# Fokker-Planck equation for a square lattice of coupled anharmonic oscillators and the two-dimensional Ising model



1985 J. Phys. A: Math. Gen. 18 1239

(http://iopscience.iop.org/0305-4470/18/8/024)

J. Phys. A: Math. Gen. 18 (1985) 1239-1254. Printed in Great Britain

# Fokker-Planck equation for a square lattice of coupled anharmonic oscillators and the two-dimensional Ising model

A Muñoz Sudupe and R F Alvarez-Estrada

Departamento de Física Teórica, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain

Received 27 July 1984, in final form 27 November 1984

**Abstract.** We calculate the lowest non-zero eigenvalue of the Fokker-Planck equation for an infinite square lattice of coupled overdamped anharmonic oscillators (bistable potentials) through a variational calculation. It generalises previous work for only one oscillator in a non-trivial way. We reduce that calculation to that of a suitable ratio of partition functions for the 2D Ising model, for which an exact analytical expression is obtained. Numerical results are also given and discussed.

## 1. Introduction

Much attention has been paid to the understanding of self-organisation and cooperative behaviour in non-equilibrium systems (Haken 1975, 1977, Dawson 1983 and references therein, Desai and Zwanzig 1978, Weindenmuller and Jing-Shang 1984). To describe these systems stochastic nonlinear partial differential equations, typically Fokker-Planck, Langevin or Itô equations, are used. Recently, numerical analysis of the so-called cellular automata have also been investigated, showing self-organisation (Wolfram 1983).

In this paper we consider a planar lattice of bistable potentials, each of which is coupled to its nearest neighbours. The bistable potential is represented by a quartic overdamped anharmonic oscillator. Thermal fluctuations, which drive the system towards equilibrium, have been taken into account through Gaussian-correlated white noise. The time dependent probability density for a given configuration of the 'positions' $q_{i,j}$ of the oscillators, $f(\{q_{i,j}\}, t)$, obeys a nonlinear Fokker-Planck equation. We calculate the lowest non-zero eigenvalue, $E_1$, of the time-independent version of the Fokker-Planck equation in a suitable limit ('discrete spin limit'), in which the position of each oscillator is allowed to take just two values, $+1$, or $-1$ (§ 2). In such a limit, all other (higher) non-vanishing eigenvalues become very large (and, eventually, diverge). We reduce the calculation of $E_1$ to that of a specific ration of partition functions for the 2D Ising model, and make full use of the fact that the latter can be solved exactly. This fact allows us to determine that ratio of partition functions (§ 3). Numerical results are also obtained and analysed (§ 4).

As is well known, the continuous nonlinear Fokker-Planck equation (Muñoz Sudupe and Alvarez-Estrada 1983) is deeply related to the $\lambda\phi^4$ quantum field theory: in fact, the former is a 'dynamical version' of the $\lambda\phi^4$ model, as it can be seen through the fluctuation-dissipation theorem. On the other hand, the $\lambda\phi^4$ theory on a lattice gives, in an appropriate limit, the Ising model (Glimm and Jaffe 1976). Then, it is to be expected that the Fokker-Planck equation on a lattice, in a similar limit, will give information about the dynamics of the Ising model. In some sense, we are investigating the rate at which the 2D system under consideration reaches equilibrium (see our comments below (2.8)).

Our study has certain formal similarities (but it does not seem to coincide exactly) with the Glauber model (Glauber 1963) for the dynamics of the Ising model.

Larson and Kostin (1978) have studied the same problem for just one overdamped anharmonic oscillator: they found the eigenvalue $E_1$ (as well as the remaining higher eigenvalues) in the same limit, through a variational-like calculation. The case of one oscillator has also been studied recently and the eigenvalue $E_1$ has been calculated using supersymmetry and a variational principle (Bernstein and Brown 1984).

In an earlier work, we have generalised non-trivially the Larson-Kostin arguments to an infinite *linear chain* of coupled overdamped anharmonic oscillators (Alvarez-Estrada and Muñoz Sudupe 1984) finding the leading behaviour of $E_1$ in the 'discrete spin limit': we do not give the details of these calculations here as they are simpler than the ones we require to study the infinite planar lattice.

We shall also mention briefly that a relationship seems to exist between our work and the so-called instanton calculus (Zinn-Justin 1984), but we shall not deal with the latter here.

On the other hand, Desai and Zwanzig (1978) and Dawson (1983) have analysed an infinite chain of anharmonic oscillators (mean-field model), in which each of the latter interacts, in some sense, with every other oscillator, not just with its nearest neighbours. They obtained a phase transition through numerical simulation and a perturbation theory for Markov processes. So, our work, *in which every oscillator interacts only with its nearest neighbours,* is complementary to their work. In principle, we do not pretend to perform here a proper and detailed calculation in the region of parameters where a phase transition is to be expected. Nevertheless, some (perhaps vague) signal of a phase transition is seen to appear: see the discussion in § 4.2 and the table in appendix 3.

## 2. Square lattice of coupled anharmonic oscillators

We consider an infinite 2D square lattice of overdamped anharmonic oscillators coupled together through nearest-neighbour interactions. The potential energy of an arbitrary configuration $\{q_{i,j}\}$, where $-\infty < q_{ij} < \infty$ for any $i$, $j$ is

$$V(\{q_{i,j}\}) = \sum_{i,j=-\infty}^{+\infty} \{\tfrac{1}{2}\alpha q_{i,j}^2 + \tfrac{1}{4}\beta q_{i,j}^4 + \tfrac{1}{2}\gamma[(q_{i+1,j} - q_{i,j})^2 + (q_{i,j+1} - q_{i,j})^2]\}. \tag{2.1}$$

The equations of motion for the planar lattice of coupled overdamped anharmonic oscillators without fluctuations read $\mathrm{d}q_{j,l}/\mathrm{d}t = -\partial V/\partial q_{j,l}$. It is easy to see that the set $q_{j,l} = +1$ for all $j$, $l$ constitutes a stable solution. In fact, by analysing the small perturbations about it, namely, $q_{j,l} = 1 + \sigma^{(0)} \exp \mathrm{i}(k_1 j + k_2 l + \omega t)$ where $\sigma^{(0)}$ is a small amplitude, independent on $j$, $l$, one gets directly: $\omega = \mathrm{i}2\{\beta + \gamma[(1 - \cos k_1) + (1 - \cos k_2)]\}$ which implies stability. Similarly, the set $q_{j,l} = -1$ for any $j$, $l$ is another stable solution, while $q_{jl} = 0$ for any $j$, $l$ is an unstable one.

If one includes white-noise fluctuations, the corresponding Langevin equation is ($i, j = 0, \pm 1, \pm 2, \ldots, \pm\infty$):

$$\mathrm{d}q_{i,j}/\mathrm{d}t = -\partial V/\partial q_{i,j} + \xi_{i,j}(t) \tag{2.2}$$

where $\langle \xi_{i,j} \rangle = 0$ and $\langle \xi_{i,j}(t)\xi_{k,l}(t') \rangle = Q\delta_{i,k}\delta_{j,l}\delta(t-t')$. Equivalently, we may write the associated Fokker-Planck equation for the probability density of the configuration $\{q_{i,j}\}$, $f(\{q_{i,j}\}, t)$, as

$$\frac{\partial f}{\partial t} = \sum_{i,j=-\infty}^{+\infty} \frac{\partial}{\partial q_{i,j}}\left(\frac{\partial V}{\partial q_{i,j}} f + \frac{Q}{2}\frac{\partial f}{\partial q_{i,j}}\right). \tag{2.3}$$

Later on, we shall consider a finite lattice with $M \times M$ sites, occasionally, and then take the limit $M \to \infty$.

The stationary probability density $f_0(\partial f_0/\partial t = 0)$ is:

$$f_0 = N \exp[-2Q^{-1}V(\{q_{i,j}\})] \tag{2.4}$$

where $N$ is a normalisation constant, so as to satisfy

$$\int \left(\prod_{i,j=-\infty}^{+\infty} \mathrm{d}q_{i,j}\right) f_0 = 1.$$

In order to see the relation of the system under consideration and the 2D Ising model, let us compute $f_0$ in the 'discrete spin limit': $\beta \to +\infty$, $\alpha \to -\infty$ with $\beta = -\alpha$, $\gamma$, $Q$ being fixed. The result is, by using $\lim_{\lambda\to\infty} \exp(-\lambda x^2) = (\pi/\lambda)^{1/2}\delta(x)$:

$$f_0(\{q_{i,j}\}) = \frac{1}{Z}\left(\prod_{i,j=-\infty}^{+\infty} [\delta(q_{i,j}+1) + \delta(q_{i,j}-1)]\right)\left(\exp 2\gamma Q^{-1} \sum_{i,j=-\infty}^{+\infty} (q_{i+1,j}q_{i,j} + q_{i,j+1}q_{i,j})\right)$$
$$\equiv Z^{-1}\exp(-H) \tag{2.5}$$

where the normalisation constant $Z$ is seen to coincide with the partition function of the 2D Ising model and $H$ is the interaction energy between neighbouring spins with coupling $2\gamma Q^{-1}$. It may also be verified easily from (2.5) that the equal-time correlation function for (2.3)-(2.4) gives, in the same limit, the correlation function of the 2D Ising model.

The probability density $f$ can be formally written, in general, as

$$f(\{q_{i,j}\}, t) = f_0(\{q_{i,j}\})\left(\sum_{n=0}^{\infty} h_n(\{q_{i,j}\}) \exp(-E_n t)\right) \tag{2.6}$$

where $E_0 = 0$ and $h_0 = 1$, and the positive eigenvalues $E_n$ of the time-independent version of (2.3) increase with $n$. As we are interested in the long-time behaviour of $f$, we retain the term corresponding to the lowest non-vanishing eigenvalue ($n = 1$) in the right-hand side of (2.6). Upon substituting (2.6) into (2.3), we may write the resulting equation for $h_1$ ($\alpha = -\beta$) as

$$-E_1 h_1 = \sum_{i,j=-\infty}^{+\infty}\left(\frac{Q}{2}\frac{\partial^2 h_1}{\partial q_{i,j}^2} - [\beta(q_{i,j}^2 - 1)q_{i,j} - \gamma(q_{i+1,j} + q_{i,j+1} + q_{i-1,j} + q_{i,j-1} - 4q_{i,j})]\frac{\partial h_1}{\partial q_{i,j}}\right). \tag{2.7}$$

Upon multiplying both sides of (2.7) by $h_1$ and integrating by parts on the right-hand side, the first eigenvalue $E_1$, which determines the long-time behaviour of $f$, may be written as:

$$E_1 = \frac{Q}{2} \frac{\int \left( \prod_{i,j=-\infty}^{+\infty} \mathrm{d}q_{i,j} \right) f_0(\{q_{i,j}\}) \sum_{i,j=-\infty}^{+\infty} \left( \frac{\partial h_1}{\partial q_{i,j}} \right)^2}{\int \left( \prod_{i,j=-\infty}^{+\infty} \mathrm{d}q_{i,j} \right) f_0(\{q_{i,j}\}) h_1^2} \equiv \frac{Q}{2} \frac{N}{D}. \tag{2.8}$$

This formula will be used to compute $E_1$ for large $\beta$ ($\beta = -\alpha$; $\gamma$, $Q$ being fixed) through a variational-like calculation which will consititute a non-trivial generalisation of that of Larson and Kostin (1978) for the case of only one oscillator ($i = j = M = 1$).

They showed that, in such a limit, $E_1$ is, essentially, the rate constant which controls the long-time behaviour of the systems consisting of just one oscillator and, hence, how the latter approaches equilibrium. One is tempted to argue that, in the actual case of an infinite planar lattice of such oscillators, $E_1$ could play a similar role. We recall that in the case of only one oscillator, Larson and Kostin expressed the corresponding analogue of $h_1$ as an error function. Two essential remarks about their calculation (see equations (2.11)-(2.14) in their paper) follow:

(1) The derivative of their $h_1$ gives non-negligible contributions to the analogue of $N$ only for values of $q$ close to zero.

(2) On the other hand, the same $h_1$ turned out to be essentially constant except for values of $q$ close to zero and, hence, it was seen to give appreciable contributions to the analogue of $D$ only for values of $q$ close to $\pm 1$. We shall generalise these facts to our present case, in a non-trivial way.

The approximate solution of (2.7) with $E_1 = 0$ on the left-hand side and generic configurations in which all the oscillator coordinates nearly take on the values $q_{i,j} = \pm 1$, except for the one located at the $(k, l)$-site where $q_{k,l} \approx 0$, will be adopted, by extending the choice of Larson and Kostin. These configurations correspond heuristically to the tunnelling of the spin at the $(k, l)$-site between its two stable configurations $q_{k,l} = \pm 1$. This unique function $h_1$ will be used both in $N$ and $D$ of (2.8). We shall outline below the explicit construction of $h_1$ and of its derivative, and the calculation of their contributions to $N$ and $D$.

### 2.1. *Approximate expression for $h_1$*

The solution $h_1$ may be approximately factorised for large $\beta$ ($\beta = -\alpha$, $\gamma$ and $Q$ being fixed) as

$$h_1(\{q_{i,j}\}) \approx \tilde{h}_1(\{q_{i,j}\}, (i,j) \neq (k, l)) \cdot \tilde{h}(q_{k,l}) \tag{2.9}$$

where we have neglected terms of $\mathrm{O}(\gamma/\beta)$.

The function $\tilde{h}(q_{k,l})$ is an error function with derivative

$$\frac{\mathrm{d}\tilde{h}}{\mathrm{d}q_{k,l}} = C \exp[-Q^{-1}(\beta - 4\gamma) q_{k,l}^2 - 2\gamma Q^{-1}(\varepsilon_{k+1,l} + \varepsilon_{k-1,l} + \varepsilon_{k,l+1} + \varepsilon_{k,l-1}) q_{k,l}] \tag{2.10a}$$

$C$ being a constant, $\varepsilon_{k\pm 1,l}^2 = \varepsilon_{k,l\pm 1}^2 = 1$ and

$$\tilde{h}_1(\{q_{i,j}\}, (i,j) \neq (k, l)) = \text{constant}. \tag{2.10b}$$

The justification of (2.9) and (2.10*a*, *b*) starting from (2.7) is outlined in appendix 1.

It is easy to show that $h_1$ gives approximately a true trial function in the sense of the Ritz variational principle, when terms of order $\gamma^2/\beta$ are neglected. In fact, (2.8) can be cast into an equivalent Hamiltonian form by using the transformation $h \to \phi = f_0^{1/2} h$, as in appendix 2. We only need to show that $\phi_1 = f_0^{1/2} h_1$ is approximately orthogonal to $\phi_0 = f_0^{1/2}$, that is, that

$$\int \left( \prod_{i,j=-\infty}^{+\infty} \mathrm{d}q_{i,j} \right) \phi_1(\{q_{ij}\}) \phi_0(\{q_{ij}\}) = \int \left( \prod_{i,j=-\infty}^{+\infty} \mathrm{d}q_{ij} \right) h_1(\{q_{ij}\}) f_0(\{q_{ij}\})$$

vanishes approximately. In fact the right-hand side of (2.10$a$) is even when the term $-2\gamma Q^{-1}(\varepsilon_{k+1,l} + \varepsilon_{k-1,l} + \varepsilon_{k,l+1} + \varepsilon_{k,l-1}) q_{k,l}$ (that is, terms of relative order $\gamma^2/\beta$) is neglected and, hence, $h_1$ is approximately odd under $q_{kl} \to -q_{kl}$ while $f_0$ is even.

### 2.2. *Calculation of N*

Upon introducing (2.10$a$) and (2.4) into $N$, one realises that the main contributions as $\beta$ is large ($\gamma$ and $Q$ being fixed) come from values of $q_{kl}$ close to zero and from the remaining $q_{ij} = \pm 1$ for $(i, j) \neq (k, l)$. We stress that this is precisely the natural generalisation to the planar lattice of the corresponding step made by Larson and Kostin (1978) in their variational calculation for only one anharmonic oscillator: compare with (2.11)-(2.13) and related remarks in their paper.

Notice that all this amounts to replacing $f_0$ by

$$Z^{-1}\left( \prod_{i,j=1}^{+\infty}{}' [\delta(q_{i,j}+1) + \delta(q_{i,j}-1)] \right) \left\{ 2\left( \frac{\beta}{2\pi Q} \right)^{1/2} \exp\left[ -\left( \frac{\beta - 8\gamma}{2Q} \right) \right] \exp\left( \frac{\beta - 4\gamma}{Q} q_{k,l}^2 \right) \right\}$$
$$\times \exp\left[ \frac{2\gamma}{Q} \left( \sum_{i,j=-\infty}^{+\infty}{}' (q_{i+1,j} + q_{i,j+1}) q_{i,j} \right.\right.$$
$$\left.\left. + (q_{k+1,l} + q_{k-1,l} + q_{k,l+1} + q_{k,l-1}) q_{k,l} \right) \right] \tag{2.11}$$

where the prime over $\Pi$ and $\Sigma$ indicates that all terms containing $q_{k,l}$ have to be excluded. We have replaced the $\varepsilon$'s appearing in (2.10$a$) by $q$'s, since the latter fulfil $q^2 = 1$.

Notice that the factor $\exp\{[(\beta - 4\gamma)/Q] q_{kl}^2\}$ in (2.11) is overcome by twice a similar factor coming from the square of (2.10$a$) using (2.10$a$, $b$) and (2.11) in $N$ (2.8), the Gaussian integral over $q_{k,l}$ can be easily calculated and finally yields

$$N = \frac{\sqrt{2}}{Z} C_1^2 \exp\left[ -\left( \frac{\beta - 8\gamma}{2Q} \right) \right] \sum_{\substack{\{q_{i,j}\} \\ q_{i,j} = \pm 1}}{}' \exp\left( \frac{2\gamma}{Q} \sum_{i,j}{}' (q_{i+1,j} + q_{i,j+1}) q_{i,j} \right) \tag{2.12}$$

where we have neglected terms of $\mathrm{O}(\gamma/\sqrt{\beta})$ (coming from 2.10$a$)) and $C_1$ is a constant. The sum over configurations (excluding all terms containing the $(k, l)$-spin) in the right-hand side of (2.12) is the partition function for an Ising model, in which the $(k, l)$ spin has been removed. Let us call it $Z_{k,l}$. So, we have

$$N = \sqrt{2}\, C_1^2 \exp\left[ -\left( \frac{\beta - 8\gamma}{2Q} \right) \right] \frac{Z_{k,l}}{Z}. \tag{2.13}$$

### 2.3. Calculation of D

Upon integrating (2.10$a$) in $(0, q_{kl})$ one sees that $\tilde{h}(q_{kl})$ is nearly constant except for values of $q_{kl}$ close to zero and so on if one integrates it in $(-q_{kl}, 0)$: compare with the comments in Larson and Kostin, after their equations (2.10) and (2.13). Consequently, by considering $D$ and recalling (2.4), the integrations over all $q_{ij}$ (including $q_{kl}$) are significant only for $q_{ij} = \pm 1$. This is equivalent to replacing $f_0$ in $D$ by the right-hand side of (2.5) for all $q_{ij}$ (including $q_{kl}$). It turns out that the normalisation factor $Z^{-1}$ in (2.5) cancels with a similar factor arising from the integration over all $q_{ij}$.

So, we obtain for $\beta \gg 1$, $\beta = -\alpha$, $\gamma$ and $Q$ being fixed:

$$D = (\pi Q/4\beta)C_1^2. \tag{2.14}$$

Using (2.13) and (2.14) in (2.8) we get the main result which determines the smallest non-vanishing eigenvalue for (2.7)

$$E_1 = \frac{2\sqrt{2}}{\pi}\beta \exp\left[-\left(\frac{\beta - 8\gamma}{2Q}\right)\right]\frac{Z_{k,l}}{Z}. \tag{2.15}$$

Equation (2.15) for the case of only one oscillator coincides with (2.16) of Larson and Kostin, since $Z_{kl}/Z$ becomes $\frac{1}{2}$ in such a case.

We remark, at this point, that the limit that we are considering, that is, $\beta$ large, $\gamma$ and $Q$ fixed, amounts, somehow, to 'freezing' the dynamics, which is reflected in the term $\beta \exp(-\frac{1}{2}\beta Q^{-1})$. The 'static' part, namely, the quotient $Z_{k,l}/Z$ may still display 'signals' of some static critical behaviour, if $\gamma(\gamma \ll \beta)$ is not small (see later). The point is that we have set fixed the magnitude of the random pushes, represented by the diffusion parameter $Q$, while we have increased the potential barrier between $q_{i,j} = 1$ and $q_{i,j} = -1$ (as $\beta \to \infty$, with $\beta = -\alpha$): the dynamical effect is the tunnelling between the two minima.

At this point, it may be interesting to recall the following result of Larson and Kostin (1978) for just one overdamped anharmonic oscillator. Equation (2.16) in their paper turns out to approximate the numerical (say, exact) results for the first eigenvalue with error less than 10% for $\frac{1}{2}\beta Q^{-1} \geq 4$: the error is 4% for $\frac{1}{2}\beta Q^{-1} \geq 10$ and decreases to zero as $\frac{1}{2}\beta Q^{-1}$ increases (see table 1 in Larson and Kostin 1978). This suggests that (2.15), which is the generalisation of their result for the infinite planar lattice may also be reasonably accurate for finite values of $\beta$ (provided that they are larger than $\gamma$). Equation (2.15) which is a highly non-perturbative result regarding the $\beta$ dependence is the leading term of an asymptotic expansion for large $\beta$. Higher-order terms could be obtained in principle by generalising the procedure outlined in Larson and Kostin, which led to their (2.25); we shall not do it here because such a task lies outside the scope of this work.

One may ask, *a posteriori*, whether other configurations, different from those considered above, could give rise to sizeable contributions to $E_1$ or whether another (finite) structure for $E_1$, different from (2.15), could exist. The fact that our procedure, so far, is the simplest and most natural (albeit non-trivial) generalisation to an infinite planar lattice of coupled anharmonic oscillators of the method used by Larson and Kostin (1978) for only one, already seems a very strong indication that the answers to the above two questions are negative. In appendix 2, we shall provide further arguments, which also lead to negative answers for them.

The quotient of partition functions in (2.15) which is, obviously, non-negative may be calculated using the transfer matrix method (Huang 1963) and introducing fermion operators (Schultz *et al* 1964). This will be the subject of the next section.

## 3. Evaluation of $Z_{k,l}/Z$

Consider now the lattice to be finite, having $M\times M$ sites with periodic boundary conditions: $q_{i,M+1}=q_{i,1}$, $q_{M+1,j}=q_{1,j}$. We denote the $r$th row of that lattice as $\mu_r$, that is $\mu_r\equiv(q_{r,1},\ldots,q_{r,M})$. We may write the partition function $Z_{kl}$ as (notice that the $k$th row is excluded):

$$Z_{kl}=\sum_{\{\mu_i\}}{}'\,\langle\mu_{k+1}|P|\mu_{k+2}\rangle\ldots\langle\mu_{k-2}|P|\mu_{k-1}\rangle\langle\mu_{k-1}|P'_{kl}|\mu_{k+1}\rangle. \tag{3.1}$$

In (3.1) $P$ is the usual transfer matrix of the 2D Ising model:

$$P=\left(2\sinh\frac{4\gamma}{Q}\right)^{M/2}\left(\exp\frac{\gamma}{Q}\sum_{i=-M}^{M}\tau_i^z\tau_{i+1}^z\right)\left(\exp\theta\sum_{i=-M}^{M}\tau_i^x\right).$$
$$\times\left(\exp\frac{\gamma}{Q}\sum_{i=-M}^{M}\tau_i^z\tau_{i+1}^z\right)\equiv\left(2\sinh\frac{4\gamma}{Q}\right)^{M/2}V_2^{1/2}V_1V_2^{1/2} \tag{3.2}$$

with $\tanh\theta=\exp(-4\gamma Q^{-1})$ and $\tau_i^z$, $\tau_i^x$ being the appropriate $2^M\times2^M$ Pauli spin matrices (tensor products of $2\times2$ unit matrices $\mathbb{1}_i$, and $2\times2$ ordinary spin Pauli matrices $\sigma_i^z$, $\sigma_i^x$, located at the $i$th site) (see Schultz *et al* 1964, Huang 1963).

The matrix $P'_{kl}$ which 'transfers' between the rows $\mu_{k-1}$ and $\mu_{k+1}$ has matrix elements of the form:

$$\langle\mu_{k-1}|P'_{kl}|\mu_{k+1}\rangle=\exp\left(\frac{\gamma}{Q}\sum_{i=-M}^{M}(q_{k+1,i}q_{k+1,i+1}+q_{k-1,i}q_{k-1,i+1})\right)$$
$$\times\sum_{\{q_{kj}\}}{}'\left[\exp\left(\frac{2\gamma}{Q}\sum_{j=-M}^{M}{}'\,[(q_{k-1,j}+q_{k+1,j})q_{k,j}+q_{k,j}q_{k,j+1}]\right)\right] \tag{3.3}$$

and may be written, after some algebra, as

$$P'_{kl}=V_2^{1/2}F_l(2\sinh4\gamma Q^{-1})^{M-1}[V_1\exp(-\theta\tau_l^x)]$$
$$\times[V_2\exp[-2\gamma Q^{-1}\tau_l^z(\tau_{l+1}^z+\tau_{l-1}^z)]][V_1\exp(-\theta\tau_l^x)]V_2^{1/2} \tag{3.4}$$

where $F_l=\mathbb{1}_1\times\ldots\times(\mathbb{1}_l\times\sigma_l^x)\times\ldots\times\mathbb{1}_M$ ensures that the sum over row configurations in (3.1) does not include those corresponding to the $k$th row.

Now taking into account that the matrix $\{V_2\exp[-2\gamma Q^{-1}\tau_l^z(\tau_{l+1}^z+\tau_{l-1}^z)]\}$ commutes with $[\exp(-\theta\tau_l^x)]$, as none of them depends on the $l$th spin, the trace in (3.1) may be expressed as:

$$Z_{kl}=\mathrm{Tr}\,[\![(2\sinh4\gamma Q^{-1})^{M^2/2-1}F_l[\exp[-2\theta\tau_l^x)]$$
$$\times\{\exp[-2\gamma Q^{-1}\tau_l^z(\tau_{l+1}^z+\tau_{l-1}^z)]\}(V_2V_1)^M]\!]. \tag{3.5}$$

On the other hand, the partition function of the ordinary 2D Ising model takes on the form (Schultz *et al* 1964)

$$Z=(2\sinh4\gamma Q^{-1})^{M^2/2}\,\mathrm{Tr}\{(V_2V_1)^M\}. \tag{3.6}$$

By following Schultz *et al* (1964), we perform the canonical transformation $\tau_l^x \to -\tau_l^z$, $\tau_l^z \to \tau_l^x$.

Let $|0\rangle$ be the eigenstate associated to the maximum eigenvalue ('the vacuum': see also the comments after (3.11)) of the product matrix $V_2 V_1$. By using equations (3.5)-(3.6), the quotient $Z_{kl}/Z$ in (2.16) can be written, in the thermodynamic limit ($M \to \infty$) as

$$Z_{kl}/Z = 2\sinh(4\gamma Q^{-1})]^{-1}\langle 0|F_l \exp(2\theta\tau_l^z)\exp[-2\gamma Q^{-1}\tau_l^x(\tau_{l+1}^x + \tau_{l-1}^x)]|0\rangle. \tag{3.7}$$

The exponentials of the Pauli spin matrices can be readily evaluated as

$$\exp 2\theta\tau_l^z = \cosh 2\theta + \tau_l^z \sinh 2\theta$$

$$\exp[-2\gamma Q^{-1}\tau_l^x(\tau_{l+1}^x + \tau_{l-1}^x)]$$
$$= (\cosh 2\gamma Q^{-1} - \tau_l^x\tau_{l+1}^x \sinh 2\gamma Q^{-1})(\cosh 2\gamma Q^{-1} - \tau_{l-1}^x\tau_l^x \sinh 2\gamma Q^{-1}). \tag{3.8}$$

Next, also by following Schultz *et al* (1964), we introduce the Jordan-Wigner transformation:

$$\tau_l^+ = \prod_{i=1}^{l-1}(1 - 2C_i^+C_i)C_l^+, \qquad \tau_l^- = \prod_{i=1}^{l-1}(1 - 2C_i^+C_i)C_l \tag{3.9}$$

with $\tau_l^+ = \tau_l^x + \mathrm{i}\tau_l^y$ and $\tau_l^- = \tau_l^x - \mathrm{i}\tau_l^y$. We have introduced in (3.9) the fermion operators $C_i$, $C_i^+$ with anticommutation rules:

$$\{C_i, C_j^+\} = \delta_{i,j}, \qquad \{C_i, C_j\} = \{C_i^+, C_j^+\} = 0. \tag{3.10}$$

Finally, by using (3.8)-(3.10) the quotient (3.7) may be cast as follows

$$Z_{kl}/Z = [2\sinh(4\gamma Q^{-1})]^{-1}\langle 0|(\exp -2\theta)[(1 - C_l^+C_l)\cosh^2 2\gamma Q^{-1}$$
$$+ C_l(C_{l+1}^+ + C_{l+1} - C_{l-1} + C_{l-1}^+)\sinh 2\gamma Q^{-1}\cosh 2\gamma Q^{-1}$$
$$-(C_{l+1}^+ + C_{l+1})(C_{l-1} - C_{l-1}^+)C_lC_l^+ \sinh^2 2\gamma Q^{-1}]|0\rangle. \tag{3.11}$$

We recall that the 'vacuum' $|0\rangle$ is strictly associated with the new fermion operators $\xi_q$, $\xi_q^+$ which, at the end, diagonalise the transfer matrix ($\xi_q|0\rangle = 0$ for all $\xi_q$). In turn, the latter are related to the $C_l$, $C_l^+$ operators through the expression (Schultz *et al* 1964) as

$$\begin{aligned} C_l &= M^{-1/2}[\exp(-\mathrm{i}\tfrac{1}{4}\pi)]\sum_q(\exp \mathrm{i}ql)(\cos\phi_q\xi_q - \sin\phi_q\xi_{-q}^+) \\ C_l^+ &= M^{-1/2}(\exp \mathrm{i}\tfrac{1}{4}\pi)\sum_q(\exp -\mathrm{i}ql)(\cos\phi_q\xi_q^+ - \sin\phi_q\xi_{-q}). \end{aligned} \tag{3.12}$$

In (3.12) the $q$'s range over one of the following sets

$$\begin{aligned} q &= 0, \pm\frac{2\pi}{M}, \ldots, \pm\frac{(M-2)\pi}{M}, \pi \qquad &\text{(cyclic)} \\ q &= \pm\frac{\pi}{M}, \pm\frac{3\pi}{M}, \ldots, \pm\frac{M-1}{M}\pi \qquad &\text{(anticyclic)} \end{aligned} \tag{3.13}$$

and the angles $\phi_q$ are defined by ($q \neq 0, \pi$):

$$\tan\phi_q = \frac{2\sinh 2\gamma Q^{-1}\sin q(\cosh 2\theta\cosh 2\gamma Q^{-1} - \sinh 2\theta\sinh 2\gamma Q^{-1}\cos q)}{\exp\varepsilon_q - [\exp(-2\theta)](\cosh 2\gamma Q^{-1} + \sinh 2\gamma Q^{-1}\cos q)^2 - (\exp 2\theta)(\sinh 2\gamma Q^{-1}\sin q)^2} \tag{3.14}$$

where the following determination will be understood

$$\phi_q \equiv -\phi_{-q}, \qquad \phi_0 = \phi_\pi = 0.$$

In (3.14), $\varepsilon_q$ is the positive root of

$$\cosh \varepsilon_q = \cosh 4\gamma Q^{-1} \cosh 2\theta - \sinh 4\gamma Q^{-1} \sinh 2\theta \cos q. \tag{3.15}$$

The operators $\xi$, $\xi^+$ introduced in (3.12) satisfy

$$\xi_q^+|0\rangle = |q\rangle, \qquad \xi_q|q'\rangle = \delta_{qq'}|0\rangle. \tag{3.16}$$

It turns out that, in order to evaluate the right-hand side of (3.11) we need to calculate the following expectation value:

$$a_{rj} = \langle 0|\mathrm{i}C_r^y C_j^x|0\rangle \tag{3.17}$$

where $\mathrm{i}C_k^y = C_k^+ - C_k$ and $C_k^x = C_k^+ + C_k$. Using (3.12) and (3.15), $a_{rj}$ may be written (Schultz *et al* 1964) successively as

$$\begin{aligned} a_{rj} &= -\frac{1}{M}\sum_q [\exp -\mathrm{i}q(j-r)][\exp(-\mathrm{i}2\phi_q)] \\ &= -\frac{1}{M}\sum_q \cos[2\phi_q + (j-r)q] \end{aligned} \tag{3.18}$$

since $\phi_q$ is an odd function of $q$. Equation (3.18) leads directly to the following results

$$\begin{aligned} &\langle 0|C_l^+ C_l|0\rangle = -\frac{1}{2M}\sum_q (1+\cos 2\phi_q) = \frac{1}{M}\sum_q \sin^2\phi_q \\ &\langle 0|C_l(C_{l+1}^+ + C_{l+1} - C_{l-1} + C_{l-1}^+)|0\rangle = \frac{2}{M}\sum_q \cos(2\phi_q + q) \\ &\langle 0|C_{l+1}^+ + C_{l+1})(C_{l-1} - C_{l-1}^+)C_l C_l^+|0\rangle \\ &\quad = \frac{1}{M^2}\sum_{q,q'} \cos^2\phi_q \cos(2\phi_{q'} + 2q') - \frac{1}{2M^2}\left(\sum_q \cos(2\phi_q + q)\right)^2 \end{aligned} \tag{3.19}$$

where Wick's theorem has been used. That is, we associate fermion operators in pairs, replace each pair (contraction) by its 'vacuum' expectation value (3.17), multiply the product of these contractions by $(-1)^P$ (where $P$ is the signature of the permutation necessary to bring paired operators next to each other starting from the original ordering) and finally, sum over all pairings.

Collecting the previous results, we arrive at the following explicit expression for the quotient of partition functions:

$$\begin{aligned} \frac{Z_{kl}}{Z} = \frac{1}{2\cosh^2(2\gamma Q^{-1})} \bigg\{ &\cosh^2(2\gamma Q^{-1}) \frac{1}{M}\sum_q \cos^2\phi_q + \sinh(2\gamma Q^{-1})\cosh(2\gamma Q^{-1}) \\ &\times \frac{1}{M}\sum_q \cos(2\phi_q + q) + \sinh^2(2\gamma Q^{-1}) \\ &\times \left[\frac{1}{2M^2}\left(\sum_q \cos(2\phi_q + q)\right)^2 - \frac{1}{M^2}\sum_{q,q'} \cos^2\phi_q \cos(2\phi_{q'} + 2q')\right]\bigg\}. \end{aligned} \tag{3.20}$$

## 4. Discussion of the results

### *4.1. Bounds on the ratio $Z_{kl}/Z$*

We shall discuss some general features of $Z_{kl}/Z$. We concentrate on the four spins $q_{k\pm1,l}$, $q_{k,l\pm1}$ and introduce the auxiliary positive quantity

$$Z_{kl}(q_{k\pm1,l}, q_{k,l\pm1}) \equiv \sum_{\substack{\{q_{i,j}\}, q_{i,j}=\pm1 \\ q_{k\pm1,l}, q_{k,l\pm1} \\ \text{fixed}}}' \exp\left(\frac{2\gamma}{Q}\sum_{i,j}' q_{i,j}(q_{i+1,j}+q_{i,j+1})\right). \tag{4.1}$$

The dependence of $Z_{kl}(q_{k\pm1,l}, q_{k,l\pm1})$ upon $q_{k\pm1,l}$, $q_{k,l\pm1}$ comes from the fact that the exponential on the right-hand side of (4.1) does depend upon them but no summation over those four spins is carried out. Then, we shall introduce the three positive quantities

$$Z_{kl}^{(2)} = \sum_{q_{k\pm1,l}, q_{k,l+1}=\pm1}^{(2)} Z_{kl}(q_{k\pm1,l}, q_{k,l\pm1}) \tag{4.2}$$

$$Z_{kl}^{(3)} = \sum_{q_{k\pm1,l}, q_{k,l+1}=\pm1}^{(3)} Z_{kl}(q_{k\pm1,l}, q_{k,l\pm1}) \tag{4.3}$$

$$Z_{kl}^{(4)} = \sum_{q_{k\pm1,l}, q_{k,l\pm1}=\pm1}^{(4)} Z_{kl}(q_{k\pm1,l}, q_{k,l\pm1}) \tag{4.4}$$

where $\Sigma^{(n)}_{q_{k\pm1,l}, q_{k,l\pm1}=\pm1}$ indicates that one sums over the possible values of $q_{k\pm1,l}$ and $q_{k,l\pm1}$, with the restriction that $n(=2, 3, 4)$ of those values have to be equal. Then, it is easy to see that

$$Z_{kl} = Z_{kl}^{(2)} + Z_{kl}^{(3)} + Z_{kl}^{(4)} \tag{4.5}$$

$$Z = 2[Z_{kl}^{(2)} + \cosh(4\gamma Q^{-1})Z_{kl}^{(3)} + \cosh(8\gamma Q^{-1})Z_{kl}^{(4)}]. \tag{4.6}$$

Equations (4.5)–(4.6) imply the following general properties

(a) $Z_{kl}/Z \to \frac{1}{2}$ if $\gamma/Q \to 0$

(b) $[2\cosh(8\gamma Q^{-1})]^{-1} \leqslant Z_{kl}/Z < \frac{1}{2}$

(c) $Z_{kl}/Z \to \exp(-8\gamma Q^{-1})$ as $\gamma Q^{-1} \to +\infty$.

In fact, it is well known that, as $\gamma Q^{-1}$ increases, the 2D Ising model has a phase transition, so that, for suitably large $\gamma Q^{-1}$ above the critical point, practically all spins are in one of the two ordered phases (either $q_{ij}=+1$ or $q_{ij}=-1$, for any $i$, $j$). This implies that $Z_{kl}^{(4)}$ dominates in such a regime, which yields to the stated property.

### *4.2. Numerical analysis*

We have studied (3.20) numerically for several values of $M$ (number of spins in each row or column) and of $\gamma Q^{-1}$ respectively. The results that we have obtained, part of which are collected in appendix 3, are in good agreement with the bounds presented in the preceding subsection, that is: (i) $Z_{kl}/Z \to \frac{1}{2}$ as $\gamma Q^{-1}$ decreases, (ii) $Z_{kl}/Z \to 0$ like $\exp(-8\gamma Q^{-1})$ for $\gamma Q^{-1}$ large.

Above the critical point of the 2D Ising model (which corresponds to $2\gamma Q^{-1} = \frac{1}{2}\ln(1+\sqrt{2}) = 0.440\,687$) the results are insensitive to $M$, that is, the same ratio $Z_{kl}/Z$ is obtained for $M = 10^3$ or $M = 10^4$, for values of $2\gamma Q^{-1} = 0.43$. In contrast, below the critical point the results decrease more rapidly with increasing $M$.

Another important feature, which clearly appears for any $M$, is a zero in the second derivative of $Z_{kl}/Z$ with respect to $2\gamma Q^{-1}$ at the critical point (see table 1). The slope

**Table 1.**

| $K=2\gamma Q^{-1}$ | $Z_{kl}/Z$ | $\mathrm{d}(Z_{kl}/Z)/\mathrm{d}K$ |
|---|---|---|
| 0.440 682 | 0.275 583 | −3.656 779 |
| 0.440 683 | 0.275 579 | −3.656 883 |
| 0.440 684 | 0.275 576 | −3.656 965 |
| 0.440 685 | 0.275 562 | −3.657 024 |
| 0.440 686 | 0.275 568 | −3.657 060 |
| 0.440 687 | 0.275 565 | −3.657 075 |
| 0.440 688 | 0.275 561 | −3.657 066 |
| 0.440 689 | 0.275 557 | −3.657 035 |
| 0.440 690 | 0.275 554 | −3.656 981 |

$M=6000$.

of $Z_{kl}/Z$ with respect to $2\gamma Q^{-1}$ becomes more negative with greater values of $M$. In fact, the numerical results would seem to suggest a divergence of the first derivative of $Z_{kl}/Z$ with respect to $2\gamma Q^{-1}$ as it decreases from approximately $-3$ for $M=10^3$ to $-4$ for $M=10^4$. Unfortunately, it is very difficult to go on to higher values of $M$ because of rounding-off errors, that accumulate with $M$, yielding nonsensical results.

Nevertheless, there are analytical arguments which support the existence of a divergence in the first derivative of $Z_{kl}/Z$ at the critical point. In fact, let us write the quotient $Z_{kl}/Z$ in the following way

$$Z_{kl}/Z=\tfrac{1}{2}\langle\exp[-2\gamma Q^{-1}(q_{k+1,l}+q_{k-1,l}+q_{k,l+1}+q_{k,l-1})q_{kl}]\rangle \tag{4.7}$$

where the $\frac{1}{2}$ factor is introduced in order to eliminate the summation over the two possible values of $q_{k,l}=\pm1$, which was not in $Z_{kl}$. Expanding the exponential in (4.7), the ratio $Z_{kl}/Z$ may be expressed as a linear combination of two-point correlation functions, between nearest and next-nearest neighbours, and four-point correlation functions among the $(k,l)$-spin and its four nearest neighbours. As it is shown by McCoy and Wu (1973), the two-point correlation functions between nearest and next-nearest neighbours have an inflexion point with a logarithmically divergent slope at the critical point, which agrees with what our numerical computations suggest.

**Acknowledgments**

We are indebted to Professor A Sokal for many valuable comments. This work has received partial financial support from Comisión Asesora de Investigación Científica y Tecnológica, Spain.

**Appendix 1. Justification of (2.9) and (2.10*a*, *b*)**

The starting point is (2.7), where we set $E_1\simeq0$. We stress that we are searching for an approximate solution for it, to be used at a later stage (see § 2.1) in order to evaluate $N$ and, then, to get a more accurate (variational) expression for $E_1$. We set $q_{ij}=\varepsilon_{ij}+\sigma_{ij}$ for $(i,j)\neq(k,l)$, $\varepsilon_{ij}^2=+1$, where $|\sigma_{ij}|$ and $q_{kl}$ are assumed to be small compared to unity. Then, it is allowed to approximate $q_{ij}^3-q_{ij}\simeq2\sigma_{ij}$, $q_{kl}^3-q_{kl}^2\simeq-q_{kl}$ in (2.7), which becomes

$$-\frac{Q}{2}\left(\frac{\partial^2}{\partial q_{kl}^2}+\sum_{i,j=\langle k,l\rangle}\frac{\partial^2}{\partial\sigma_{ij}^2}\right)h_1+\left[(-\beta+4\gamma)q_{kl}-\gamma\left(\sum_{i,j=\langle k,l\rangle}(\varepsilon_{ij}+\sigma_{ij})\right)\right]$$

$$\times\frac{\partial h_1}{\partial q_{kl}}+\sum_{i,j=\langle k,l\rangle}[(2\beta+4\gamma)\sigma_{ij}-\gamma q_{kl}]\frac{\partial h_1}{\partial\sigma_{ij}}+B_1+B_2\simeq 0. \qquad \text{(A1.1)}$$

In (A1.1), $\Sigma_{i,j=\langle k,l\rangle}$ denotes a finite sum for $(i,j)=(k+1,l),(k-1,l),(k,l+1),(k,l-1)$ while $B_1$ contains all contributions to the right-hand side of (2.7) which depend on all $\sigma_{ij}$ (and derivatives thereof) for any $(i,j)\neq(k,l),(k\pm 1,l),(k,l\pm 1)$. On the other hand, $B_2$ is the remainder, namely, the sum of four terms: the first is

$$-\gamma(\varepsilon_{k+2,l}+\varepsilon_{k+1,l+1}+\varepsilon_{k+1,l-1}-4\varepsilon_{k+1,l}+\sigma_{k+2,l}+\sigma_{k+1,l+1}+\sigma_{k+1,l-1})\partial h_1/\partial\sigma_{k+1,l}$$

and so on for the other three.

At this point, we shall perform the following changes of variables

(i) $\sigma_{k+1,l}+\sigma_{k-1,l}=A_{kl}^{(1)}$, $\qquad \sigma_{k+1,l}-\sigma_{k-1,l}=a_{kl}^{(1)}$

$\sigma_{k,l+1}+\sigma_{k,l-1}=A_{kl}^{(2)}$, $\qquad \sigma_{k,l+1}-\sigma_{k,l-1}=a_{kl}^{(2)}$

(ii) $A_{kl}^{(1)}+A_{kl}^{(2)}=A_+$, $\qquad A_{kl}^{(1)}-A_{kl}^{(2)}=A_-$.

Then, (A1.1) becomes

$$-\frac{Q}{2}\left[\frac{\partial^2}{\partial q_{kl}^2}+4\left(\frac{\partial^2}{\partial A_+^2}+\frac{\partial^2}{\partial A_-^2}\right)\right]h_1+\left((-\beta+4\gamma)q_{kl}-\gamma\sum_{i,j=\langle k,l\rangle}\varepsilon_{ij}-\gamma A_+\right)\frac{\partial h_1}{\partial q_{kl}}$$

$$-4\gamma q_{kl}\frac{\partial h_1}{\partial A_+}+(2\beta+4\gamma)\left(A_+\frac{\partial}{\partial A_+}+A_-\frac{\partial}{\partial A_-}\right)h_1+B_1+B_2+B_3=0 \qquad \text{(A1.2)}$$

$$B_3=-Q\left(\frac{\partial^2}{\partial a_{kl}^{(1)2}}+\frac{\partial^2}{\partial a_{kl}^{(2)2}}\right)h_1+(2\beta+4\gamma)\left(a_{kl}^{(1)}\frac{\partial}{\partial a_{kl}^{(1)}}+a_{kl}^{(2)}\frac{\partial}{\partial a_{kl}^{(2)}}\right)h_1. \qquad \text{(A1.3)}$$

Equation (A1.2) is almost ready to arrive at the desired approximate results, since, for $\beta\gg\gamma$, the dependence of $h_1$ upon the variable $q_{kl}$ can be decoupled from that of the remaining ones. In fact, by performing the last change of variables

$$\begin{pmatrix} q_{kl}\\ A_+\end{pmatrix}\to\begin{pmatrix} q'_{kl}\\ A'_+\end{pmatrix}=\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix} q_{kl}\\ (A_+/2)\end{pmatrix} \qquad \text{(A1.4)}$$

one looks for the angle $\theta$ such that the coefficients of $q'_{kl}\,\partial h_1/\partial A'_+$ and $A'_+\partial h_1/\partial q'_{kl}$ vanish. One finds $\tan 2\theta=4\gamma/3\beta$, which is very small if $\beta\gg\gamma$. By keeping track of the dependence of $B_2$ upon $q_{kl}$ and carrying through the preceding changes of variables, one sees that it contains $\gamma\sin\theta\partial/\partial q'_{kl}$ and $\gamma\cos\theta\partial/\partial A'_+$ times sums of terms like $\sigma_{k\pm 2,l}$, $\sigma_{k,l\pm 2}$, $\sigma_{k\pm 1,l+1}$, $\sigma_{k\pm 1,l-1}$. No such contributions appear in either $B_1$ or $B_3$. Clearly, the term $\gamma\cos\theta\partial/\partial A'_+$ can be included into the terms which do not depend upon $q'_{kl}$, so that the only coupling between $q'_{kl}$ and the other variables comes from the term $\gamma\sin\theta\partial/\partial q'_{kl}$. Consequently, for $\beta\gg\gamma$, the factorised form

$$h_1=\tilde{h}(q'_{kl})\tilde{h}_1[\{\sigma_{ij}\},(i,j)\neq(k,l),(k\pm 1,l),(k,l\pm 1);a_{kl}^{(1)},a_{kl}^{(2)},A_-,A'_+] \qquad \text{(A1.5)}$$

is an approximate solution of (A1.2), when coupling terms between $\tilde{h}$ and $\tilde{h}_1$ of order $\gamma\sin\theta$ are neglected. Finally, by setting $\theta\simeq 0$, $q'_{kl}\simeq q_{kl}$ and $\tilde{h}_1=$ constant, one arrives directly at (2.9) and (2.10*a*, *b*).

## Appendix 2. On the uniqueness of (2.15) and of the configurations leading to it

One may ask whether other configurations corresponding to $n(\geqslant 2)$ 'spins' located at the sites $(k_1 l_1) \ldots (k_n l_n)$, all of which would be 'performing the tunnelling' between $+1$ and $-1$, could also contribute to $N$ (2.8). The additional requirement that those $n$ 'tunnelling spins' be suitably separated from one another seems a *sufficient* condition to ensure that the procedure outlined in appendix 1 (in particular, the decoupling of a 'tunnelling spin' from its neighbours) could be generalised to them. Consequently, an approximate solution of (2.7) with $E_1 \simeq 0$ for $n$ 'tunnelling spins' would be

$$h_1(\{q_{ij}\}) \simeq \left(\prod_{r=1}^{n} \tilde{h}(q_{k_r l_r})\right) \tilde{h}_1(\{q_{ij}\}, (i,j) \neq (k_1 l_1) \ldots (k_n l_n)) \tag{A2.1}$$

where $\tilde{h}_1(\{q_{ij}\}, (i,j) \neq (k_1 l_1) \ldots (k_n l_n))$ can be regarded as a constant and each $\tilde{h}(q_{k_r l_r})$ is given by (2.10$a$) (with $(k, l) \to (k_r, l_r)$), Consequently, a new variational calculation should be undertaken for $N$, using (A2.1) together with the obvious generalisation of (2.11) for $n$ 'tunnelling spins'.

Then, one sees immediately that $N$ is proportional to

$$\sum_{r=1}^{n} \int \left(\prod_{s=1}^{n} \mathrm{d}q_{k_s l_s}\right) \exp\left[\sum_{t=1}^{n} \left(\frac{\beta - 4\gamma}{Q}\right) q_{k_t l_t}^2 - \frac{2}{Q}(\beta - 2\gamma) q_{k_r l_r}^2 + (\gamma \text{ terms})\right] \tag{A2.2}$$

where ($\gamma$ terms) denotes a quadratic form of the $q$'s (which is independent of $\beta$), whose detailed form can be inferred easily from (2.10$a$) and (2.11) but turns out to be immaterial, here. In fact, for $\beta$ suitably larger than $\gamma$ and $n \geqslant 2$, one sees immediately that (A2.2) diverges. Consequently, configurations with $n(\geqslant 2)$ well separated 'tunnelling spins' cannot contribute to $E_1$.

It is unclear, *a priori*, whether the above argument could be applied directly when there is, at least, two 'tunnelling spins' which lie close to each other. Then, we shall analyse the extreme situation where *all* spins in the infinite planar lattice are performing the tunnelling. This amounts to assuming that $\beta(q_{ij}^3 - q_{ij}) \simeq -\beta q_{ij}$ for any $(i, j)$ in (2.3) and (2.1). Notice that, then, $f_0$ becomes unnormalisable $(\int \Pi_{i,j=-\infty}^{+\infty} \mathrm{d}q_{ij}] f_0 = +\infty)$ as $\beta$ is larger than $\gamma$. We shall find all eigenvalues of the corresponding Fokker-Planck equation under the above (crude) approximation and see that all of them diverge and, hence, turn out to be completely different from $E_1$, as given by (2.15). For that purpose, it is simpler to go over to an equivalent Hamiltonian formulation, through the transformation $f \to \varphi = f_0^{-1/2} f$ ($f_0$ being given through (2.1), (2.4) with $\alpha = -\beta$ and all $\beta q_{ij}^4/4$ terms omitted). One finds that $\varphi$ satisfies

$$H\varphi = -\partial\varphi/\partial t \tag{A2.3}$$

$$H = \sum_{r,s=-\infty}^{+\infty} \{\tfrac{1}{2}P_{rs}^2 + \tfrac{1}{2}Q^{-1}[-\beta q_{rs} - \gamma(q_{r+1,s} + q_{r-1,s} + q_{r,s+1} + q_{r,s-1} - 4q_{rs})]^2 - \tfrac{1}{2}(-\beta + 4\gamma)\} \tag{A2.4}$$

$$P_{rs} = -\mathrm{i}Q^{1/2}\partial/\partial q_{rs}. \tag{A2.5}$$

Our task reduces to diagonalising $H$. This can be done by a direct generalisation of the procedure discussed in § 3.1.1 of Itzykson and Zuber (1980). One introduces the creation and annihilation operators $a^+(\iota_1, \iota_2)$, $a(\iota_1, \iota_2)$ through

$$q_{rs} = \int_{-\pi}^{+\pi} \frac{\mathrm{d}\iota_1\, \mathrm{d}\iota_2}{(2\pi)} [a(\iota_1, \iota_2) \exp \mathrm{i}(\iota_1 r + \iota_2 s) + \text{HC}] \tag{A2.6}$$

$$P_{rs} = \mathrm{i}\int_{-\pi}^{+\pi} \frac{\mathrm{d}\iota_1\,\mathrm{d}\iota_2}{(2\pi)}[a(\iota_1, \iota_2)\exp \mathrm{i}(\iota_1 r + \iota_2 s) - \mathrm{HC}] \tag{A2.7}$$

$$[a(\iota_1, \iota_2), a^+(\iota_1', \iota_2')] = \delta(\iota_1 - \iota_1')\delta(\iota_2 - \iota_2') \tag{A2.8}$$

so that $H$ becomes

$$H = \int_{-\pi}^{+\pi} \mathrm{d}\iota_1\,\mathrm{d}\iota_2\,\omega(\iota_1, \iota_2)a^+(\iota_1, \iota_2)a(\iota_1, \iota_2) + H_0 \tag{A2.9}$$

$$H_0 = \tfrac{1}{2}\sum_{r,s=-\infty}^{+\infty}\left(\int_{-\pi}^{+\pi}\frac{\mathrm{d}\iota_1\,\mathrm{d}\iota_2}{(2\pi)^2}\,\omega(\iota_1, \iota_2) - (-\beta + 4\gamma)\right) \tag{A2.10}$$

$$\omega(\iota_1, \iota_2) = \beta - 2\gamma[(1 - \cos\iota_1) + (1 - \cos\iota_2)]. \tag{A.2.11}$$

Notice that $H_0$ is the overall 'zero-point energy'. Since

$$H_0 = \sum_{r,s=-\infty}^{+\infty}(\beta - 4\gamma) \tag{A2.12}$$

it follows that all eigenvalues of $H_0$ diverge, as they have $H_0$ as a lower bound. Consequently, none of them has the structure of $E_1$ (2.15)).

One could ask whether the first non-vanishing eigenvalue should not correspond to a long-wavelength excitation. In fact, for $\beta = 0$ and arbitrary $\alpha$, $\gamma$, (2.3) can be transformed by using $f = f_0^{+1/2}\phi$ into (A2.3) with

$$H = \sum_{rs}\{\tfrac{1}{2}P_{rs}^2 + \tfrac{1}{2}Q^{-1}[\alpha q_{rs} - \gamma(q_{r+1,s} + q_{r-1,s} + q_{r,s+1} + q_{r,s-1} - 4q_{r,s})]^2 - \tfrac{1}{2}(\alpha + 4\gamma)\}. \tag{A2.13}$$

By using the transformation (A2.6)-(A2.8), (A2.13) becomes (A2.9) with $H_0 = 0$ and $\omega = \alpha + 2\gamma[(1 - \cos\iota_1) + (1 - \cos\iota_2)]$.

For $\alpha = 0$ and small $\iota_1$, $\iota_2$, the smallest eigenvalue would correspond to the state formed by applying $a^+(\iota_1, \iota_2)$ upon 'the vacuum' and its value would be $\gamma(\iota_1^2 + \iota_2^2)$ which could indeed be interpreted as a long-wavelength excitation. However this is no longer true for large $\beta$, which is the case treated in this paper. In fact, let us consider small fluctations about the configurations where all oscillators are at $q_{ij} = +1$, that is $q_{ij} = 1 + \sigma_{ij}$, where all $\sigma_{ij}$ are small. By keeping leading-order terms, using $f = f_0^{1/2}\phi$ and (A2.6)-(A2.8) one arrives at (A2.3) and (A2.9) where now, $H_0 = 0$ and

$$\omega = 2[\beta + \gamma(1 - \cos\iota_1 + 1 - \cos\iota_2)] \tag{A2.14}$$

(compare with the remarks between (2.1) and (2.2)).

For small $\iota_1$, $\iota_2$ (A2.14) becomes

$$\omega \simeq 2|\beta + \tfrac{1}{2}\gamma(\iota_1^2 + \iota_2^2)|$$

which is much larger than (2.15) since $\beta$ is large.

As in the infinite linear chain of overdamped coupled anharmonic oscillators with noise, $E_1/[\beta\exp(-\frac{1}{2}\beta Q^{-1})]$ increases for small values of $\gamma$ and then it decreases as $\gamma$ becomes sufficiently large.

The region of small $\gamma$ is where the calculation is more reliable. The reliability of the calculation as $\gamma$ increases is limited by our previous neglect of terms, which was fully justified when $\gamma^2/\beta$ and, hence, $\gamma/\beta$ are small.

## Appendix 3. Numerical results for the ratio $Z_{kl}/Z$

| $K = 2\gamma Q^{-1}$ | $Z_{kl}/Z$ | $d(Z_{kl}/Z)/dK$ | $\exp(4\gamma Q^{-1})Z_{kl}/Z$ |
|---|---|---|---|
| 0.03 | 0.4993 | −0.038 | 0.5302 |
| 0.04 | 0.4988 | −0.053 | 0.5403 |
| 0.05 | 0.4981 | −0.068 | 0.5505 |
| 0.06 | 0.4973 | −0.083 | 0.5607 |
| 0.07 | 0.4963 | −0.099 | 0.5709 |
| 0.08 | 0.4951 | −0.115 | 0.5811 |
| 0.09 | 0.4938 | −0.131 | 0.5912 |
| 0.10 | 0.4924 | −0.147 | 0.6014 |
| 0.11 | 0.4907 | −0.163 | 0.6115 |
| 0.12 | 0.4889 | −0.180 | 0.6216 |
| ⋮ | ⋮ | ⋮ | ⋮ |
| 0.41 | 0.3271 | −1.200 | 0.7426 |
| 0.42 | 0.3137 | −1.339 | 0.7266 |
| 0.43 | 0.2982 | −1.549 | 0.7047 |
| 0.44 | 0.2778 | −2.044 | 0.6697 |
| 0.45 | 0.2554 | −2.237 | 0.6282 |
| 0.46 | 0.2399 | −1.552 | 0.6019 |
| 0.47 | 0.2268 | −1.312 | 0.5805 |
| 0.48 | 0.2152 | −1.158 | 0.5620 |
| 0.49 | 0.2047 | −1.045 | 0.5455 |
| 0.50 | 0.1952 | −0.095 | 0.5306 |
| ⋮ | ⋮ | ⋮ | ⋮ |
| 0.90 | 0.0422 | −0.016 | 0.2552 |
| 0.91 | 0.0407 | −0.015 | 0.2511 |
| 0.92 | 0.0392 | −0.014 | 0.2470 |
| 0.93 | 0.0378 | −0.014 | 0.2431 |
| 0.94 | 0.0365 | −0.013 | 0.2391 |
| 0.95 | 0.0352 | −0.013 | 0.2352 |
| 0.96 | 0.0339 | −0.013 | 0.2314 |
| 0.97 | 0.0327 | −0.102 | 0.2277 |
| 0.98 | 0.0315 | −0.012 | 0.2240 |
| 0.99 | 0.0304 | −0.011 | 0.2203 |

$M = 10\,000$.

## References

Alvarez-Estrada R F and Muñoz Sudupe A 1984 in *Applications of Field Theory to Statistical Mechanics. Lecture Notes in Physics* ed L Garrido (Berlin: Springer)
Bernstein M and Brown L S 1984 *Phys. Rev. Lett.* **52** 1933
Dawson D A 1983 *J. Stat. Phys.* **31** 29
Desai R C and Zwanzig R 1978 *J. Stat. Phys.* **19** 1
Glauber R J 1963 *J. Math. Phys.* **4** 2
Glimm J and Jaffe 1976 in *New Developments in QFT and Statistical Mechanics, Cargese* (New York: Plenum)
Haken H 1975 *Rev. Mod. Phys.* **47** 1
—— 1977 *Synergetics: an Introduction* (Berlin: Springer)
Huang K 1963 *Statistical Mechanics* (New York: Wiley)
Itzykson C and Zuber J B 1980 *Quantum Field Theory* (New York: McGraw-Hill)
Larson R S and Kostin M D 1978 *J. Chem. Phys.* **69** 4821
McCoy B M and Wu T T 1973 *The Two-Dimensional Ising Model* (Cambridge, Mass.: Harvard University Press)

Muñoz Sudupe A and Alvarez-Estrada R F 1983 *J. Phys. A: Math. Gen.* **16** 3049
Schultz T D, Mattis D C and Lieb E H 1964 *Rev. Mod. Phys.* **36** 856
Weindenmuller H A and Jing-Shang Z 1984 *J. Stat. Phys.* **34** 191
Wolfram S 1983 *Rev. Mod. Phys.* **55** 3
Zinn-Justin J 1984 in *Recent Advances in Field Theory and Statistical Mechanics, Les Houches,* 1982 *session XXXIX* ed J B Zuber and R Stora (Amsterdam: North-Holland)