$:

$$a(T) = |\operatorname{Re} \varepsilon_1(q_{c1})| = |2|K_1| + \ln \mathfrak{T}_{|\bar{K}_1|}| , \tag{6.18}$$

$$b(T) = \left.\frac{\partial^2 \varepsilon_1(q)}{\partial q^2}\right|_{q_{c1}} \tag{6.19}$$
$$= \mathfrak{S}_{2|K_1|} \{(\mathfrak{C}_{2K_1} \mathfrak{C}_{2\bar{K}_1} - \mathfrak{S}_{2|K_1|})^2 - \mathfrak{S}^2_{2\bar{K}_1}\}^{-1/2} ,$$

and $a(T)$ is related to the correlation length $\xi_1^<(T)$ of an infinite homogeneous (1) lattice [22] at $T < T_{c1}$ by

$$a = 1/(2 \xi_1^<) . \tag{6.20}$$

Unfortunately (6.15) cannot be shown to hold uniformly for all l: for $l \to \infty$ the lower bound in n_1 for relative smallness of the corrections to (6.15) might well go to infinity. Thus one cannot be sure that the result of the infinite l-sum in (6.8),

$$\boxed{\ln[m_e^{(1)}(n_1)/m_1] \sim A(T)\, n_1^{-3/2}\, e^{-n_1/(2\xi_1^<)}}$$
$$\text{for } n_1 \to \infty \tag{6.21}$$

with

$$A(T) = -\alpha_0' R\, b^{-3/2} (2\pi)^{-1/2} , \tag{6.22}$$

$$\left.\begin{aligned} R(T) &= \sum_{l=1}^{\infty} l (\mathfrak{T}_{|\bar{K}_1|^*})^l \{(\mathfrak{T}_{|K_1|})^{-l} - (\mathfrak{T}_{|K_1|})^l\} \\ &= \mathfrak{S}_{2|K_1|} \mathfrak{S}_{2|\bar{K}_1|} (\mathfrak{C}_{2K_1} - \mathfrak{S}_{2|K_1|} \mathfrak{C}_{2\bar{K}_1})^{-2} \end{aligned}\right\} \tag{6.23}$$

will be the correct asymptotic expression. However, *the n_1-dependence* of (6.21) can be shown to be correct (by discussion of the double integral (5.9b), see Appendix B). Moreover, the T-dependence of $A(T)$ shows the physically expected behaviour, at least in the simplest case of purely ferromagnetic couplings

$$\bar{J}_1 = J_1 > 0 , \quad \bar{J}_2 = J_2 > 0 , \tag{6.24}$$

see Figure 6. Here we find [13]

$$\operatorname{sgn} A(T) = \operatorname{sgn}(T_{c2} - T_{c1}) \text{ for all } T , \tag{6.25}$$
$$A(T) \sim \text{const} \cdot |T - T_{c1}|^{-3/2} \text{ for } T \to T_{c1} , \tag{6.26}$$
$$A(T) \sim 2\sqrt{2}\, e^{-K_1} (e^{-4K_1} - e^{-4K_2}) \text{ for } T \to 0 . \tag{6.27}$$

The sign relation (6.25) means that $m_e^{(1)} \gtreqless m_1$ for $T_{c2} \gtreqless T_{c1}$, as is to be expected. The divergence (6.26) of $A(T)$ at $T = T_{c1}$ can be understood as follows: In the case $T_{c2} > T_{c1}$ we have $\tilde{T}_c > T_{c1}$ (but $\tilde{T}_c \to T_{c1}$ for $n_1 \to \infty$, see Appendix A). So m_1 will vanish at T_{c1} while $m_e^{(1)}$ remains finite up to $\tilde{T}_c > T_{c1}$, and thus $\ln m_e^{(1)}/m_1 \to +\infty$ for $T \to T_{c1}$. In the opposite case $T_{c2} < T_{c1}$, $m_e^{(1)}$ vanishes at $\tilde{T}_c < T_{c1}$ while m_1 remains finite up to T_{c1}, so $\ln m_e^{(1)}/m_1 \to -\infty$ for $T \to \tilde{T}_c$, i. e. for $T \to T_{c1}$ since $\tilde{T}_c \to T_{c1}$ for $n_1 \to \infty$. – Finally, the behaviour (6.27) at $T \to 0$ might be related to the corresponding asymptotics of the Onsager-Yang magnetizations m_1 and m_2:

$$m \sim 1 - 2 e^{-8K} \quad \text{for } T \to 0 \tag{6.28}$$

though the appearance of the exponents $-4K$ in (6.27) instead of the $-8K$ in (6.28) is not yet understood.

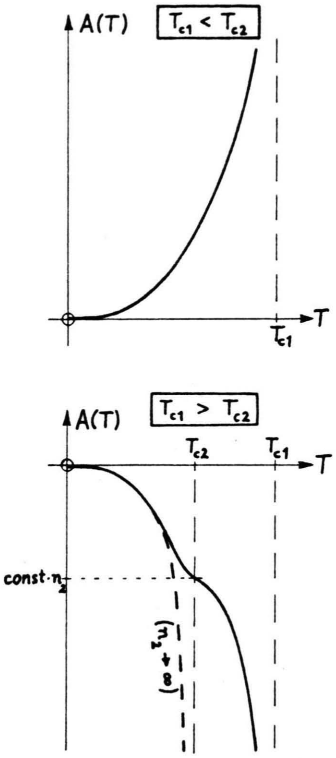

Fig. 6. Qualitative temperature dependence of $A(T)$, (6.22), for $\bar{J}_1 = J_1 > 0$, $\bar{J}_2 = J_2 > 0$ in the two cases $T_{c1} < T_{c2}$ and $T_{c1} > T_{c2}$. In the latter case $A(T_{c2})$ depends linearly on n_2, and for $n_2 \to \infty$ a singularity $\sim |T - T_{c2}|^{-1}$ appears.

In conclusion, there is large evidence that not only the n_1 dependence of (6.21) is correct (see Appendix B) but also the factor $A(T)$.

6.2. $m(l_0)$ far from an Interface

To deduce on the basis of our result (6.21) on $m_e^{(1)}$ $(n_1 \to \infty)$ the asymptotic decay of $m(l_0)$ far from an interface, we need $m_e^{(2)}$ $(n_1 \to \infty)$ too. As mentioned in Chapter 5, Eq. (5.9) will give $m_e^{(2)}$ if we write

$$f(q) = \tilde{\varphi}^{(2)}(q, n_1) + \varphi_2(q) + q/2 \qquad (6.29)$$

instead of (5.8) and determine $\tilde{\varphi}^{(2)}$ from (3.40) with interchange of $(n_1, \varepsilon_1, \varphi_1)$ and $(n_2, \varepsilon_2, \varphi_2)$. Thus we get from (3.40)

$$\cot 2\tilde{\varphi}^{(2)} = \cot 2\tilde{\varphi}_\infty^{(2)} + 2\,\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1) \frac{\mathfrak{S}_{n_2\varepsilon_2}}{\mathrm{S}_{2(\varphi_1-\varphi_2)}} \frac{e^{-2n_1|\mathrm{Re}\,\varepsilon_1|}}{1 - e^{-2n_1|\mathrm{Re}\,\varepsilon_1|}} \qquad (6.30)$$

where $\tilde{\varphi}_\infty^{(2)}$ is defined by

$$\left.\begin{aligned} \cot 2\tilde{\varphi}_\infty^{(2)} &= \lim_{n_1\to\infty} \cot 2\tilde{\varphi}^{(2)} \\ &= \mathrm{sgn}(\mathrm{Re}\,\varepsilon_1)\,\mathfrak{C}_{n_2\varepsilon_2} \\ &\cdot \{\mathfrak{T}_{n_2\varepsilon_2} + \mathrm{C}_{2(\varphi_1-\varphi_2)}\,\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1)\}/\mathrm{S}_{2(\varphi_1-\varphi_2)} \end{aligned}\right\} \qquad (6.31)$$

for $T < T_{c1}$. Now if there exists a finite N_2 such that for $n_1 \gtrsim N_2$ the relation

$$\frac{2|\mathfrak{T}_{n_2\varepsilon_2}|}{1 + (\tan 2\tilde{\varphi}_\infty^{(2)})^2} \frac{e^{-2n_1|\mathrm{Re}\,\varepsilon_1|}}{|\mathfrak{T}_{n_2\varepsilon_2} + \mathrm{C}_{2(\varphi_1-\varphi_2)}\,\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1)|} \ll 1 \qquad (6.32\text{ a})$$

is fulfilled (supplemented by

$$\tfrac{4}{3}\,(\mathfrak{S}_{n_2\varepsilon_2}/\mathrm{S}_{2(\varphi_1-\varphi_2)})^2\, e^{-4n_1|\mathrm{Re}\,\varepsilon_1|} \ll 1 \qquad (6.32\text{ b})$$

if $|\cot 2\tilde{\varphi}_\infty^{(2)}| \ll 1$) we may, for $n_1 \gtrsim N_2$, insert (6.30) into the Taylor series of the arc cot and truncate after the linear term:

$$\tilde{\varphi}^{(2)}(q) \sim \tilde{\varphi}_\infty^{(2)}(q) - \Phi(q)\, e^{-2n_1|\mathrm{Re}\,\varepsilon_1(q)|} \qquad (n_1 \to \infty) \qquad (6.33)$$

where

$$\Phi(q) = \mathrm{sgn}(\mathrm{Re}\,\varepsilon_1)\,\mathfrak{S}_{n_2\varepsilon_2}(\mathrm{S}_{2\tilde{\varphi}_\infty^{(2)}})^2/\mathrm{S}_{2(\varphi_1-\varphi_2)}\,. \qquad (6.34)$$

The two conditions (6.32) [as well as (6.12)] can, for all q, only be fulfilled for *finite* $n_2\varepsilon_2$. For, with $|\mathfrak{T}_{n_2\varepsilon_2}| \to 1$ there exist certain q values with $\{\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1) + \mathfrak{T}_{n_2\varepsilon_2}\mathrm{C}_{2(\varphi_1-\varphi_2)}\} = 0$ [in case of (6.12)] or

$$\{\mathfrak{T}_{n_2\varepsilon_2} + \mathrm{C}_{2(\varphi_1-\varphi_2)}\,\mathrm{sgn}(\mathrm{Re}\,\varepsilon_1)\} = 0 \quad \text{and} \quad \mathrm{S}_{2(\varphi_1-\varphi_2)} = 0 \qquad [\text{in case of } (6.32)]\,.$$

Now, in the limit $\bar{J}_2 \to 0$ we have for $T > 0$

$$|\mathrm{Re}\,\varepsilon_2(q)| \to \infty \qquad (\bar{J}_2 \to 0) \qquad (6.35)$$

for *all* q. Thus for $\bar{J}_2 \to 0$ the conditions (6.12) and (6.32) cannot be fulfilled uniformly for all q. [Likewise $a(q)$ is not bounded in this case.] — The physical meaning of this limit is quite clear: according to Fig. 2, the layered lattice decomposes into uncoupled (1) strips of finite width with uncoupled (2) chains lying between them. That is, we have $\tilde{T}_c \to 0$, and no magnetization will be present at all.

We see that, apart from the case $\bar{J}_2 \to 0$, the $N_2 < \infty$ mentioned in (6.32) will always exist for all q, i. e. (6.33) is valid uniformly in q. So we may take over the formalism [(6.1) to (6.21)] to the calculation of $\ln m_e^{(2)}(n_1)$, replacing $\varphi_1(q)$ with $\varphi_2(q) + \tilde{\varphi}_\infty^{(2)}(q)$ and $\tilde{\varphi}(q, n_1)$ with $-\Phi(q)\, e^{-2n_1|\mathrm{Re}\,\varepsilon_1|}$.

Since we don't, however, explicitly know $k_l^{(2)}$, the Fourier coefficient of $\varphi_2+\tilde{\varphi}_\infty^{(2)}$, we cannot actually perform the calculation. But we can infer the n_1 dependence of $\ln m_e^{(2)}$:

$$\ln[m_e^{(2)}(n_1)/m_e^{(2)}(\infty)] \sim B(T)\, n_1^{-3/2}\, e^{-n_1/\xi_1^<} \quad \text{for } n_1\to\infty \tag{6.36}$$

with unknown $B(T)$. [The same result follows from the double integral (5.9 b), cf. Appendix B.]

Thus we have shown to exist a finite N_1 such that for $n_1>N_1$ (6.21) is the leading asymptotic term of $\ln m_e^{(1)}$, and a finite N_2 such that for $n_1>N_2$ (6.36) is the leading term of $\ln m_e^{(2)}$. Therefore there will also exist a finite $\bar{N}_1$ such that for $n_1\geqq\bar{N}_1$ one has

$$\ln[m_e^{(1)}(n_1)/m_1]\leqq e^{-\varrho}\ll 1\,, \tag{6.37}$$

and a $\bar{N}_2<\infty$ such that for $n_1\geqq\bar{N}_2$ one has

$$\ln[m_e^{(2)}(n_1)/m_e^{(2)}(\infty)]\leqq e^{-\varrho}\ll 1\,, \tag{6.38}$$

where ϱ is defined just by $e^{-\varrho}\ll 1$. Now we define $\hat{N}$ to be the maximum of these four lower bounds:

$$\hat{N}=\mathrm{Max}\,\{N_1, N_2, \bar{N}_1, \bar{N}_2\}<\infty\,. \tag{6.39}$$

Then we may use, for $n_1>\hat{N}$, the asymptotic forms (6.21), (6.36):

$$\left.\begin{aligned}\ln[m_e^{(1)}(n_1)/m_1] &\sim A(T)\, n_1^{-3/2}\, e^{-n_1/(2\xi_1^<)}\,,\\ \ln[m_e^{(2)}(n_1)/m_e^{(2)}(\infty)] &\sim B(T)\, n_1^{-3/2}\, e^{-n_1/\xi_1^<}\end{aligned}\right\} \tag{6.40}$$

and define a $\Delta\hat{N}$ such that for $n_1\geqq\hat{N}+\Delta\hat{N}$ one has

$$\left|\frac{\ln[m_e^{(2)}(n_1)/m_e^{(2)}(\infty)]}{\ln[m_e^{(1)}(n_1)/m_1]}\right|\equiv\left|\frac{B(T)}{A(T)}\right| \cdot e^{-n_1/(2\xi_1^<)}\leqq e^{-\varrho}\ll 1\,. \tag{6.41}$$

From this we get

$$\hat{N}+\Delta\hat{N}=2\,\xi_1^<[\varrho+\ln|B(T)/A(T)|]\,. \tag{6.42}$$

If therefore $|B(T)|<\infty$ (which should be expected on physical grounds at least for ferromagnets at $0\leqq T<T_{c1}$) and $A(T)\neq 0$, $\hat{N}+\Delta\hat{N}$ will be *finite* for $T<T_{c1}$. Then, for $n_1>\hat{N}+\Delta\hat{N}$ we have from (6.37) and (6.41):

$$\left|\ln\frac{m_e^{(2)}(n_1)}{m_e^{(2)}(\infty)}\right|\ll\left|\ln\frac{m_e^{(1)}(n_1)}{m_1}\right|\ll 1\,. \tag{6.43}$$

This is a more precise statement of the observation that, according to (6.40), $\ln[m_e^{(2)}(n_1)/m_e^{(2)}(\infty)]$ for $n_1\to\infty$ decreases twice as fast as $\ln[m_e^{(1)}(n_1)/m_1]$. This different behaviour of (6.21) and (6.36) may be interpreted as follows: The periodically spaced (2) layers cause perturbations in the logarithm $\ln m_1$ of the magnetization of the underlying (1) lattice. For $n_1>\hat{N}+\Delta\hat{N}$ interactions among these perturbations become negligible, as (6.43) shows, and $\ln m(l_0)$ is the mere superposition of these independent contributions. So one may deduce directly from (6.21) the asymptotic decay of $\ln m(l_0)$ in sublayer (1) at large distance d from a (1) – (2) interface (i. e. $n_1>2d$!):

$$\ln[m(d)/m_1]\sim\frac{\sqrt{2}}{8}\,A(T)\,d^{-3/2}\,e^{-d/\xi_1^<}\,. \quad (d\to\infty) \tag{6.44}$$

For those values of d at which [in analogy to (6.37)]

$$\ln[m(d)/m_1]\ll 1\,, \tag{6.45}$$

that is,

$$2\,d>\hat{N}+\Delta\hat{N}\,, \tag{6.46}$$

one may linearize the logarithm in (6.44):

$$m(d)\sim m_1\left\{1+\frac{\sqrt{2}}{8}\,A(T)\,d^{-3/2}\,e^{-d/\xi_1^<}\right\}. \quad (d\to\infty) \tag{6.47}$$

The reasoning leading to (6.44) is obviously independent of the regularity or randomness of the distribution of (2) layers, provided the separation between them satisfies (6.42). Thus (6.44/47) is valid also for a single perturbing (2) layer in a homogeneous (1) lattice, i. e. a grain boundary.

7. Discussion

According to (6.47) the spontaneous magnetization near a layer-shaped inhomogeneity in an otherwise homogeneous (1) lattice decays, for $T<T_{c1}$, exponentially with a decay length equal to the spin-spin correlation length $\xi_1^<$. A similar behaviour has been found in the past for some other systems. Near the free surface of a three-dimensional Ising lattice at $T<T_c$, Monte Carlo studies [23] approximately yielded the same exponential behaviour (of course without any factors like our denominator $d^{3/2}$). The Landau theory too gives such an exponential decay for $T<T_c$ as well as for $T>T_c$, in either case with the decay length equal to the corresponding spin-spin correlation length [13, 24, 28]. On the other hand, near the free surface of a three-dimensional quantum Heisenberg model spin-wave theory [25] yielded a power-law behaviour of the magnetization for $T \ll T_c$ which again is accompanied by a power-law behaviour of the spin-spin correlation functions in the corresponding infinite homogeneous system [26]. (The only known inconsistency between the asymptotics of the magnetization and of correlations is for the classical three-dimensional Heisenberg model: Monte Carlo studies [23] yield approximately a power-law behaviour of the magnetization whereas on the basis of transfer matrix theory (p. 955 in [27]) the pair correlations are known to decay exponentially.)

It is, however, not at all obvious that the decay of the spontaneous magnetization should reflect the behaviour of the *spin-spin* correlation. On the basis of the picture developed in the derivation of (6.44) the magnetization responds to the differing coupling constants within the inhomogeneity, i. e. a variation of the local energy density. Accordingly the *spin-energy density* correlation

$$G_{\mathrm{SE}}(\boldsymbol{r}) = \langle \sigma_{\boldsymbol{0}}\, \sigma_{\boldsymbol{r}}\, \sigma_{\boldsymbol{r}+\boldsymbol{\delta}} \rangle \qquad (7.1)$$

should come into play. ($\boldsymbol{\delta}$ is a vector connecting nearest neighbours.) For classical systems $G_{\mathrm{SE}}(T < T_c, H = 0)$ indeed decays with the same correlation length as $\langle \sigma_{\boldsymbol{0}} \sigma_{\boldsymbol{r}} \rangle$ [Eq. (2.29 d) of [28]; ch. III c, (3.17, 31, 34) of [29]]. This would explain (6.47) as well as the Monte Carlo results of [23] on the three-dimensional Ising model. For the other systems cited above there seem to be no results on G_{SE} up to now, which prevents a further check of our hypothesis. (The results of [27] on the exponential decay of pair correlations hold as well for G_{SE}. So the inconsistencies with the classical Heisenberg model mentioned above persist even when G_{SE} is taken into consideration. On the other hand, the Monte Carlo results of [23] yield the magnetization only in the 12 to 15 layers next to the surface, which might be too poor to make a reliable statement on asymptotic decay.)

An understanding of the denominator $d^{3/2}$ in (6.47) should be possible by a thorough investigation of correlations near interfaces as reported in [30] for free surfaces.

Acknowledgements

I would like to thank Prof. H. Hahn for suggesting this problem, for many helpful discussions, and a steady encouragement during the work.

Appendix A: The Global Critical Temperature $\tilde{T}_c$

According to (3.49 a) $\tilde{T}_c$ is defined as that temperature at which $\mathrm{Re}\,\tilde{\varepsilon}(q)$ becomes zero for $q = \tilde{q}_c = 0$ or $= \pi$. Using (3.5) we therefore have from (3.49 a) for $T = \tilde{T}_c$:

$$n_1(2\,K_1\,C_{\tilde{q}_c} + \ln \mathfrak{T}_{|\bar{K}_1|}) + n_2(2\,K_2\,C_{\tilde{q}_c} + \ln \mathfrak{T}_{|\bar{K}_2|}) = 0 \qquad (A\,1)$$

or

$$2\,(n_1 K_1 + n_2 K_2) \cos \tilde{q}_c = n_1 \ln \coth |\bar{K}_1| + n_2 \ln \coth |\bar{K}_2| \,. \qquad (A\,2)$$

[Cf. (31) in [4].] Since the right-hand side of (A 2) is positive one has

$$\cos \tilde{q}_c = \mathrm{sgn}\,(n_1 J_1 + n_2 J_2) \,. \qquad (A\,3)$$

In the following we want to discuss (A 1) in the limit $n_1 \to \infty$ with fixed n_2, i. e. $n_1/n_2 \to \infty$. In this case $\tilde{q}_c \to q_{c1}$ from comparison of (A 3) and (6.11), and (A 1) becomes identical with the condition $\mathrm{Re}\,\varepsilon_1(q) = 0$ for $T = T_{c1}$. Hence one has

$$\tilde{T}_c \to T_{c1} \,. \qquad (n_1/n_2 \to \infty) \qquad (A\,4)$$

To investigate the asymptotics of $\tilde{T}_c$ in this case we therefore expand (A1) in powers of $(\tilde{T}_c - T_{c1})/T_{c1}$. Taking only linear terms one gets

$$\frac{\tilde{T}_c - T_{c1}}{T_{c1}} \sim \frac{n_2}{n_1} \left\{ \frac{K_2\, \mathrm{sgn}\, J_1 - \frac{1}{2} \ln \coth |\bar{K}_2|}{|K_1| + \bar{K}_1/\sinh 2\,\bar{K}_1} \right\}_{T = T_{c1}} \quad (n_1/n_2 \to \infty) \,. \qquad (A\,5)$$

Using the conditions for T_{c1} and T_{c2},

$$|K_1| - |\bar{K}_1|^* = 0 \,, \quad \text{resp.,} \quad |K_2| - |\bar{K}_2|^* = 0 \,, \qquad (A\,6)$$

one finds from (A 5) that for large n_1/n_2

1. $\tilde{T}_c < T_{c1}$ for $T_{c2} < T_{c1}$ (A 7)
2. $\tilde{T}_c \gtrless T_{c1}$ for $T_{c2} > T_{c1}$ and $J_1 J_2 \gtrless 0$. (A 8)

Hence the naive assumption that $\tilde{T}_c$ will always lie *between* T_{c1} and T_{c2} is correct only for $J_1 J_2 > 0$.

For $J_1 J_2 < 0$ even $\tilde{T}_c = 0$ is possible in spite of $T_{c1} \neq 0$, $T_{c2} \neq 0$. To discuss this case we consider (A 2) for $\tilde{T}_c \to 0$ and get

$$|n_1 J_1 + n_2 J_2| \sim n_< k_B \tilde{T}_c \exp\{-2\,|\bar{J}_<|/k_B \tilde{T}_c\} \quad (\tilde{T}_c \to 0) \qquad (A\,9)$$

where

$$|\bar{J}_<| = \mathrm{Min}\,\{|\bar{J}_1|, |\bar{J}_2|\}$$

and $n_<$ is the corresponding sublayer width n_1 or n_2. Thus the function $\tilde{T}_c(n_1/n_2)$ has a (nonanalytic) zero at

$$n_1/n_2 = -J_2/J_1 . \quad \text{(A 10)}$$

At this point the critical wavenumber $\tilde{q}_c$ is undefined, cf. (A 3): there is strong competition between the two sublayers with respect to the sign of order (remember that $J_1 J_2 < 0$!), so no order will develop at all. This behaviour is analogous to that of the antiferromagnetic triangular lattice ([31], § 3.5.4). – The conclusions of this appendix are summarized in the temperature-"concentration" phase diagram Figure 7.

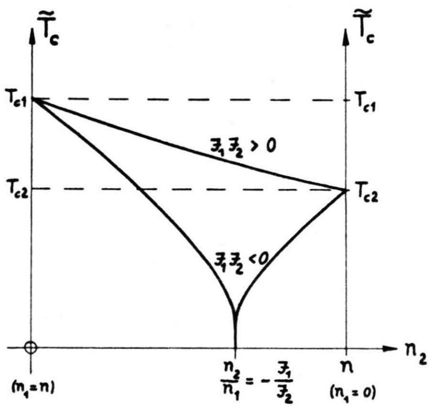

Fig. 7. Qualitative dependence of the global critical temperature $\tilde{T}_c$ on the widths n_1 and n_2 of the two sublayers. The parameters $\bar{J}_1$, J_1, $\bar{J}_2$, J_2, and $n=n_1+n_2$ are held fixed.

Appendix B: Asymptotics of $m_e^{(1)}(n_1 \to \infty)$

In this appendix we shall verify the n_1 dependence of (6.21) by considering the double integral (5.9 b):

$$\ln m_e^{(1)}(n_1) = -\frac{1}{4}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\int_{-\pi}^{\pi}\frac{d\bar{q}}{2\pi}\left(\frac{f(q,n_1)-f(\bar{q},n_1)}{\sin\frac{1}{2}(q-\bar{q})}\right)^2 \quad \text{(B 1)}$$

with

$$f(q,n_1) = \tilde{\varphi}(q,n_1) + \varphi_1(q) + q/2 . \quad \text{(B 2)}$$

A decomposition of $f(q,n_1)$ similar to (6.4) yields three terms in (B 1):

$$\ln m_e^{(1)}(n_1) = T_0 + T_1 + T_2 \quad \text{(B 3)}$$

with

$$T_0 = -\frac{1}{4}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\int_{-\pi}^{\pi}\frac{d\bar{q}}{2\pi}[g_0(q,\bar{q})]^2 = \ln m_1 , \quad \text{(B 4)}$$

$$T_1 = -\frac{1}{2}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\int_{-\pi}^{\pi}\frac{d\bar{q}}{2\pi}g_0(q,\bar{q})\,g_{n_1}(q,\bar{q}) , \quad \text{(B 5)}$$

$$T_2 = -\frac{1}{4}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\int_{-\pi}^{\pi}\frac{d\bar{q}}{2\pi}[g_{n_1}(q,\bar{q})]^2 , \quad \text{(B 6)}$$

where

$$g_0(q,\bar{q}) = \{[\varphi_1(q) + q/2] - [\varphi_1(\bar{q}) + \bar{q}/2]\}/\sin\tfrac{1}{2}(q-\bar{q}) , \quad \text{(B 7)}$$

$$g_{n_1}(q,\bar{q}) = \{\tilde{\varphi}(q,n_1) - \tilde{\varphi}(\bar{q},n_1)\}/\sin\tfrac{1}{2}(q-\bar{q}) . \quad \text{(B 8)}$$

Again T_1 is the first-order correction in the limit $n_1 \to \infty$, T_2 the second-order term. So one has

$$\ln[m_e^{(1)}(n_1)/m_1] \sim T_1 \quad \text{for } n_1 \to \infty . \quad \text{(B 9)}$$

The integrand of (B 5),

$$G_{n_1}(q,\bar{q}) := g_0(q,\bar{q})\,g_{n_1}(q,\bar{q}) , \quad \text{(B 10)}$$

has some symmetries, due to the antisymmetry properties (4.4, 5):

$$G_{n_1}(q,\bar{q}) = G_{n_1}(\bar{q},q) = G_{n_1}(-\bar{q},-q) . \quad \text{(B 11)}$$

(The same symmetries hold for g_0 and g_{n_1} either.) With the help of Fig. 3 the qualitative $(q,\bar{q})$-dependence of g_0 can be sketched for a typical set of parameters at $T<T_{c1}$, Figure 8. (In the following we restrict ourselves to the case $J_1>0$, i.e. $q_{c1}=0$. The case $q_{c1}=\pi$ can be treated similarly.) To sketch g_{n_1} too we use the fact that, for large n_1, $\tilde{\varphi}(q,n_1)$ is appreciably different from zero only in the neighbourhood of $q=q_{c1}$ [cf. (6.14)]: $\mathrm{Re}\,\varepsilon_1(q)$

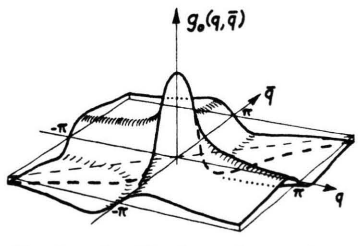

Fig. 8. Qualitative $(q,\bar{q})$ dependence of g_0, (B 7), for $T<T_{c1}$.

has a well-defined minimum here while $a(q)$ has a zero of first order. The height and width of this double peak can be estimated in this limit $n_1 \to \infty$ as given in Figure 9. From this behaviour the qualitative $(q, \bar{q})$-dependence of g_{n_1} follows as shown in Figure 10. In Figs. 8 and 10 we have used the following limiting properties:

$$\left.\begin{aligned} g_0 &\to \pm\left(2\,\frac{\partial \varphi_1}{\partial q}+1\right) && \text{for } q-\bar{q} \to \{{}^{0}_{\pm 2\pi}, \\ g_{n_1} &\to \pm\, 2\,\frac{\partial \tilde{\varphi}}{\partial q} && \text{for } q-\bar{q} \to \{{}^{0}_{\pm 2\pi}. \end{aligned}\right\} \quad \text{(B 12)}$$

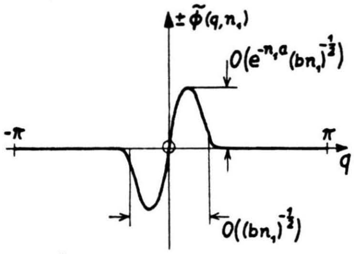

Fig. 9. Qualitative q dependence of $\tilde{\varphi}(q, n_1)$ for large n_1 and $T < T_{c1}$.

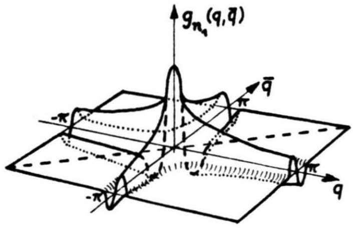

Fig. 10. Qualitative $(q, \bar{q})$ dependence of g_{n1}, (B 8).

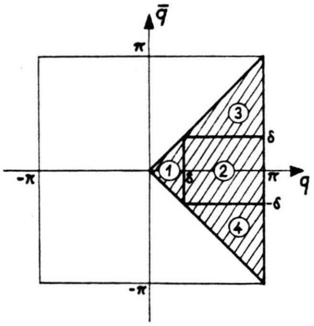

Fig. 11. The integration regions in (B 15).

Due to the symmetries (B 11) the integration region in (B 5) can be reduced to the hatched triangle shown in Figure 11. The special double-ribbed structure of g_{n_1} in Fig. 10 suggests a further division into the four subregions indicated in Fig. 11, where $\delta > 0$ is fixed but small enough to make the expression

$$a_0'\, q \exp\{-n_1(a + b\, q^2/2)\} \qquad \text{(B 13)}$$

a good approximation to $\tilde{\varphi}(q, n_1)$ in the interval $-\delta \leqq q \leqq \delta$. [The coefficients $a_0'(T)$, $a(T)$, $b(T)$ are defined in (6.16 – 19).] With these four subregions we may write

$$T_1 = 4(T_1^{(1)} + T_1^{(2)} + T_1^{(3)} + T_1^{(4)}) \qquad \text{(B 14)}$$

where

$$T_1^{(1)} = -\frac{1}{2}\int_0^{\delta} \frac{dq}{2\pi}\int_{-q}^{q} \frac{d\bar{q}}{2\pi}\, G_{n_1}(q, \bar{q}), \qquad \text{(B 15.1)}$$

$$T_1^{(2)} = -\frac{1}{2}\int_{\delta}^{\pi} \frac{dq}{2\pi}\int_{-\delta}^{\delta} \frac{d\bar{q}}{2\pi}\, G_{n_1}(q, \bar{q}), \qquad \text{(B 15.2)}$$

$$T_1^{(3)} = -\frac{1}{2}\int_{\delta}^{\pi} \frac{dq}{2\pi}\int_{\delta}^{q} \frac{d\bar{q}}{2\pi}\, G_{n_1}(q, \bar{q}), \qquad \text{(B 15.3)}$$

$$T_1^{(4)} = -\frac{1}{2}\int_{\delta}^{\pi} \frac{dq}{2\pi}\int_{-q}^{-\delta} \frac{d\bar{q}}{2\pi}\, G_{n_1}(q, \bar{q}), \qquad \text{(B 15.4)}$$

In the following we shall discuss these four terms and show that, for $n_1 \to \infty$, $T_1^{(3)}$ and $T_1^{(4)}$ decay faster than $T_1^{(1)}$ and $T_1^{(2)}$.

$T_1^{(1)}(n_1 \to \infty)$: The smallness of δ allows the use of (B 13) instead of $\tilde{\varphi}(q, n_1)$, and similarly $\varphi_1(q)$ and $\sin\frac{1}{2}(q - \bar{q})$ can be replaced by approximations:

$$\left.\begin{aligned} \varphi_1(q) + q/2 &\sim (\varphi_1' + 1/2)\, q \\ \sin\tfrac{1}{2}(q-\bar{q}) &\sim \tfrac{1}{2}(q-\bar{q}) \end{aligned}\right\} \text{for small } q, \bar{q}, \quad \text{(B 16)}$$

where $\varphi_1' = (\partial \varphi_1/\partial q)_{q_{c1}}$. [A rigorous estimation of the higher terms neglected in (B 15.1) by use of (B 13, 16) is rather difficult.] With these approximations we get for $T_1^{(1)}$:

$$\begin{aligned} T_1^{(1)} \sim \frac{1}{2\pi^2}\,(\varphi_1' + 1/2)\, a_0'\, e^{-n_1 a} \int_{-\delta}^{\delta} dq \int_{-\delta}^{\delta} d\bar{q} \\ \times (q\, e^{-b n_1 q^2/2} - \bar{q}\, e^{-b n_1 \bar{q}^2/2})/(q - \bar{q}) \\ \text{for } n_1 \to \infty,\ \delta \text{ small}. \qquad \text{(B 17)} \end{aligned}$$

Here we have extended again the integration region to the full square $-\delta \leqq q, \bar{q} \leqq \delta$ and consequently multiplied by $1/4$. With the substitutions

$$x^2 = b\, n_1\, q^2, \quad y^2 = b\, n_1\, \bar{q}^2 \qquad \text{(B 18)}$$

we get

$$T_1^{(1)} \sim \frac{(2\varphi_1'+1)\,a_0'\,e^{-n_1 a}}{4\pi^2 b\, n_1} K(\delta \sqrt{b\, n_1}) \qquad \text{(B 19)}$$

with

$$K(N) = \int_{-N}^{N} \mathrm{d}x \int_{-N}^{N} \mathrm{d}y\, (x\, e^{-x^2/2} - y\, e^{-y^2/2})/(x-y)\,. \qquad \text{(B 20)}$$

To evaluate $K(N\rightarrow\infty)$ we again use the symmetries (B 11) [which hold for (B 20) too] to bisect the integration region:

$$\begin{aligned} K(N) &= 2\int_0^N \mathrm{d}x \int_{-N}^{N} \mathrm{d}y\, (x\, e^{-x^2/2} - y\, e^{-y^2/2})/(x-y) \\ &= -2\int_0^N \mathrm{d}x\, x\, e^{-x^2/2} \oint_{-N}^{N} \frac{\mathrm{d}y}{y-x} - 2\int_{-N}^{N} \mathrm{d}y\, y\, e^{-y^2/2} \oint_0^N \frac{\mathrm{d}x}{x-y} \\ &= 2\int_0^N \mathrm{d}x\, x\, e^{-x^2/2} \ln\frac{N+x}{N-x} + 2\int_{-N}^{N} \mathrm{d}y\, y\, e^{-y^2/2} \ln\frac{|y|}{N-y} \\ &= 4\int_0^N \mathrm{d}x\, x\, e^{-x^2/2} \ln\frac{N+x}{N-x} \\ &= 4N^2 \int_0^1 \mathrm{d}x\, x\, e^{-N^2x^2/2} \ln\frac{1+x}{1-x}\,. \end{aligned} \qquad \text{(B 21)}$$

The integrand of (B 21) has, for $N\rightarrow\infty$, a peak near $x=0$ and an (integrable!) logarithmic singularity at $x=1$. Therefore, to discuss $K(N\rightarrow\infty)$, we divide the interval $(0,1)$ into two parts $(0,x_0)$ and $(x_0,1)$ with fixed x_0. The first part yields the integral

$$\begin{aligned} 4N^2 &\int_0^{x_0} \mathrm{d}x\, x\, e^{-N^2x^2/2} \ln\frac{1+x}{1-x} \\ &= 4N^2 \left(\int_0^\infty - \int_{x_0}^\infty\right) \mathrm{d}x\, x\, e^{-N^2x^2/2} \ln\frac{1+x}{1-x} \qquad \text{(B 22)} \\ &= 4N^2 \left\{ \sqrt{\frac{\pi}{2}}\, \frac{1}{N^3} + \mathrm{O}(x_0\, e^{-N^2x_0^2/2} N^{-2}) \right\}. \end{aligned}$$

In the second part we replace the integrand by

$$x_0\, e^{-N^2x_0^2/2} \ln\frac{1+x}{1-x} \qquad \text{(B 23)}$$

which in $x_0<x<1$ is larger than the integrand. So we find

$$\begin{aligned} 4N^2 \int_{x_0}^1 \mathrm{d}x\, x\, e^{-N^2x^2/2} \ln\frac{1+x}{1-x} &< 4N^2 x_0\, e^{-N^2x_0^2/2} \\ \cdot \left\{ 2\ln 2 - \ln(1-x_0^2) - x_0 \ln\frac{1+x_0}{1-x_0} \right\}. \end{aligned} \qquad \text{(B 24)}$$

Thus for a fixed x_0 and $N\rightarrow\infty$ the first term of (B 22) is the leading one:

$$K(N) \sim \sqrt{\frac{\pi}{2}}\, \frac{4}{N}\,, \quad (N\rightarrow\infty) \qquad \text{(B 25)}$$

and we get from (B 19)

$$T_1^{(1)} \sim \sqrt{\frac{2}{\pi^3}}\, (\varphi_1'+1/2)\, a_0' (b\, n_1)^{-3/2} e^{-n_1 a}/\delta \qquad (n_1\rightarrow\infty,\ \delta \text{ small})\,. \qquad \text{(B 26)}$$

The somewhat strange δ dependence of (B 26) deserves a comment. At (B 13) δ was defined to be small enough to make possible the approximations (B 13, 16), so the case $\delta\rightarrow\infty$ is excluded. On the other hand δ has to be chosen finite, so as to include in the regions (1) and (2) of Fig. 11 the double ribs of g_{n_1}, Figure 10. Only after letting $n_1\rightarrow\infty$ δ may be chosen arbitrarily small. [This way of performing the limits is also implicit in (B 25) where we have $N=\delta\sqrt{b\, n_1}\rightarrow\infty$.] The sum (B 14) of course must be independent of δ. This cannot, however, be shown here since for the remaining three terms of (B 14) only the orders of magnitude can be estimated, without explicit factors.

Concerning the asymptotic estimation of these three terms a few general remarks must be made. For each $(q,\bar q)$ with $q\neq\bar q$ there exists a *finite* lower bound $N(q-\bar q)$ such that for $n_1>N(q-\bar q)$ we have the asymptotics

$$G_{n_1}(q,\bar q) \sim \tilde\varphi(q_<, n_1) \sim -a(q_<)\, e^{-n_1|\mathrm{Re}\,\varepsilon_1(q_<)|} \qquad (n_1\rightarrow\infty) \qquad \text{(B 27)}$$

with $q_<$ chosen as to make $|q_<|=\mathrm{Min}(|q|,|\bar q|)$. For $q=\bar q$ and $q=\bar q\pm 2\pi$, however, one finds the limit (B 12), i.e.

$$G_{n_1}(q,\bar q) \sim \partial\tilde\varphi/\partial q \sim -(a'-n_1\varepsilon' a)\, e^{-n_1|\mathrm{Re}\,\varepsilon_1|} \qquad (n_1\rightarrow\infty) \qquad \text{(B 28)}$$

which for $n_1\rightarrow\infty$ predominates over (B 27) at all points $q=\bar q\,(\pm 2\pi)$ where $\varepsilon'(q)\,a(q)\neq 0$. So we have a similar non-uniformity problem here as is possibly present in (6.15): for $q-\bar q\rightarrow 0$ the lower bound $N(q-\bar q)$ for the asymptotic approximation (B 27) approaches infinity according to

$$N(q-\bar q) \sim \varrho\, |(q-\bar q)\, \partial\varepsilon_1/\partial q|^{-1} \qquad (q\rightarrow\bar q) \qquad \text{(B 29)}$$

where $e^{-\varrho}\ll 1$ is chosen to be the magnitude of the relative error neglected in (B 27). But in the present case we can estimate the effect of this non-uniformity since we know the limiting behaviour (B 28), and thus overcome the problem. We simply have to exclude a small stripe of constant width $\Delta\sqrt{2}$, surrounding the lines $q-\bar q=0,\pm 2\pi$, from the behaviour (B 27), see Figure 12. (For sim-

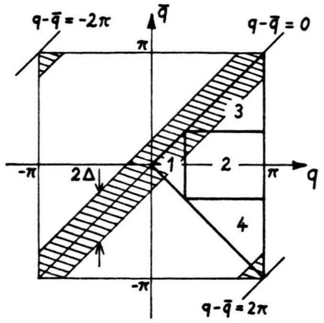

Fig. 12. The exclusion of the nonuniformity stripes of $g_{n1}(n_1 \to \infty)$ from the integration regions.

plicity we take $\Delta < \delta$.) If in this whole stripe a behaviour like (B 28), say

$$G_{n_1} \sim n_1\, e^{-n_1|\mathrm{Re}\,\varepsilon_1|} \quad (n_1 \to \infty) \tag{B 30}$$

is assumed, the asymptotic order of magnitude of the corresponding integral (B 5) will be an upper limit for the order of magnitude of the real T_1.

$T_1^{(2)}(n_1 \to \infty)$: Sparing for a moment the hatched corner of area 2 in Fig. 12, we are left with the integral

$$\int_{\delta}^{\pi} \frac{\mathrm{d}q}{2\pi} \int_{-\delta}^{x(q)} \frac{\mathrm{d}\bar q}{2\pi}\, G_{n_1}(q, \bar q) \tag{B 31}$$

with

$$x(q) = \mathrm{Min}\,\{\delta, q - \Delta\}\,. \tag{B 32}$$

Since $\bar q < \delta < q$ in this area one can neglect $\tilde\varphi(q, n_1)$ compared to $\tilde\varphi(\bar q, n_1)$ which can be approximated by (B 13). Further one may replace $\varphi_1(\bar q) + \bar q/2$ by $(\varphi_1' + 1/2)\,\bar q$ according to (B 16), and replace the denominator of G_{n_1} by the truncated expansion

$$[\sin \tfrac{1}{2}(q - \bar q)]^{-2} \sim \left(\sin \frac{q}{2}\right)^{-2} + \bar q\, \frac{2}{\sin q}\, \frac{1 + \cos q}{1 - \cos q} + O(\bar q^2) \qquad (\bar q \to 0)\,.$$

So one has

$$(\text{B 31}) \sim a_0'\, e^{-n_1 a} \int_{\delta}^{\pi} \frac{\mathrm{d}q}{2\pi} \int_{-\delta}^{x(q)} \frac{\mathrm{d}\bar q}{2\pi} \cdot \left\{ \frac{2\,\varphi_1(q) + q}{1 - \cos q} + \bar q\, F(q) + O(\bar q^2) \right\} \bar q\, e^{-b n_1 \bar q^2/2} \tag{B 33}$$

with

$$F(q) = \{[2\,\varphi_1(q) + q]\,(1 + \cos q)/\sin q - (2\,\varphi_1' + 1)\}/(1 - \cos q)\,. \tag{B 34}$$

For those values of q for which $x(q) = +\delta$ the $\bar q$-free term in the bracket of (B 33) yields no contribution to the $\bar q$ integral, whereas for the remaining q values one gets from this term a contribution of the order

$$e^{-n_1 a} \int_{-\delta}^{q-\Delta} \mathrm{d}\bar q\; \bar q\, e^{-b n_1 \bar q^2/2} = O\,[(b\,n_1)^{-1}\, e^{-n_1 a}\, e^{-b n_1 (\delta - \Delta)^2/2}]\,. \tag{B 35}$$

(The higher even powers of $\bar q$ in the bracket yield similar expressions with higher negative powers of $b\,n_1$.) The second (linear) term in the bracket yields

$$a_0'\, e^{-n_1 a} \int_{\delta}^{\pi} \frac{\mathrm{d}q}{2\pi}\, F(q) \int_{-\delta}^{x(q)} \frac{\mathrm{d}\bar q}{2\pi}\, \bar q^2\, e^{-b n_1 \bar q^2/2}\,.$$

Here one can, without altering the leading term, replace $x(q)$ by $+\delta$ for all q. Thus one gets for this term:

$$a_0'\, e^{-n_1 a} \int_{\delta}^{\pi} \frac{\mathrm{d}q}{2\pi}\, F(q)\, (b\,n_1)^{-3/2}/\sqrt{2\pi} = O\,[(b\,n_1)^{-3/2}\, e^{-n_1 a}]\,, \tag{B 36}$$

i. e. the same order of magnitude as $T_1^{(1)}$, since $F(q)$ has no zeros inside (δ, π). Finally the contribution of the hatched corner has to be estimated. Up to a factor independent of n_1, the integrand will be of the order (B 30), i. e.

$$n_1\, e^{-n_1 a}\, e^{-b n_1 \delta^2/2} \tag{B 37}$$

in this region. Since the area of the corner is chosen independent of n_1 the integral over this corner will be of order (B 37) too. Thus (B 36) is the leading term of $T_1^{(2)}$:

$$T_1^{(2)} \sim O\,[(b\,n_1)^{-3/2}\, e^{-n_1 a}]\,. \tag{B 38}$$

$T_1^{(3)}(n_1 \to \infty)$: Again we first discuss the unhatched area of region 3, which is of order O(1). The modulus of the integrand takes its maximum at the boundary $\bar q = \delta$:

$$G_{n_1}(q, \bar q = \delta) \sim \tilde\varphi(\bar q = \delta, n_1) \sim O\,(e^{-n_1 a}\, e^{-b n_1 \delta^2/2}) \tag{B 39}$$

whence the integral over this area is of the same order. The hatched stripe contributes a term of the order

$$n_1\, e^{-n_1 a}\, e^{-b n_1 \delta^2/2} \tag{B 40}$$

which dominates (B 39) but is in turn dominated by (B 38).

$T_1^{(4)}(n_1 \to \infty)$: The unhatched area of region 4 yields a term

$$O[\tilde{\varphi}(\bar{q}=\delta, n_1)] \sim O(e^{-n_1 a} e^{-b n_1 \delta^2/2}) \quad \text{(B 41)}$$

while the hatched corner gives $O(\partial\tilde{\varphi}/\partial q|_{q=\pi})$. With (B 28) and $\varepsilon_1'(\pi) = a(\pi) = 0$ this is

$$O(e^{-n_1 a} e^{-n_1[\varepsilon_1(\pi) - \varepsilon_1(0)]}) \quad \text{(B 42)}$$

which decays faster than (B 41). However, (B 41) decays faster than (B 38), $T_1^{(2)}$, so we may neglect $T_1^{(3)}$ and $T_1^{(4)}$ for $n_1 \to \infty$. In conclusion we see that both $T_1^{(1)}$ and $T_1^{(2)}$ yield a term of order

$$(b\, n_1)^{-3/2} e^{-n_1 a}.$$

Now from (B 26) and (B 36) both terms are seen to have the sign of $a_0'(\varphi_1' + 1/2)$. So they do not cancel, and the n_1 dependence of (6.21) is proven. – Quite similar considerations lead to (6.36).

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