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TOPICAL REVIEW

The absence of finite-temperature phase transitions in low-dimensional many-body models: a survey and new results

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Abstract
After a brief discussion of the Bogoliubov inequality and possible generalizations thereof, we present a complete review of results concerning the Mermin–Wagner theorem for various many-body systems, geometries and order parameters. We extend the method to cover magnetic phase transitions in the periodic Anderson model as well as certain superconducting pairing mechanisms for Hubbard films. The relevance of the Mermin–Wagner theorem to approximations in many-body physics is discussed on a conceptual level.

1. Introduction

The quest for criteria for the existence, or absence, of phase transitions in physical systems has been a dominant theme in theoretical physics ever since the phenomenological concept of a *phase* was introduced in the context of equilibrium thermodynamics which is associated with the names of Boltzmann, Gibbs, Ehrenfest and many others. The pioneering work in the phenomenological theory of phase transitions was soon supplemented by attempts to provide a detailed theoretical description of macroscopic phenomena via microscopic many-body theories. The Lenz–Ising model (1925) was the first such model, and Onsager's solution of the 2D Ising model (1944) is evidence that, by then, the mathematical physics of phase transitions had become a subject in its own right. Other landmark developments of the 1950s and 1960s were the famous Yang and Lee papers (1952) providing a mathematically rigorous scenario of how phase transitions can occur in the thermodynamic limit, and the papers by Hohenberg (1967) and Mermin and Wagner (1966) excluding certain phase transition in low-dimensional systems.

It is the latter result, generally known as the Mermin–Wagner theorem, which we shall discuss in this article. In doing so, our goal is threefold. First, we discuss applications, and possible generalizations, of the Bogoliubov inequality, which underlies the proof of the

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Mermin–Wagner theorem. Then we present a survey of existing proofs of the absence of finite-temperature phase transitions in low-dimensional systems along with recent generalizations. Finally, by means of a simple example, we discuss the relevance and validity of the Mermin–Wagner theorem in approximate theories designed to describe a magnetic phase transition.

2. Mathematical tools

The occurrence of a phase transition is often intimately related to the failure of one of the phases to exhibit a certain symmetry property of the underlying Hamiltonians. Crystals, for example, by their very lattice structure, break the translational symmetry encountered in the continuum description of fluids; ferromagnets, in addition to the spatial symmetry breaking due to their crystal structure, are not invariant under rotations in spin space, even though the underlying Hamiltonians describing the system may well be. Less obvious types of symmetry breaking occur in other quantum systems, such as superfluids and superconductors, where a breaking of gauge invariance occurs.

2.1. Bogoliubov quasi-averages

Bogoliubov has devised a method for describing the occurrence of spontaneous symmetry breaking in terms of *quasi-averages* [1, 2]. Normally, for systems in statistical equilibrium, the expectation value of an operator A is given by the trace over the equilibrium *density* (or *statistical) operator* $\rho = \exp(-\beta\mathcal{H})$ times the observable A. Thus, for the infinite system ($V \to \infty$) one must calculate

$$\langle A\rangle \equiv \lim_{V\to\infty} \operatorname{tr}(\rho A) = \lim_{V\to\infty} \operatorname{tr}(\mathrm{e}^{-\beta\mathcal{H}} A) \tag{1}$$

where $\mathcal{H}$ is the grand-canonical Hamiltonian, $\mathcal{H} = H - \mu\hat{N}$ ($\hat{N}$: number operator). However, it turns out that under certain conditions such averages may be unstable with respect to an infinitesimal perturbation of the Hamiltonian. If a corresponding additive contribution $H_\nu \equiv \nu H'$ of the order of ν is added (where ν is a small positive number which will eventually be taken to zero: $\nu \to 0$), i.e.,

$$\mathcal{H}_\nu = H + H_\nu - \mu\hat{N} \tag{2}$$

one can define the *quasi-average* of A in the following way:

$$\langle A\rangle_q \equiv \lim_{\nu\to 0}\lim_{V\to\infty} \operatorname{tr}(\mathrm{e}^{-\beta\mathcal{H}_\nu} A). \tag{3}$$

The average (1) and the quasi-average (3) need not coincide, since the two limits in (3) may fail to commute within some parameter region (i.e. for some combination of μ and β).

Quasi-averages are appropriate for cases in which spontaneous symmetry breaking occurs, as can be shown by a simple argument. Suppose the Hamiltonian $\mathcal{H}$ displays a continuous symmetry $\mathcal{S}$, i.e. it commutes with the generators $\Gamma^i_{\mathcal{S}}$ of the corresponding symmetry group,

$$[\mathcal{H}, \Gamma^i_{\mathcal{S}}]_- = 0. \tag{4}$$

If some operator B is not invariant under the transformations of $\mathcal{S}$,

$$[B, \Gamma^i_{\mathcal{S}}]_- \equiv C^i \neq 0 \tag{5}$$

the (normal) average of the commutator C^i vanishes:

$$\langle C^i\rangle = 0 \tag{6}$$

as can be readily seen from equation (1) by use of cyclic invariance of the trace. In those instances, however, where the perturbative part H_ν of (2) does not commute with Γ^i_S, this will give a *non-vanishing quasi-average*:

$$\langle C^i \rangle_q = \lim_{\nu \to 0} \mathrm{tr}(\mathrm{e}^{-\beta \mathcal{H}_\nu} [B, \Gamma^i_S]_-) \neq 0. \tag{7}$$

Thus, even though one might naïvely expect the quasi-average to coincide with the 'normal' average in the limit $\nu \to 0$, quite generally this will not be the case. Note that the quasi-average depends on the nature of the perturbation added to the 'original' Hamiltonian.

As a first example, let us examine the Heisenberg model

$$H = -\sum_{ij} J_{ij} (\vec{S}_i \cdot \vec{S}_j) \tag{8}$$

which is invariant under the continuous rotation group generated by the total spin vector $\vec{S} = \sum_i \vec{S}_i$ because $[H, \vec{S}]_- = 0$. Thus, we can take $\vec{S}$ as the operator B, and from (6) one finds $\langle [S^\alpha, S^\beta]_- \rangle = 0$, where S^α, S^β are the components of the total spin vector $\vec{S}$. Considering this together with the commutation relations for spin operators, e.g. $[S^x, S^y]_- = \mathrm{i}\hbar S^z$, it is obvious that the conventional average of the magnetization vanishes. This is just a manifestation of the fact that on the macroscopic level, for an ideal, infinitely extended system, there is no preferred direction in space. One can think of this situation as a 'degeneracy' with respect to spatial orientation. Adding an external field, $\vec{B}_0 = B_0 \vec{e}_z$ along the z-axis for example, lifts this degeneracy and via the contribution $H_b \sim B_0 M(T, B_0)$ to the Hamiltonian (M: magnetization) one can, thus, construct appropriate quasi-averages for arbitrary operators according to equation (3).

2.2. *Order parameters*

In the theory of phase transitions, the first step is to identify a quantity whose (quasi-)average vanishes on one side of the transition, but takes on a finite value on the other side. This quantity is called the *order parameter*. In a continuous phase transition, the order parameter may gradually evolve from zero at the critical point to a finite value on one side (usually the low-temperature side) of the transition. For different kinds of phase, different order parameters must be chosen. From a phenomenological point of view, one must consider each physical system anew. We have already mentioned the liquid–vapour and the ferromagnetic–paramagnetic transition as prototypes for phase transitions. In the former, the obvious choice for the order parameter would be the difference between the mean densities, i.e. $\rho - \rho_{\mathrm{vapour}}$; in the latter the relevant order parameter is the magnetization M. Within a given many-body model, the magnetization can be defined in microscopic terms, as we shall see shortly.

Sometimes, as in the transition to the superconducting state, it may even be possible to characterize the *same* type of phase transition by use of different order parameters. According to the standard theories of superconductivity, at low temperatures electrons with opposite spins form Cooper pairs. Thus, a possible order parameter would be the average probability amplitude for finding a Cooper pair at a given lattice site in the crystal. Alternatively, one could characterize the phase transition through the gap parameter whose modulus is the difference in energy per electron of the Cooper pair condensate and the energy at the Fermi level. We shall briefly return to the problem of superconductivity when we consider the possibility of pairing at finite temperatures in film systems.

2.3. Bogoliubov inequality

The Bogoliubov inequality is a rigorous relation between two essentially arbitrary operators A and B and a valid Hamiltonian H of a physical system. In its original form, proposed in [1], it is given by

$$|\langle[C, A]_-\rangle|^2 \leqslant \frac{\beta}{2}\langle[A, A^\dagger]_+\rangle\langle[C^\dagger, [H, C]_-]_-\rangle \tag{9}$$

where $\beta = 1/k_B T$ is the inverse temperature and $\langle\cdots\rangle$ denotes the thermodynamic expectation value. A and B do not necessarily have an obvious physical interpretation from the very beginning, so the physical significance of (9) will depend on the suitable choice for the operators involved. The inequality can be proved by introducing a scalar product which is based on the energy eigenvalues E_n and the orthogonality of the corresponding energy eigenstates $|n\rangle$ of the Hamiltonian H and to which one then applies the Schwarz inequality. The details of the proof are readily accessible elsewhere (see e.g. the textbook [3]); however, we briefly note that as a result of this derivation, the two factors on the RHS of (9) each are *upper bounds to a norm* and can, thus, be bounded from below by zero. In particular, if, for example, the double commutator depends on some parameter k, one will always find

$$\langle[[C, H]_-, C^\dagger]_-\rangle(k) + \langle[[C, H]_-, C^\dagger]_-\rangle(k') \geqslant \langle[[C, H]_-, C^\dagger]_-\rangle(k). \tag{10}$$

Dividing both sides of (9) by the double commutator and summing over all wave vectors $\vec{k}$ associated with the first Brillouin zone in the reciprocal lattice, one arrives at

$$\sum_{\vec{k}} \frac{|\langle[C, A]_-\rangle|^2}{\langle[[C, H]_-, C^\dagger]_-\rangle(\vec{k})} \leqslant \frac{\beta}{2}\sum_{\vec{k}}\langle[A, A^\dagger]_+\rangle(\vec{k}). \tag{11}$$

2.4. Generalized Bogoliubov-type inequalities

The use of inequalities in the theory of phase transitions has developed into a subdiscipline of its own right within the field of mathematical physics [4, 5]; consequently, this article is not intended to give a complete account of such approaches. The close kinship between some of these methods and the Bogoliubov inequality, however, justifies a brief discussion of what one might call *generalized Bogoliubov-type inequalities.* The common feature of these inequalities is the fact that certain algebraic properties of the quantities involved allow one to use the Cauchy–Schwarz inequality, thus leading to upper, or lower, bounds for physical observables, such as the dynamical structure factor

$$\begin{aligned} C_{BA}(\vec{k}', \vec{k}; E') &= \int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}E't/\hbar} \sum_n \frac{\mathrm{e}^{-\beta E_n}}{N\Xi}\langle n|\mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar} B(\vec{k}', 0)\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar} A(\vec{k}, 0)|n\rangle \\ &= 2\pi\hbar \sum_{mn} \frac{\mathrm{e}^{-\beta E_n}}{N\Xi}\langle m|A(\vec{k}, 0)|n\rangle\langle n|B(\vec{k}', 0)|m\rangle\delta(E' - (E_m - E_n)) \end{aligned} \tag{12}$$

(where the sum runs over all energy eigenstates $|n\rangle$, $|m\rangle$ corresponding to eigenvalues E_n, E_m), or the susceptibility

$$\chi_{AB}(\vec{k}, \vec{k}'; E, \mathrm{i}\eta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}E'\ \frac{(1 - \mathrm{e}^{-\beta E'})C_{BA}(E')}{E - E' + \mathrm{i}\eta}.$$

Wagner [6] discusses the static susceptibility χ_{AB}, defined as

$$\chi_{AB}(\vec{k}, \vec{k}') = \Re\left(\lim_{E,\eta\to 0} \chi_{AB}(\vec{k}, \vec{k}'; E, \mathrm{i}\eta)\right) = \mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}E'\ \frac{S_{AB}(\vec{k}, \vec{k}'; E')}{E'} \tag{13}$$

in terms of the spectral density which, in its spectral representation, is given by

$$S_{AB}(\vec{k},\vec{k}';E') = \frac{\hbar}{\Xi}\sum_{nm}\langle n|A(\vec{k},0)|m\rangle\langle m|B(\vec{k}',0)|n\rangle e^{-\beta E_m}(e^{\beta E'}-1)\delta(E'-(E_m-E_n)). \tag{14}$$

It can then be shown [6, 49] that

$$\langle A(\vec{k}); B(\vec{k}')\rangle := \chi_{AB}(\vec{k},\vec{k}') \tag{15}$$

is a valid scalar product in the space of operators A, B. The Schwarz inequality for the static susceptibility then reads

$$|\chi_{AB}(\vec{k},\vec{k}')|^2 \leqslant \chi_{AA^\dagger}(\vec{k})\chi_{B^\dagger B}(\vec{k}'). \tag{16}$$

Physically significant relations can be deduced from this general statement by an appropriate choice of operators A and B. If A is taken to be a time derivative of another operator [6], i.e.,

$$A_{\vec{k}}(t) := i\hbar\frac{\partial}{\partial t}Q_{\vec{k}}(t) \tag{17}$$

the inequality

$$\mathcal{P}\int_{-\infty}^{\infty} dE\,\frac{S_{B^\dagger B}(\vec{k};E)}{E} \geqslant \frac{|\langle[Q_{\vec{k}},B_{\vec{k}'}]_-\rangle|^2}{\langle[[Q_{\vec{k}},H]_-,Q_{\vec{k}}^\dagger]_-\rangle} \tag{18}$$

follows, which relates the response function for the observable B to commutators that can, in principle, be calculated directly from one's knowledge of Q, B and H. If for a given many-body Hamiltonian H one specifies Q and B further, it is possible to obtain bounds for non-trivial order parameters. Thus, for the planar magnetization M_p defined as

$$M_p(T,\tilde{B}_0) := \frac{1}{N}\sum_i\langle\alpha_i\sigma_i^y + \beta_i\sigma_i^x\rangle \tag{19}$$

(where i runs over all lattice sites, σ_i^x and σ_i^y denote the respective components of the spin and the real constants α_i and β_i can be chosen so as to take into account various kinds of spin ordering within the xy-plane), evaluating (18) with operators Q and B given by

$$Q_{\vec{k}} = \sum_j e^{-i\vec{k}\cdot\vec{R}_j}(\beta_j\sigma_j^y - \alpha_j\sigma_j^x)$$

and

$$B_{\vec{k}} = \sum_j e^{-i\vec{k}\cdot\vec{R}_j}\sigma_j^z = \sigma^z(\vec{k})$$

gives an upper bound for M_p in terms of the longitudinal susceptibility $\chi^{zz}(\vec{k})$. Since for the latter, rigorous limits and estimates have been established, e.g. for the attractive Hubbard model [7], these carry over to the order parameter M_p.

Before turning to exact results concerning finite-temperature phase transitions, let us discuss how correlation inequalities can be put to use in the zero-temperature case. Pitaevskii and Stringari [8] have suggested defining a scalar product simply through the anticommutator:

$$\langle A; B\rangle := \langle[A^\dagger, B]_+\rangle \tag{20}$$

which gives the Schwarz inequality

$$\langle[A^\dagger, A]_+\rangle\langle[B^\dagger, B]_+\rangle \geqslant |\langle[A^\dagger, B]_+\rangle|^2. \tag{21}$$

It is then possible to define auxiliary operators, denoted by a tilde, such that

$$\begin{aligned}\langle n|\tilde{C}|0\rangle &:= \langle n|C|0\rangle \\ \langle 0|\tilde{C}|n\rangle &:= -\langle 0|C|n\rangle\end{aligned} \tag{22}$$

from which it follows that

$$\begin{aligned}\langle n|\tilde{C}^\dagger|0\rangle &= -\langle n|C^\dagger|0\rangle \\ \langle 0|\tilde{C}^\dagger|n\rangle &= \langle 0|C^\dagger|n\rangle.\end{aligned} \tag{23}$$

At $T = 0$ the expectation values in (21) are evaluated in the ground state $|0\rangle$, and if instead of B the newly defined operator $\tilde{B}$ is used, one deduces from

$$\begin{aligned}\langle 0|[A^\dagger, \tilde{B}]_+|0\rangle &= \langle 0|[A^\dagger, B]_-|0\rangle \\ \langle 0|[\tilde{B}^\dagger, \tilde{B}]_+|0\rangle &= \langle 0|[B^\dagger, B]_+|0\rangle\end{aligned} \tag{24}$$

that the Schwarz inequality holds not only for the anticommutator on the RHS but also for the commutator, so (writing down (21) for the operators A, $\tilde{B}$, and making use of (24) to express $\tilde{B}$ in terms of B) one finds

$$\langle [A^\dagger, A]_+\rangle\langle [B^\dagger, B]_+\rangle \geqslant |\langle [A^\dagger, B]_-\rangle|^2. \tag{25}$$

With this in mind, one can turn to the dynamical structure factor, which for the transverse spin–spin correlation function at $T = 0$ is given by

$$\begin{aligned}C^{+-}(\vec{q}, E)\big|_{T=0} &\equiv \frac{1}{N}\int_{-\infty}^{\infty} \mathrm{d}t\; \mathrm{e}^{\mathrm{i}Et/\hbar}\langle \sigma^+(\vec{q}, t)\sigma^-(-\vec{q}, 0)\rangle\big|_{T=0} \\ &= \frac{1}{N}\int_{-\infty}^{\infty} \mathrm{d}t\; \mathrm{e}^{\mathrm{i}Et/\hbar}\sum_m \langle 0|\mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar}\sigma^+(\vec{q}, 0)\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}|m\rangle\langle m|\sigma^-(-\vec{q}, 0)|0\rangle \\ &= \frac{2\pi\hbar}{N}\sum_m \delta(E - (E_m - E_0))|\langle 0|\sigma^+(\vec{q}, 0)|m\rangle|^2.\end{aligned} \tag{26}$$

Since E_0 is the ground-state energy, we have $E_m \geqslant E_0$, so the δ-function only gives a contribution if $E \geqslant 0$. As a corollary

$$EC^{+-}(\vec{q}, E)\begin{cases}\geqslant 0 & \text{if } E > 0 \\ = 0 & \text{if } E \leqslant 0.\end{cases} \tag{27}$$

If one defines

$$C_\perp(\vec{q}, E) = \frac{1}{2}(C^{+-}(\vec{q}, E) + C^{-+}(-\vec{q}, E)) = \frac{1}{2}\langle [\sigma^+(\vec{q}, E), \sigma^-(-\vec{q}, E)]_+\rangle \tag{28}$$

and

$$C_\perp(\vec{q}) = \int \mathrm{d}E\; C_\perp(\vec{q}, E) \tag{29}$$

one can make use of (25) for operators $\sigma^+(\vec{q} + \vec{Q})$, $\sigma^-(-\vec{q})$ to get

$$C_\perp(\vec{q} + \vec{Q})C_\perp(\vec{q}) \geqslant |M(\vec{Q})|^2 \tag{30}$$

where the magnetization

$$M(\vec{Q}) = \frac{2\hbar}{N}\left\langle \sum_i \sigma_i^z \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{R}_i}\right\rangle \tag{31}$$

has been introduced (the reciprocal-lattice vector $\vec{Q}$ as usual accounts for possible antiferromagnetic order). Equation (27) tells us that $C_\perp(\vec{q}, E)$ is non-vanishing only for $E > 0$, where it is positive, so the integral quantity $C_\perp(\vec{q})$ may be formally written as

$$C_\perp(\vec{q}) = \int \mathrm{d}E\ \sqrt{EC_\perp(\vec{q}, E)}\sqrt{\frac{C_\perp(\vec{q}, E)}{E}}. \tag{32}$$

In this form, one can apply *Hölder's inequality* which states that for real-valued function f and g for which $|f(x)|^p$ and $|g(x)|^q$ are integrable (where p and q are numbers satisfying the relations $p^{-1} + q^{-1} = 1$ and $p > 1$) the following inequality holds:

$$\int_a^b \mathrm{d}x\ f(x)g(x) \leqslant \left(\int_a^b \mathrm{d}x\ |f(x)|^p\right)^{1/p}\left(\int_a^b \mathrm{d}x\ |g(x)|^q\right)^{1/q}. \tag{33}$$

For $p = q = 2$ and with f, g defined as

$$\begin{aligned} f(x) &= \sqrt{EC_\perp(\vec{q}, E)} \\ g(x) &= \sqrt{\frac{C_\perp(\vec{q}, E)}{E}} \end{aligned} \tag{34}$$

Hölder's inequality (33) applied to (32) gives

$$C_\perp(\vec{q}) \leqslant \sqrt{\int \mathrm{d}E\ EC_\perp(\vec{q}, E)}\sqrt{\int \mathrm{d}E\ \frac{C_\perp(\vec{q}, E)}{E}}. \tag{35}$$

The first of the integrals can in many cases be bounded from above by

$$\int \mathrm{d}E\ EC_\perp(\vec{q}, E) = \langle[\sigma^+(\vec{q}, E), [\mathcal{H}, \sigma^-(-\vec{q}, E)]_-]_-\rangle \equiv f(\vec{q})Nq^2 \leqslant \text{constant} \times Nq^2 \tag{36}$$

which suggests writing

$$\left(\int \mathrm{d}E\ EC_\perp(\vec{q}, E)\right)\Big/\left(\int \mathrm{d}E\ \frac{C_\perp(\vec{q}, E)}{E}\right) \equiv \omega^2(\vec{q})q^2 \tag{37}$$

thus defining the new quantity $\omega(\vec{q})$. Inequality (30) can be strengthened using (35) and rearranged by use of (37) to give

$$C_\perp(\vec{q} + \vec{Q}) \geqslant \frac{|M(\vec{Q})|^2}{\omega(\vec{q})q\chi^{+-}(\vec{q})}. \tag{38}$$

This equation relates the order parameter M, the transverse susceptibility χ^{+-} and the structure factor C^{+-} (via $C_\perp$). The relation between these quantities can be made even more pronounced by summing both sides of (38) over the first Brillouin zone. One can then go on to show that in the thermodynamic limit a relation of the form

$$\xi_0 \geqslant \frac{v^{(d)}}{(2\pi)^d}\int_{1.\mathrm{B.Z.}} \mathrm{d}^d\vec{q}\ \frac{1}{q}\frac{|M(\vec{Q})|^2}{\omega(\vec{q})\chi^{+-}(\vec{q})} \tag{39}$$

holds (where ξ_0 turns out to be a model-dependent constant). Provided that $\omega(\vec{q})$ and $\chi^{+-}(\vec{q})$ remain finite in the limit $q \to 0$, this means that in 1D not even at zero temperature can there be a transition to a state with non-vanishing $M(\vec{Q})$, as this would lead to a logarithmic divergence of the RHS and thus would contradict ξ_0 being a constant.

It seems to us that the range of applications of correlation inequalities has not yet been fully exhausted. Using the mathematical tools discussed in the previous paragraphs, and variations thereof, should serve as a starting point for the derivation of similar relations for other order parameters and many-body models.

3. The Mermin–Wagner theorem: a survey

Having established the wide range of relationships the Bogoliubov, and related, inequalities can generate, we shall now turn to a narrower range of applications, namely results concerning the absence of finite-temperature phase transitions in low-dimensional systems.

Hohenberg [9] was the first to note that the Bogoliubov inequality could be used to exclude phase transitions, showing that there could be no finite-temperature phase transition in one- and two-dimensional superfluid systems. At roughly the same time Mermin and Wagner, following a suggestion by Hohenberg, considered the case of spontaneous magnetization in the Heisenberg model [10]. Since Mermin and Wagner's proof has become the exemplar for studies concerning the absence of phase transitions, we shall briefly outline the paradigmatic procedure (see also [11]). The general idea is to use the Bogoliubov inequality (11) to find an upper bound $f(B_0, M)$ for the order parameter in question, e.g. the spontaneous magnetization M:

$$M \leqslant f(B_0, M). \tag{40}$$

As indicated, the upper bound will normally depend on the external (e.g. magnetic) field that couples to the order parameter, and (implicitly) on the order parameter itself. To answer the question of whether or not a phase transition to a state with a non-zero value of the order parameter occurs, one must consider the case $B_0 \to 0$, i.e. the behaviour of the upper bound in the case of vanishing external field. The subsequent argument against a phase transition proceeds by *reductio ad absurdum*: if the assumption $M \neq 0$ can be shown to lead to a violation of (40) in the limit $B_0 \to 0$, where equation (40) is derived from the Bogoliubov equation (which is known to hold for the corresponding many-body system), it must be dropped. This, then, leaves as the only conclusion that $M \underset{B_0\to 0}{\longrightarrow} 0$, the case of vanishing order parameter and no phase transition. This argument, of course, only succeeds if the initial inequality is indeed true '*a priori*', and the most straightforward way to achieve this is to resort to the Bogoliubov inequality. From this it follows that, once one has specified a many-body model by its Hamiltonian H, the operators A and C in the Bogoliubov inequality must be carefully chosen so as to give the desired order parameter.

As an example, consider the Heisenberg model

$$H_{(Hei)} = -\sum_{ij=1,\ldots,N} J_{ij}(S_i^+ S_j^- + S_i^z S_j^z) - b \sum_{i=1,\ldots,N} \mathrm{e}^{-\mathrm{i}\vec{K}\cdot\vec{R}_i} S_i^z \tag{41}$$

(where the term $b\sum_i \mathrm{e}^{-\mathrm{i}\vec{K}\cdot\vec{R}_i} S_i^z$ is due to the interaction with an external magnetic field $b = g_J \mu_B B_0/\hbar$). The relevant order parameter is the magnetization

$$M = \frac{1}{N}\frac{g_J \mu_B}{\hbar} \sum_i \mathrm{e}^{-\mathrm{i}\vec{K}\cdot\vec{R}_i} \langle S_i^z \rangle \tag{42}$$

where the factor $\mathrm{e}^{-\mathrm{i}\vec{K}\cdot\vec{R}_i}$ already accounts for antiferromagnetic order by changing the sign of the spins in one sublattice (given that $\vec{K}$ has been properly chosen to achieve just that). This suggests that an upper bound for $\langle S^z \rangle$ is essential. Comparison with (11) suggests the choice

$$A = S^-(-\vec{k} - \vec{K}) \tag{43}$$

$$C = S^+(\vec{k}) \tag{44}$$

as, by virtue of the commutation relations,

$$[S^+(\vec{k}_1), S^-(\vec{k}_2)]_- = 2\hbar S^z_\alpha(\vec{k}_1 + \vec{k}_2) \tag{45}$$

this will indeed give a contribution proportional to the magnetization on the left-hand side of the Bogoliubov inequality:

$$\langle [C, A]_- \rangle = \xi_1 N M(T, B_0). \tag{46}$$

($\xi_{(i)}$ denote constants depending, at most, on fixed parameters of the many-body model, i.e. in this case the Heisenberg exchange integrals.) The other (anti-)commutators that feature in the Bogoliubov inequality can be bounded from above, as has been shown by Mermin and Wagner:

$$\langle [[C, H]_-, C^\dagger]_- \rangle \leqslant \xi_2^2 N(|B_0 M(T, B_0)| + \xi_3 \vec{k}^2) \tag{47}$$

$$\sum_{\vec{k}} \langle [A, A^\dagger]_+ \rangle \leqslant 2\xi_4 N^2. \tag{48}$$

For the Bogoliubov inequality,

$$\sum_{\vec{k}} \frac{|\langle [C, A]_- \rangle|^2}{\langle [[C, H]_-, C^\dagger]_- \rangle} \leqslant \frac{\beta}{2} \sum_{\vec{k}} \langle [A, A^\dagger]_+ \rangle \tag{49}$$

one finds in this case

$$\sum_{\vec{k}} \frac{\xi_1^2 N^2 M^2(T, B_0)}{\xi_2^2 N(|B_0 M(T, B_0)| + \xi_3 \vec{k}^2)} \leqslant \xi_4 \beta N^2.$$

In the thermodynamic limit, the only situation where one can at all hope for a phase transition, the sum is to be replaced by an integral, e.g. for the two-dimensional case

$$\sum_{\vec{k}} \hat{=} \frac{L^2}{(2\pi)^2} \int_{\vec{k}} \mathrm{d}^2\vec{k} \tag{50}$$

where $L^2/(2\pi)^2$ is the area in k-space associated with one quantum state. Restricting the support of the integral to a finite-volume sphere inscribed into the first Brillouin zone only strengthens the inequality, so

$$\left(\frac{\xi_1}{\xi_2}\right)^2 \frac{1}{2\pi} \frac{L^2}{N} M^2(T, B_0) \int_0^{k_0} \mathrm{d}k \, \frac{k}{|B_0 M(T, B_0)| + \xi_3 k^2} \leqslant \xi_4 \beta \tag{51}$$

where k_0 is the cut-off corresponding to the sphere in k-space. In the thermodynamic limit under consideration, L and N approach infinity in such a way that the specific volume $v_0^{(2)} = L^2/N$ remains finite throughout. Evaluating the integral, one then arrives at

$$M^2(T, B_0) \leqslant \xi \frac{\beta}{\ln(1 + \xi_3 k_0^2/|B_0 M(T, B_0)|)}. \tag{52}$$

As $B_0 \to 0$, the denominator diverges logarithmically, thus forcing the magnetization to vanish. This result is independent of the original choice of the auxiliary wave vector $\vec{K}$ (see (42)), so ferromagnetic and antiferromagnetic order are both ruled out in the two-dimensional Heisenberg model. One easily verifies that a similar divergence of the denominator rules out spontaneous magnetic order in the one-dimensional case.

The main steps in any proof of the Mermin–Wagner type are:

(a) choice of a many-body model characterized by its Hamiltonian H;
(b) identification of the order parameter for the phase transition to be discussed;
(c) adequate choice of operators A and B in the Bogoliubov inequality so as to single out the order parameter;
(d) search for non-trivial upper bounds for the (anti-)commutators in the Bogoliubov inequality;

(e) proof that in the thermodynamic limit the assumption of a spontaneous non-zero value for the order parameter will be self-refuting in the one- or two-dimensional cases (and, possibly, other cases as well).

This basic scheme has been applied to a wide range of different models and order parameters. The remainder of this section attempts to present a survey of established as well as new results, along with brief discussions and related references.

Shortly after the papers by Hohenberg [9] and Mermin and Wagner [10] appeared, Mermin showed that a classical Bogoliubov-type inequality holds if in equation (9) one replaces the commutators by Poisson brackets and also requires certain quantities in the corresponding classical thermal averages to vanish. For short-range interactions, one can then rule out phase transitions for the 'classical', i.e. infinite-spin limit [12].

Walker used the Bogoliubov inequality to rule out the possibility of a phase transition, in one and two dimensions, to an excitonic insulating state [13]. The main idea behind the formation of the insulating state involved the assumption that certain conditions might favour bound electron–hole pairs forming if a semiconductor with a very small gap, or a semimetal with a very small band overlap, was to be cooled to a sufficiently low temperature. The proof that such a state is impossible in the low-dimensional case is straightforward for electrons interacting via a potential which falls off faster than $|\vec{r}|^{-D}$ (D: number of dimensions); it can be generalized to cover certain simplified Hamiltonians with weaker convergence behaviour. A generalization to an isotropic two-band model can also be given [13].

The Bogoliubov inequality, together with an analogous classical inequality, also rules out the possibility of crystalline ordering in two dimensions, thus confirming earlier suggestions by Peierls and Landau that there could be no two-dimensional crystalline ordered state [14]. This is significant, since the extension to crystalline ordering is not quite straightforward: contrary to the case for types of ordering where the energies of fluctuations that cause the disorder are kinetic (e.g. superfluid, superconducting or excitonic interactions), the relevant energy in the crystalline case is potential. Also, one cannot simply posit that one particle only interacts with a finite number of neighbours (as one can in the case of spin systems; see the next section), because a given particle may well diffuse through the crystal and interact with many, and possibly all, others. The proof can nevertheless be achieved by assuming a system of identical particles with pair potential $\Phi(\vec{r})$, where Φ as well as the related function

$$\Psi(\vec{r}) = \Phi(\vec{r}) - \lambda|\vec{r}|^2|\Delta\Phi(\vec{r})| \tag{53}$$

are required to satisfy the criteria for the existence of a proper thermodynamic limit for a sufficiently small positive value of λ [15]. While this includes Lennard-Jones-type potentials, it does not cover hard-core potentials.

The corresponding result for the quantum case, only sketched in [14] in an appendix, has been reproduced in detail by Fernández [16]. The paper discusses an electrically neutral system of nuclei and electrons which is confined to one or two finite dimension(s) with the remaining two or one dimension(s) being infinite. The paradigmatic examples for such geometrically restricted systems are the infinite slab and the rod with rectangular cross section and infinite length (see section 3.2 below for further examples of this kind). One then proceeds to show that for systems of this kind, no *maximum* long-range crystalline order can exist, or, formally:

$$\langle\Psi_{\vec{K}}\rangle = 0 \qquad \text{for any } \vec{K} \neq 0 \tag{54}$$

where

$$\langle\Psi_{\vec{K}}\rangle = \lim_{N\to\infty} \langle\rho_{\vec{K}}\rangle \big/ N \tag{55}$$

with

$$\rho_{\vec{K}} = \int \mathrm{d}\vec{r}\ \rho(\vec{r}) \exp(-\mathrm{i}\vec{K} \cdot \vec{r}) \tag{56}$$

and $\rho(\vec{r})$ is the number-density operator, and the limit is taken with N/V being held constant (V: volume of the system).

Kishore and Sherrington [17] considered a quite general Hamiltonian of electrons interacting non-relativistically among themselves, and with spatially ordered or disordered scatterers, excluding spontaneous low-dimensional magnetic order. The restriction to non-relativistic interactions means that spin–orbit effects are excluded from the problem, thus not ruling out a phase transition for Ising-type, or other suitable anisotropies. The role of disorder and impurities has also been discussed by Schuster [18], who discusses the influence of a static random field conjugate to the order parameter. Such random fields might be generated by electrically charged or magnetic impurities in certain quenched systems. The Bogoliubov inequality, in that case, allows one to exclude magnetic order for a classical XY model with Gaussian-distributed random field in less than or equal to four dimensions. The proof makes use of Mermin's classical analogue of the Bogoliubov inequality mentioned earlier in this section [12]. The significance of the Mermin–Wagner theorem for the XY model and its characteristic Kosterlitz–Thouless–Berezinskii transition is discussed in [19]. For the XY model it has also been pointed out [20] that finite-size magnetization may obscure Mermin–Wagner-type behaviour for any realizable physical system.

3.1. Spin systems

Much research has been carried out in order to extend the statement to spin systems other than the simple Heisenberg model considered by Mermin and Wagner. Wegner [21] considered a model describing a system with locally interacting itinerant electrons with pseudo-spins $\vec{\sigma}$, to which the B_0-field couples, giving a contribution $\sim B_0 \sum_{\vec{k}} (a^\dagger_{\vec{k}\uparrow} a_{\vec{k}\uparrow} - a^\dagger_{\vec{k}\downarrow} a_{\vec{k}\downarrow})$ to the Hamiltonian. The dynamics of the electrons, in this model, are governed solely by the kinetic energy

$$T_e = \sum_{\vec{k}\sigma} \frac{k^2}{2m} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}.$$

The interaction V of the electrons with the nuclei and among themselves is further assumed to satisfy the condition

$$[C, V]_- = 0 \tag{57}$$

(where C is the operator that appears in the Bogoliubov inequality).

A more realistic model has been discussed by Walker and Ruijgrok [22]: it includes Coulomb and exchange effects, with possible non-local interaction. The authors consider a model for which Lieb and Mattis had previously ruled out ferromagnetic ordering in one dimension [23], and which turns out to be a special case of their general many-band model for interacting electrons in a metal. Ghosh [24], more specifically, recovered the Mermin–Wagner theorem for the Hubbard model given by

$$H_{Hub} = \sum_{ij} \sum_{\sigma} T_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\sigma} n_{i-\sigma} + \tilde{B}_0 \sum_l (n_{l\uparrow} - n_{l\downarrow}) \exp(-\mathrm{i}\vec{K} \cdot \vec{R}_l). \tag{58}$$

Van den Bergh and Vertogen [25] present a proof of the Mermin–Wagner model for the s–d interaction model characterized by the Hamiltonian

$$H_{\mathrm{s-d}} = \sum_{lm\sigma} T_{lm} c^\dagger_{l\sigma} c_{m\sigma} - \sum_{lm} J_{lm} ((c^\dagger_{l\uparrow} c_{l\uparrow} - c^\dagger_{l\downarrow} c_{l\downarrow}) S^z_m + c^\dagger_{l\uparrow} c_{l\downarrow} S^-_m + c^\dagger_{l\downarrow} c_{l\uparrow} S^+_m). \tag{59}$$

Just as in the case discussed by Walker and Ruijgrok, the s–d interaction does not satisfy Wegner's criterion (57). Furthermore, the system is composed of two subsystems, so one has to show that both the conduction electron system and the system of localized magnetic moments fail to exhibit a magnetic phase transition in 1D and 2D.

Robaszkiewicz and Micnas have generalized the proof for the s–d model by including interactions within the spins of each subsystem and Hubbard-type interactions; the model, thus, covers the modified Zener model, the extended Hubbard model and s–d models as particular cases [26].

The range of validity of the Mermin–Wagner model can, of course, also be extended by discussing more general geometries: Baryakhtar and Yablonskii [27], for example, have shown that the Mermin–Wagner theorem remains valid for systems with an arbitrary number of magnetic sublattices, and also excludes non-collinear magnetic order when an external field is applied. Thorpe [28] considers the case of ferromagnetism in phenomenological models with double and higher-order exchange terms; similar results were obtained in the multi-sublattice case by Krzemiński [29]. These methods differ from others in that the Hamiltonian is written as a series expansion in terms of spin spherical harmonics, thus offering a more systematic way of evaluating the Bogoliubov inequality using the defining properties of spin spherical harmonics. A closely related proof, using spherical tensor operators, has been put forward for the problem of ordering in quadrupolar systems of restricted dimensionality [30].

Uhrig [31] has shown that, at finite temperatures, there can be no planar magnetic order in the one- and two-dimensional generalized multiband Hubbard model

$$H_{gen.Hub} = -\sum_{\substack{ij\sigma\\ \alpha\gamma}} T_{i\alpha,j\gamma} c^{\dagger}_{i\alpha\sigma} c_{j\gamma\sigma} + \sum_{\substack{ij\\ \alpha\gamma}} U_{i\alpha,j\gamma} n_{i\alpha} n_{j\gamma}. \tag{60}$$

Planar magnetic order, in this case, is taken to be characterized by an order parameter of the form

$$M_{plan} = \sum_{i\alpha} (\eta_{i\alpha}\sigma^x_{i\alpha} + \zeta_{i\alpha}\sigma^z_{i\alpha}) \tag{61}$$

where $\sigma^{(x,y,z)}_{i\alpha}$ denote the pseudo-spin components at lattice site i, α is the band index and $\eta_{i\alpha}$, $\zeta_{i\alpha}$ are essentially arbitrary real constants that fix the direction and the norm of the order parameter M_{plan}. Except for the choice of operators C and A in the Bogoliubov inequality, the proof of the Mermin–Wagner theorem carries through in the usual way.

Attempts to generalize the Mermin–Wagner theorem to anisotropic models with nth-nearest-neighbour exchange interactions produce results that seem somewhat artificial [32]. Similarly, attempts to extend the Mermin–Wagner theorem to special cases in three dimensions remain somewhat inconclusive [33]. In both cases, a certain circularity enters the argument: the parameters of the respective models are chosen '*ex post facto*' so as to enforce the absence of a phase transition.

A comparatively large class of many-body models has been discussed by Proetto and Lopez [34]. They confirm the Mermin–Wagner theorem for Anderson and Kondo lattices, which is of interest since the nature of the exchange interaction e.g. in the Anderson model is quite different from those in the Heisenberg model and variants thereof. The effective exchange interactions are higher-order functions of the hybridization matrix elements and are mediated by the conduction band. As can be shown via a canonical transformation, at higher order multisite interactions exist that go beyond the simpler models discussed thus far. The full Hamiltonian for this case is given by

$$H_{And} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \varepsilon_f \sum_{i\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} + \frac{U}{2} \sum_{i\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} f^{\dagger}_{i-\sigma} f_{i-\sigma} + \frac{G}{2} \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} c^{\dagger}_{i-\sigma} c_{i-\sigma}$$

$$+ J\sum_{i}\left(\sum_{\sigma} f_{i\sigma}^{+} f_{i\sigma}\right)\left(\sum_{\sigma'} c_{i\sigma'}^{\dagger} c_{i\sigma'}\right) + \sum_{ij\sigma}(V(\vec{R}_i - \vec{R}_j)c_{i\sigma}^{\dagger} f_{i\sigma} + \text{h.c.})$$
$$- \frac{\tilde{B}_0}{2}\sum_{l}((f_{l\uparrow}^{\dagger} f_{l\uparrow} - f_{l\downarrow}^{\dagger} f_{l\downarrow}) + (c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow}))\exp(-\mathrm{i}\vec{K}\cdot\vec{R}_l) \tag{62}$$

thus covering the Hubbard model, Anderson model, Falikov–Kimball model and Kondo-lattice model as special cases. The Anderson model has also been discussed by Noce and Cuoco who rederive the Mermin–Wagner theorem for the magnetic phase transition. Their paper [35] also presents analogous proofs for different pairing mechanisms and the corresponding superconducting phase transitions. For the Hubbard model, a proof of the absence of superconducting long-range order for different kinds of pairing has been given in reference [36]. A generalization of these cases will be discussed in section 3.3 below, along with its implications for superconductivity in thin films.

3.2. Partially restricted systems

Soon after the publication of the papers by Hohenberg, Mermin and Wagner, some authors expressed their doubt as to the applicability of the Mermin–Wagner scheme for systems of finite cross section (or finite thickness). As we have seen in the previous section, the scheme based on Bogoliubov's inequality ultimately rests on the divergence of the integral

$$\int_{k\leqslant k_0}\frac{\mathrm{d}^D\vec{k}}{k^2} \tag{63}$$

in one or two dimensions ($D = 1, 2$). The doubts were founded on the observation that the wave function of a system in a box of finite cross section must vanish on the walls, thus forcing the wave function to have some non-zero curvature even in the ground state. This is not compatible with the wave function assuming a uniform value—which, it was believed, should correspond to the $\vec{k} = 0$ value ('vanishing momentum') that gives the divergence in the first place. Chester *et al* [37] have argued that these doubts are ill-founded, since the $\vec{k}$-value is a purely mathematical index which need not be identified with any physical property of the system—just as in (10) the physical meaning of the k-values is irrelevant to the mathematical inequality. This observation indicated that it might well be possible to extend the scope of the Mermin–Wagner theorem to partially restricted systems as well.

Costache and Nenciu [38] discuss the overall magnetization of a partially finite three-dimensional Heisenberg model and reproduce the generalization expected from the arguments given by Chester *et al*. A similar, though much more exhaustive, discussion has been given by Fisher and Jasnow in two papers [39,40], where the authors discuss Bose systems with respect to off-diagonal ordering, and spin systems with respect to a magnetic phase transition. The general procedure is to embed the space Ω occupied by the physical system into an enclosing 'box' Λ and, furthermore, to allow for a decomposition of Ω into 'subdomains' Γ. This makes it possible to distinguish different boundary conditions—such as a possible 'corridor' surrounding Ω. This is of interest for the discussion of explicit bounds on e.g. the spin–spin correlation function, but also on the limiting behaviour of e.g. surface contributions in partially finite systems as the system approaches the thermodynamic limit [40]. The 'global' approach to partially restricted systems, i.e. the procedure of slicing up physical space into the system's domain, its subdomains and additional auxiliary 'boxes', however, appears to obscure the more basic question of whether or not within a given many-body system (e.g. of film geometry) a phase transition can occur. This, as will be seen in the next section, is quite independent of which numerical values certain model parameters display in certain subdomains (apart from some general symmetry requirements.)

For the Heisenberg model, Corciovei and Costache [41, 42] have discussed the role of boundary conditions imposed on partially finite systems, focusing on boundary conditions of the 'pinning case'. The authors also discuss a classical analogue of the Bogoliubov inequality (which, it appears, is derived independently of Mermin's paper [12]), which allows an alternative proof of the non-existence of magnetization in the classical case. The case of the Hubbard model of thin films is mentioned by Sukiennicki and Wojtczak [43]; unfortunately no explicit proof of the absence of a phase transition is given in their paper (contrary to what one of the authors suggests in reference [44]).

3.3. Systems with film geometries

The problem of geometrical restriction imposed on physical systems can be made much more explicit, by defining the many-body system as a film system *from the start*. Thus, no restrictions need to be imposed 'in hindsight', and any further specifications of interactions etc can be implemented on the level of the many-body model itself. A proof of the Mermin–Wagner theorem for systems with film geometries has recently been given [11] for the Heisenberg, Hubbard, s–f and Kondo-lattice models. In this section, we briefly outline the procedure, thereby extending the validity of the Mermin–Wagner system to the periodic Anderson model with film geometry (where we shall rule out a finite value of the layer magnetization), and to a superconducting pairing mechanism in Hubbard films.

The film geometry is incorporated into the many-body Hamiltonian by assigning each atom in the sample a double index (n, γ), where n represents the vector $\vec{R}_n$ of the underlying 2D Bravais lattice and the Greek index γ identifies which layer of the film is considered. We shall assume that the film system consists of d identical layers stacked on top of each other; the total number of lattice sites within one layer is N.

For the *periodic Anderson model* the film Hamiltonian then is as follows:

$$H_{PAM} = \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\beta\sigma} + \varepsilon_f \sum_{i\alpha\sigma} f_{i\alpha\sigma}^{\dagger} f_{i\alpha\sigma} + \frac{U}{2} \sum_{i\alpha} n_{i\alpha\uparrow}^{f} n_{i\alpha\downarrow}^{f} + V \sum_{i\alpha\sigma} (c_{i\alpha\sigma}^{\dagger} f_{i\alpha\sigma} + f_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma}) - b \sum_{i\alpha} \mathrm{e}^{-\mathrm{i}\vec{K}\cdot\vec{R}_i} (\sigma_{c_{i\alpha}}^{z} + \sigma_{f_{i\alpha}}^{z}) \qquad (64)$$

where the $c^{(\dagger)}$- and $f^{(\dagger)}$-operators denote fermionic annihilation (destruction) operators for the electrons of the conduction band and the f electrons, respectively. (The number-density operators $n_{i\alpha\sigma}^{f} = f_{i\alpha\sigma}^{\dagger} f_{i\alpha\sigma}$ and the z-components of the pseudo-spins, $\sigma_{c/f_{i\alpha}}^{z} = (\hbar/2)(n_{i\alpha\uparrow}^{c/f} - n_{i\alpha\downarrow}^{c/f})$, are defined in the standard way.)

For the Bogoliubov inequality the operators A and C are chosen as

$$A_{(\gamma)} = \sigma_{c_\gamma}^{-}(-\vec{k} - \vec{K}) + \sigma_{f_\gamma}^{-}(-\vec{k} - \vec{K}) \qquad (65)$$

$$C \equiv \sum_{\beta} C_{\beta} = \sum_{\beta} (\sigma_{c_\beta}^{+}(\vec{k}) + \sigma_{f_\beta}^{+}(\vec{k})) \qquad (66)$$

so that A is *layer dependent*, whereas C is *layer independent* (the sum $\sum_\beta$ extends over the whole sample). The (anti-)commutators appearing in the Bogoliubov inequality (11) can now be evaluated by making extensive use of the (anti-)commutation relations for the conduction electrons and the f electrons. The Hamiltonian-independent quantities can be calculated in a straightforward way:

$$\langle [C, A_{(\gamma)}]_{-} \rangle = \frac{2\hbar^2 N}{g_J \mu_B} M_{\gamma}(T, B_0) \qquad (67)$$

where the *layer-dependent magnetization* M_γ has been introduced (again with a phase factor $e^{-i\vec{K}\cdot\vec{R}_n}$ to account for possible antiferromagnetic ordering):

$$M_\gamma(T, B_0) = \frac{1}{N}\frac{g_J\mu_B}{\hbar}\sum_n e^{-i\vec{K}\cdot\vec{R}_n}\langle\sigma^z_{c_{n\gamma}} + \sigma^z_{f_{n\gamma}}\rangle. \tag{68}$$

The right-hand side of (11) can be bounded from above by

$$\sum_{\vec{k}}\langle[A, A^\dagger]_+\rangle \leqslant 8\hbar^2 N^2 \tag{69}$$

as can be shown by using a symmetrization procedure with subsequent application of the spectral theorem, similar to the procedure outlined in the appendix of [11].

For the Hamiltonian-dependent double commutator, one finds as an upper bound

$$\langle[[C, H]_-, C^\dagger]_-\rangle \leqslant 4Nd\hbar^2(|B_0 M(T, B_0)| + 2\tilde{q}\vec{k}^2) \tag{70}$$

where the constant $\tilde{q}$ is taken to reflect the fact that the hopping constants $t^{\alpha\beta}_{ij}$ fulfil the convergence criterion

$$\frac{1}{Nd}\sum_{\gamma\beta}\sum_{nk}|t^{\gamma\beta}_{nk}|\frac{(\vec{R}_n - \vec{R}_k)^2}{4} \equiv \tilde{q} < \infty. \tag{71}$$

Inserting these results into the (k-summed) Bogoliubov inequality, and making the transition to the thermodynamic limit as in (50), one arrives at an inequality for the layer magnetization M_γ which is similar, though not identical, to the one in (52):

$$M^2_\gamma(T, B_0) \leqslant \xi\frac{\beta d}{\ln(1 + \xi_1 k_0^2/|B_0 M(T, B_0)|)} \tag{72}$$

the main difference being the factor d (=number of layers) on the right-hand side. Interestingly, the upper bound is proportional to the inverse temperature β and the number of layers d. While for any finite β ($T \neq 0$) and for any finite number of layers ($d < \infty$) a phase transition is ruled out because of the divergence of the denominator as $B_0 \to 0$, the possibility of a phase transition opens up if either β or d is infinite, i.e. when a two-dimensional system is considered at $T = 0$, or when the system becomes *truly* three dimensional (i.e. infinitely extended in all dimensions).

As an example for a *superconducting phase transition,* we shall now consider a pairing mechanism for *Hubbard films.* Following the discussion in [36], we restrict our attention to the order parameter

$$\mathfrak{F}(\vec{K}) = \frac{1}{Nd}\sum_\alpha\sum_i e^{-i\vec{K}\cdot\vec{R}_i}\langle c^\dagger_{i\alpha\uparrow}c^\dagger_{i\alpha\downarrow}\rangle \equiv \frac{1}{d}\sum_i \mathfrak{F}_\alpha(\vec{K}) \tag{73}$$

which measures the breakdown of U(1) symmetry due to local on-site pairing ($\mathfrak{F}_\alpha(\vec{K})$ is again the layer-dependent equivalent to the bulk $\mathfrak{F}(\vec{K})$). The ordering wave vector allows one to distinguish between different types of pairing: for $\vec{K} = 0$ one would have s-wave pairing, for $\vec{K} \neq 0$ (generalized) η-pairing. The Hubbard Hamiltonian with an appropriate U(1) symmetry-breaking contribution of order λ is then given by

$$H = \sum_{ij\alpha\beta\sigma} t^{\alpha\beta}_{ij} c^\dagger_{i\alpha\sigma}c_{j\beta\sigma} + \frac{U}{2}\sum_{i\alpha\sigma} n_{i\alpha\sigma}n_{i\alpha-\sigma} - \lambda\sum_{i\alpha}(\eta^+_{i\alpha}e^{-i\vec{K}\cdot\vec{R}_i} + \eta^-_{i\alpha}e^{+i\vec{K}\cdot\vec{R}_i}) \tag{74}$$

where we have introduced the operators

$$\eta^+_{i\alpha} = c^\dagger_{i\alpha\uparrow}c^\dagger_{i\alpha\downarrow} \tag{75}$$

$$\eta^-_{i\alpha} = c_{i\alpha\downarrow}c_{i\alpha\uparrow} \tag{76}$$

$$\eta^z_{i\alpha} = \frac{1}{2}(n_{i\alpha\uparrow} + n_{i\alpha\downarrow} - 2). \tag{77}$$

With the operators A and C chosen as

$$C = \sum_{\gamma} \eta^z_\gamma(\vec{k}) \tag{78}$$

$$A = \eta^+_\alpha(-\vec{k} - \vec{K}) \tag{79}$$

the calculation of the (anti-)commutators for the Bogoliubov inequality results in

$$\langle [C, A]_- \rangle = \left\langle \sum_{\gamma} [\eta^z_\gamma(\vec{k}), \eta^+_\alpha(-\vec{k} - \vec{K})]_- \right\rangle = \langle \eta^+_\alpha(-\vec{K}) \rangle \tag{80}$$

$$\sum_{\vec{k}} \langle [A, A^\dagger]_+ \rangle = \sum_{\vec{k}} \sum_{ij} \mathrm{e}^{\mathrm{i}(\vec{k}+\vec{K})\cdot(\vec{R}_i - \vec{R}_j)} \langle [\eta^+_{\alpha j}, \eta^-_{\alpha i}]_+ \rangle = N \sum_{i} \langle [\eta^+_{\alpha i}, \eta^-_{\alpha i}]_+ \rangle \leqslant 4N^2 \tag{81}$$

$$\langle [[C, H]_-, C^\dagger]_- \rangle \leqslant Nd\tilde{q}\vec{k}^2 + 2\lambda Nd|\mathfrak{F}(\vec{K})|. \tag{82}$$

Thus, in this case as well, one gets a result of the form

$$\frac{v_0^{(2)}}{2\pi} |\mathfrak{F}_\alpha(\vec{K})|^2 \leqslant \frac{\beta d}{\ln(1 + \tilde{q}k_0^2/[2\lambda|\mathfrak{F}(\vec{K})|^2])} \tag{83}$$

which excludes a finite value of the layer-specific quantity $\mathfrak{F}_\alpha$, again due to the divergence of the denominator in the limit $\lambda \to 0$. Thus, no pairing transition of the proposed kind and hence *no corresponding superconducting phase transition can occur in Hubbard films,* provided the number of layers is finite and the temperature is non-zero.

The dependence on d of the upper bound in the film cases confirms a statement by Fisher [45], which is based on his work with Jasnow [40], where the upper bound scales with the extension of the 'box' Λ in which the physical system is embedded. Note, however, that the two approaches start from opposite ends: Fisher and Jasnow impose external geometrical constraints, whereas the approach presented here (and the related approach of reference [11]) includes the film geometry in the Hamiltonian from the very beginning.

3.4. Fractal lattices

The discussion in the previous section points to a deeper connection between the geometry of the sample and the interaction between its constituents. Hattori *et al* [46] have pointed to an interesting aspect of this relation, and we shall briefly summarize their discussion.

In the theory of phase transitions, and particularly in the versions of the Mermin–Wagner theorem discussed so far, one typically deals with a spin system on a translationally invariant lattice which is embedded into a Euclidean space of integer dimension ($D = 1$, 2 or 3). It turns out that the conditions for the (non-)existence of a phase transition are governed by the dimension of this Euclidean space. More generally, the critical properties and the scaling limits of such a many-particle system crucially depend on the Euclidean metric associated with the dimensionality: correlation functions of the form $\langle \phi_n \cdots \phi_m \rangle$ are Euclidean invariant functions in the scaling limit. This, however, poses a question which Hattori *et al* put forward in the following way: 'Why do the spins on the lattice 'know' this natural embedding into Euclidean space that should govern their critical phenomena?' After all, the only geometrical structure that spins can feel is the one given by the Hamiltonian, i.e. by the 'network structure of the interaction (the kinetic term, in terms of field theory)' [46].

As long as one is concerned with highly regular, i.e. translationally invariant lattices, this duality between the structure of the interaction (as contained in the Hamiltonian) and Euclidean dimension remains somewhat hidden. One instance where it surfaces, however, is the complementarity, mentioned in the last paragraph of the previous section, between Fisher and Jasnow's approach (which suggests that the upper bound in the Mermin–Wagner approach is $\sim\Lambda$, i.e. proportional to the linear extension of the '*embedding* box') and our calculation which proves that the upper bound in a film system is indeed proportional to the *number of layers d* (by virtue of the structure of the *Hamiltonian*).

The question becomes highly relevant for irregular lattices, where many of the techniques (e.g. Fourier transforms, or notions of 'momentum' vectors) cannot be applied any longer. As a step towards discussing such irregular systems, Hattori *et al* developed a Gaussian field theory on a general network; the authors succeed in giving a definition of the spectral dimension of general networks in terms of the critical behaviour of a spin system, and show how, for a restricted class of networks, the spectral dimension can be determined in practice. While a detailed discussion of their results would be far beyond the scope of this article, an application by Cassi [47] is of interest. By applying the Hattori *et al* results to the case of fractal and disordered lattices whose spectral dimension is less or equal to 2, it is shown that at finite temperature no spontaneous magnetization can exist for the classical $O(n)$ and the ferromagnetic (quantum) Heisenberg model. This is due to the infrared divergencies displayed by the corresponding Gaussian models and confirms once again the wide applicability of the Mermin–Wagner theorem.

4. On the validity of the Mermin–Wagner theorem in approximative theories

Surprisingly few authors have commented on the relevance of the Mermin–Wagner theorem for methods of approximation, some of which consistently predict finite-temperature phase transitions in one or two dimensions, even when applied to many-body models that obey the Mermin–Wagner theorem. Sometimes the breaking of the Mermin–Wagner theorem has been taken to be an advantage; Sukiennicki and Wojtczak, for example, believe 'that the molecular-field approximation of the Hubbard model approaches the physical reality (magnetic order in thin films does really exist) better than the Hubbard model in its exact form' [43]. While this may seem *prima facie* reasonable, it is difficult to maintain this view in the light of the advances that have been achieved within the (unmodified) Hubbard model by disposing with simple molecular-field approximations and adopting instead more refined methods of approximation. If one aspires to formulating criteria for the reliability of one's methods of approximation (other than justifying them in an *ad hoc* fashion), one will need to shed some light on the relation between the underlying many-body model, the exact results known about it and the mechanism of approximation. It would seem unsatisfactory to rely blindly on the method of approximation introducing exactly the kind of symmetry breaking needed to reflect physical reality. If it turns out that certain classes of approximation methods consistently produce reasonable results for quasi-2D cases, this needs explanation. One could even turn the argument around and question methods of approximation for the 3D case in case they violate the Mermin–Wagner result in two dimensions. As Walker puts it: '[A]pproximation schemes that have been applied to real solids can equally well be applied to one- and two-dimensional solids. If these approximation schemes predict the occurrence of spontaneous magnetization in one and two dimensions as well as in three dimensions [$\cdots$], the validity of these predictions in three dimensions should clearly be investigated more fully' [22].

Considerations of this sort set a possible agenda for future research into the relevance of exact results for the application of approximation schemes. In the rest of this section, we shall present a fairly elementary discussion of the Heisenberg model within different methods of approximation. In particular, we shall contrast two possible ways of testing 'Mermin–Wagner-type' behaviour.

Consider the spin-1/2 anisotropic Heisenberg model given by

$$H = -\sum_{\text{n.n.}ij} (J_{ij}(S_i^x S_j^y + S_i^y S_j^y) + J_{ij}^z S_i^z S_j^z) \tag{84}$$

where $J_{ij}^z = \varepsilon J_{ij} > J_{ij}$ and the summation index 'n.n.' refers to summation over nearest neighbours only. This kind of anisotropy in spin space favouring uniaxial ordering is widely used and should, even in 2D, break the symmetry of the corresponding isotropic model.

It has sometimes been claimed [48] that a modification of mean-field theory, known as Onsager reaction-field theory, can reproduce the Mermin–Wagner theorem in the case of the Heisenberg model. According to the Onsager theory, the orienting part of the mean field acting on a given spin must not include that part of the contribution from the spins in the vicinity which is due to their correlation with the given spin under consideration. Thus, one must stipulate that the full mean field decomposes into two independent contributions, the correlated and the uncorrelated one, called the *reaction field* and *cavity field*, respectively. (For a detailed discussion see [49].) Singh [50] has succeeded in applying Onsager's reaction-field idea to the anisotropic Heisenberg model as given by (84). It turns out that the Onsager reaction-field result for the critical temperature, T_c^{Ons}, is related to that of ordinary mean-field (MF) theory by the equation

$$\frac{T_c^{Ons}}{T_c^{MF}} = 1 \Big/ \left(\sum_{\vec{k}} \frac{1}{(1 - J^z(\vec{k})/J^z(\vec{K}))} \right) \tag{85}$$

where $\vec{K}$ denotes the ordering wave vector and $J^z(\vec{k})$ is the standard Fourier transform of the exchange integrals J_{ij}. From (85), however, we see that while Onsager reaction-field theory does modify the ordinary mean-field result, it is independent of the anisotropy assumed above by setting $J_{ij}^z = \varepsilon J_{ij}$, since the anisotropy parameter ε will drop out of the fraction $J^z(\vec{k})/J^z(\vec{K})$ in the denominator. Effects of dimensionality that stem from the summation $\sum_{\vec{q}}$ are, on the other hand, retained, such as the denominator's logarithmic divergence in two dimensions, which rules out a phase transition. This compliance with the Mermin–Wagner theorem, however, is rendered spurious by the fact that no anisotropy effects are captured by the Onsager approach.

It is worthwhile to explore whether more sophisticated methods of approximation are more successful in accounting for effects due to (reduced) dimensionality and (possibly anisotropic) interaction. For the Tyablikov procedure of decoupling higher-order Green's functions within the equation-of-motion scheme, this is indeed the case. As has been shown in [49], the Tyablikov procedure accords with the Mermin–Wagner theorem in two dimensions: only when an external field is applied can there be a finite value of the magnetization at non-zero temperature. The proof is based on a series expansion of the (implicit) equation for the expectation value $\langle S^z \rangle$,

$$\frac{\langle S^z \rangle}{\hbar S} = 1 \Big/ \left(\frac{1}{N} \sum_{\vec{k}} \coth\left(\frac{\beta}{2} E(\vec{k}) \right) \right) \tag{86}$$

where the energy $E(\vec{k})$ is given by $E(\vec{k}) = 2\hbar \langle S^z \rangle (J_0 - J(\vec{k})) + g_J \mu_B B_0$. As a result of the Tyablikov approximation, equation (86) is taken to be uniform for all spins in the lattice, which seems to limit the discussion to the ferromagnetic case. However, it has also been shown that an analogous result holds for the case of spontaneous sublattice magnetization in ABAB-type antiferromagnets. The corresponding formula for the Néel temperature in that case is of the following form:

$$T_N^{Tyab} = \frac{J_0}{2k_B} \Big/ \left(\frac{2}{N} \sum_{\vec{k}} \frac{1}{(1 - J^2(\vec{k})/J_0^2)} \right). \tag{87}$$

It is straightforward to show that in the thermodynamic limit the sum in the denominator diverges in two dimensions while remaining finite in three dimensions. What remains to be shown is that the Tyablikov method can make sense of anisotropy effects, i.e. perform better than the Onsager reaction-field theory in accounting for ordering due to anisotropy. One such test is whether or not the method can correctly predict the Mermin–Wagner theorem if one starts from the three-dimensional case and gradually turns off interlayer coupling. If we choose the interaction parameters J_{ij} such that (for a fixed lattice site i) $J_{ij} = J_{\parallel}$ if sites i and j lie within a plane, and $J_{ij} = J_{\perp}$ if j is located in the direction orthogonal to this plane, then, by varying the anisotropy parameter

$$\varepsilon := J_{\perp}/J_{\parallel} \tag{88}$$

we can change the coupling continuously from quasi-two-dimensional ($\varepsilon \equiv 0$) to (isotropic) three-dimensional ($\varepsilon = 1$) coupling. One can then, indeed, prove that in the quasi-2D limit of vanishing interlayer coupling ($\varepsilon \to 0$) the Néel temperature (as calculated from the Tyablikov method) vanishes as

$$T_N^{Tyab} \underset{\varepsilon \to 0}{\sim} \frac{\varepsilon}{|\ln(\varepsilon)|} \tag{89}$$

in accordance with the Mermin–Wagner theorem. In its original form, the Tyablikov method applies to the $S = 1/2$ case only, and so, by definition, do the results derived so far. An extension of the results to higher spins can, however, be given in a straightforward way [49].

In this section, we have contrasted two approximation schemes, the Onsager reaction-field theory and the Tyablikov method. The failure of reaction-field theory to capture the effect of anisotropic coupling suggests that it does not adequately capture the behaviour of the Heisenberg model as far as the existence, or absence, of a phase transition is concerned. The Tyablikov method, despite its still rather simple random-phase characteristics, seems to fare better: it can be analytically shown to produce all the relevant limiting cases of possible 'Mermin–Wagner-type behaviour', and it also correctly reproduces the qualitative change associated with the transition from three to two dimensions by introducing anisotropic (and eventually vanishing) interlayer coupling.

5. Summary

In this article, we have presented a survey of recent and established results concerning the application of Bogoliubov's inequality to the theory of phase transitions. This includes the classic papers by Hohenberg, Mermin and Wagner as well as a host of other proofs concerning a variety of different many-body models, order parameters and system geometries. In particular, new proofs for the absence of superconducting long-range order in Hubbard films, and of magnetic long-range order in periodic Anderson-model films have been presented. The complementarity between geometric constraints on the one hand and anisotropy on the other hand, has been sketched in theoretical terms, and has been applied to two specific methods of approximation, Onsager reaction-field theory and the Tyablikov method. The two methods discussed here can only give an indication as to which effects and limiting cases should be considered, if one attempts to characterize a method in terms of its accordance with the Mermin–Wagner theorem. The more general problem of the relevance of exact results for the numerical or approximative treatment of many-body models, as characterized in section 4, will almost certainly remain and in our view deserves closer attention.

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