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THE HUBBARD MODEL:
SOME RIGOROUS RESULTS AND OPEN PROBLEMS

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Dedicated to Gian Fausto Dell'Antonio on his sixtieth birthday

Abstract

The Hubbard model of interacting electrons, like the Ising model of spin-spin interactions, is the simplest possible model displaying many "real world" features, but it is much more difficult to analyze qualitatively than the Ising model. After a third of a century of research, we are still not sure about many of its basic properties. This mini-review will explore what is known rigorously about the model and it will attempt to describe some open problems that are possibly within the range of rigorous mathematical analysis.

0. Introduction

The Hubbard model is to the problem of electron correlations as the Ising model is to the problem of spin-spin interactions; it is the simplest possible model displaying many "real world" features. It is, however, much more difficult to analyze qualitatively than the Ising model. After a third of a century of research, we are still not sure about many of its basic features. It is believed, for example, to have something to do with high temperature superconductivity, and it would be nice to validate this.

One of the most intriguing questions concerns magnetism — particularly the magnetic properties of the ground state. The familiar models of interacting spins, such as the Ising or Heisenberg models, posit an underlying spin Hamiltonian that ultimately comes from a model of itinerant electrons. The mystery here is that neither the electronic kinetic nor the electronic potential energies favor ferromagnetism, but together they sometimes do so. Ferromagnetic spin models, for example, are popular, but the truth is that the antiferromagnetic preference of the kinetic energy usually seems to dominate. In fact the only known examples of saturated itinerant electron ferromagnetism come from the

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Hubbard model in a special limit (infinite repulsion and one hole) devised by Nagaoka [NY] or from the Hubbard model with finite repulsion but on special lattices devised by Mielke and Tasaki [Mi1, TH2, MT] for which the kinetic energy spectrum is macroscopically degenerate. No doubt, further study of the Hubbard model will eventually lead to a better understanding of the way in which the Pauli exclusion principle leads to magnetism.

These notes will explore what is known rigorously about the model and it will attempt to describe some open problems that are possibly within the range of rigorous mathematical analysis. The notes are not a complete review in the sense that every contribution is covered, but an attempt has been made to mention, at least, most topics that can be treated rigorously. I apologize to those authors whose works have been omitted and I hope this will be attributed to my ignorance rather than intent. Given more space I would have liked to discuss the closely related Falicov-Kimball model, for which many rigorous results are known, but which is not a Hubbard model because it does not have $SU(2)$ symmetry. Another interesting chapter would be the infinite dimensional Hubbard model—pioneered by Metzner and Vollhardt [MV]—and which opens exciting mathematical and physical avenues. It has led to a large literature, but much remains to be added in the way of mathematical rigor.

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1. Definition of the Model

Only the original short-range Hubbard model will be considered here. Like the Ising model, the Hubbard model is defined on a graph, i.e., a collection of vertices or sites (denoted by Λ and whose number is $|\Lambda|$) and (unordered) edges or bonds connecting certain distinct pairs of vertices. The word graph instead of lattice is used to avoid any possible implication of translation invariance because most of the results stated here do not depend on such invariance. One is given a **hopping matrix** T, with elements t_{xy}, with x and $y \in \Lambda$, and we assume, as a convention, that $t_{xy} = 0$ if x, y are not connected by an edge. Note that $t_{xx} = 0$. t_{xy} might be complex, signaling the presence of a magnetic field, the line integral of whose vector potential from x to y (thought of now as points in $\mathbf{R}^3$) is $\arg(t_{xy})$. However, T is always self adjoint, $t_{xy} = t^*_{yx}$, with $*$ denoting complex conjugate.

The **bipartite** graphs form an important sub-class; here $\Lambda = A \cup B$, with A and B disjoint, and such that there is no edge between x, y if $x \in A$ and $y \in A$ or if $x \in B$ and $y \in B$. The square lattice is bipartite, the triangular is not.

Electrons, i.e., spin $\frac{1}{2}$ fermions, move on Λ with kinetic energy given in second quantized form by $K = K_\uparrow + K_\downarrow$ with

$$K_\sigma = -\sum_{x,y\in\Lambda} t_{xy} c^\dagger_{x\sigma} c_{y\sigma}. \tag{1.1}$$

Here $\sigma = \pm 1$ denote the two spin states $\uparrow$ and $\downarrow$ while $c^\dagger_{x\sigma}$ is the creation operator for an electron at x with spin σ. We have $c^\dagger_{x\sigma} c_{y\tau} + c_{y\tau} c^\dagger_{x\sigma} = \delta_{xy}\delta_{\sigma\tau}$ and $c_{x\sigma}c_{y\tau} + c_{y\tau}c_{x\sigma} = 0$. The number operator is defined by $n_{x\sigma} = c^\dagger_{x\sigma}c_{x\sigma}$ and has eigenvalues 0 and 1. The total number of each spin species

$$N_\sigma = \sum_{x\in\Lambda} n_{x\sigma}$$

is a conserved quantity. The total particle number is $N = N_\uparrow + N_\downarrow$ which satisfies $0 \le N \le 2|\Lambda|$. The **half-filled band**, $N = |\Lambda|$ is especially important and especially amenable to analysis.

In the physics literature it is often assumed that $t_{xy} = \text{constant} = t > 0$ on all edges of Λ, in which case T is a discrete version of the Laplacian, but without the diagonal terms. This assumption will not generally be made here.

At each site x there is also given a number U_x which governs the on-site electron-electron interaction at x. We usually assume all $U_x \ge 0$ (repulsive case) or all $U_x \le 0$ (attractive case). The total potential energy is†

$$W = \sum_{x\in\Lambda} U_x (n_{x\uparrow} - \tfrac{1}{2})(n_{x\downarrow} - \tfrac{1}{2}). \tag{1.2}$$

The total Hubbard Hamiltonian of our system is then

$$H = K + W, \tag{1.3}$$

and most of the results discussed here are about the ground state of this H. In fact, many of the results do not require a point interaction as in (1.2); instead, terms like $U_{xy}(n_{x\uparrow} - \frac{1}{2})(n_{y\downarrow} - \frac{1}{2})$, with the matrix U_{xy} being positive semidefinite, are also allowed.

The interaction in (1.2) includes a one-body term $-\frac{1}{2}\sum_x U_x(n_{x\uparrow} + n_{x\downarrow})$ plus a trivial constant term $\frac{1}{4}\sum_x U_x$. If U_x is independent of x, as is normally assumed in almost all papers on the subject, then this one-body term is trivially a constant proportional to the fixed particle number. It is interesting to consider $U_x \ne$ constant, and the one-body term is included in (1.2) in order to be able to exploit **hole-particle symmetry**: The unitary transformation that maps $c_{x\downarrow} \to c^\dagger_{x\downarrow}$ and $c^\dagger_{x\downarrow} \to c_{x\downarrow}$ (but $c_{x\uparrow} \to c_{x\uparrow}$) is the hole-particle transformation on the down-spins and it maps $(n_{x\downarrow} - \frac{1}{2})$ into $-(n_{x\downarrow} - \frac{1}{2})$. Thus, this transformation maps the repulsive W into the attractive W and vice versa, but it changes the down-spin number from $N_\downarrow$ to $|\Lambda| - N_\downarrow$.

This hole-particle transformation may or may not map $K_\downarrow$ into $K_\downarrow$. It does map $K_\downarrow$ into $\widehat{K}_\downarrow$, defined by $\widehat{t}_{xy} = -t^*_{yx}$.

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† The usual formulation is $n_\uparrow n_\downarrow$ instead of our $(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$. If U_x varies with x the two formulations are obviously inequivalent. The formulation here is not without a physical foundation because a neutral atom (with $n_\uparrow + n_\downarrow = 1$) is locally the most stable configuration and adding or removing an electron produces a net local charge that raises the energy roughly equally.

In the special, but important case that T is real and Λ is bipartite we can make a further unitary transformation that will take $\widehat{K}_\downarrow$ into $K_\downarrow$ and $n_{x\downarrow}$ into $n_{x\downarrow}$. This unitary transformation maps $c_{x\downarrow}$ into $(-1)^x c_{x\downarrow}$ (and, of course, $c_{x\uparrow}$ into $c_{x\uparrow}$), where $(-1)^x$ denotes the function on the vertices of Λ which is $+1$ for $x \in A$ and -1 for $x \in B$. Effectively, t_{xy} is mapped into $(-1)^x(-1)^y t_{xy} = -t_{xy}$ for the down-spins. Henceforth, the hole-particle transformation on bipartite lattice is always meant to include this additional unitary $(-1)^x$, so that $K_\downarrow$ is mapped into $K_\downarrow$.

Thus, in the special real, bipartite case we can analyze the repulsive case by analyzing the attractive case. But we have to remember that $N_\downarrow \leftrightarrow |\Lambda| - N_\downarrow$ so that the particle number for one is related to the magnetization of the other. This is a non-trivial distinction and is similar to the relation between the ferromagnetic and antiferromagnetic Ising models on a bipartite graph.

The hole-particle transformation also induces a conservation law in the real, bipartite case that has no classical analogue. Like any electron system this model has an $SU(2)$, i.e., angular momentum, invariance. The generators are

$$J^3 = \tfrac{1}{2}(N_\uparrow - N_\downarrow), \qquad J^+ = \sum_{x\in\Lambda} c^\dagger_{x\uparrow} c_{x\downarrow}, \qquad J^- = (J^+)^\dagger. \tag{1.4}$$

However, the Hamiltonian H in (1.3) is the unitary transform (described above) of another H' (with U_x replaced by $-U_x$) which also has an $SU(2)$ symmetry with generators given by (1.4) in the *transformed* basis. By transforming back we obtain a different set of $SU(2)$ generators

$$\widehat{J}^3 = \tfrac{1}{2}(N_\uparrow + N_\downarrow - |\Lambda|), \qquad \widehat{J}^+ = \sum_{x\in\Lambda} (-1)^x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow}, \qquad \widehat{J}^- = (\widehat{J}^+)^\dagger \tag{1.5}$$

that also commute with H and with the J's in (1.4). We call this the **pseudospin**. This special model thus has an $SU(2)\times SU(2)$ symmetry group,§ but it must be emphasized that real T is *essential* (zero magnetic field). These operators change the quantum numbers $N_\uparrow$ and $N_\downarrow$. The operators $J^\pm$ change J^3 by one unit while $\widehat{J}^\pm$ change $\widehat{J}^3$ by one unit. The four operators together thus permit us to move around inside rectangles in $(N_\uparrow, N_\downarrow)$ space whose four vertices have the form $(n,m), (m,n), (|\Lambda|-n, |\Lambda|-m), (|\Lambda|-m, |\Lambda|-n)$. This means that to each eigenstate for $N_\uparrow = n$, $N_\downarrow = m$ there is a corresponding eigenstate with the same energy at each point in the rectangle (there are also additional eigenstates, of course). Thus, the usual operators $J^\pm$ permit us to infer all the states of our Hamiltonian from knowledge of the states on the line $N_\uparrow - N_\downarrow = 0$ or the line $N_\uparrow - N_\downarrow = 1$. The pseudospin operators $\widehat{J}^\pm$ permit us to infer everything from knowledge of the line $N_\uparrow + N_\downarrow = |\Lambda|$

§ Actually, the group is $SO(4) = SU(2) \times SU(2)/Z_2$, as pointed out by Yang and Zhang [YZ]. The reason is that the two operators $w = -\mathbf{1}$ in each $SU(2)$ corresponds to only *one* operator on our Hilbert space, i.e., $w \otimes \mathbf{1} = \mathbf{1} \otimes w$. This reduction to $SO(4)$ coincides with the observation that in every state the spin and pseudospin are either both integral or both half-integral.

(half-filled band) or the line $N_\uparrow + N_\downarrow = |\Lambda| + 1$. But we repeat that this property of $\widehat{J}^\pm$ holds *only* for the real, bipartite case.

We note, for future use, that the hole-particle transformation (*without* $(-1)^x$) applied to *both* spins (namely $c_{x\sigma} \leftrightarrow c^\dagger_{x\sigma}$). does not preserve $\vec{J}$. Indeed, $J^3 \to -J^3$, $J^\pm \to -J^\mp$, but $\mathbf{J}^2 \to \mathbf{J}^2$.

The Hubbard model describes — in the simplest possible fashion — an interacting fermion system. It can be viewed this way, as a toy model, or it can be viewed, a bit more realistically in the repulsive case, as a serious model of π-electrons hopping between localized Wannier orbitals in some molecule such as benzene (with $|\Lambda| = 6$); the half-filled band, $N = |\Lambda|$, is then especially important because it corresponds to neutrality. The ultra-short range interaction is supposed to mimic a highly screened Coulomb potential. From the latter viewpoint it was known first in the chemistry literature as the Pariser-Parr [PP]-Pople [PJ] model; molecules having a bipartite structure are called "alternant molecules". It was a decade later that Hubbard [HJ], Gutzwiller [GMC] and Kanamori [KJ] realized its importance for bulk matter.

2. One-Dimensional Exactly Solvable Model

In 1968 the ground state of H was solved for the translation invariant one-dimensional ring by Lieb and Wu [LW] using the extension of the "Bethe ansatz" technique [BH, LL1] to fermions [MJ, FL1, YC, GM]. Shortly thereafter, Ovchinnikov [OA] used these results to calculate the elementary excitation spectrum at half filling. Recently, Essler and Korepin [ES] obtained a new and illuminating derivation. Coll [CC] extended Ovchinnikov's results to arbitrary filling, as did Woynarovich [WF]. Takahashi [TM] evaluated the magnetism curve at half filling and Shiba [SH] evaluated the magnetic susceptibility for all filling. Koma [KO] has formulated a sequence of approximations to the positive temperature free energy and correlation length (obtained by using the Trotter product formula for the partition function) which converge to the exact answer and such that each approximation can be calculated using the Bethe ansatz without any assumptions, such as the "string hypothesis".

These results were obtained in the thermodynamic limit, in which sums could be replaced by integrals. Woynarovich and Eckle [WE] evaluated the asymptotics of finite size effects on the ground state energy. For small chains the general "Bethe ansatz" solution, while correct, is too complicated for numerical evaluation. Heilmann and Lieb [HL] undertook to evaluate *all* the energy levels for *all* $U > 0$ for the benzene molecule ($N = 6, |\Lambda| = 6$). To our surprise we found many instances of both level crossings and of permanent degeneracy — as a function of U — and which were not accounted for on the basis of the known invariance groups (spin, pseudospin and symmetries of the hexagon). This means that the system has *non-abelian* symmetry groups and these *are dependent on* U (i.e., the group operations commute with H but *not* with K and W separately; a well known example of this phenomenon, for the hydrogen atom, is the Runge-Lenz vector whose definition depends on the value of the electron's charge).

What are these invariants? Sixteen years later Shastry [SB] (unaware of [HL]) found many invariants and also a two-dimensional classical statistical mechanics vertex model whose transfer matrix commutes with our H. In fact he found a whole commuting family of such transfer matrices — which means that the one-dimensional model can be called "integrable". It is not clear whether all invariants of H are of Shastry's form. A few years later, Grosse [GH] (motivated by [HL]) published another derivation of some of the invariants.

Another interesting question is whether all the eigenstates of H are of the "Bethe ansatz" form. This was answered in the negative by Essler, Korepin and Schoutens [EKS] who went on to demonstrate that when the ring is bipartite (i.e., even length) the $SU(2)\times SU(2)$ generators J^+ and $\widehat{J}^+$ save the day. The lowest weight states (the ones that are annihilated by J^- and $\widehat{J}^-$) are claimed to be *all* of the "Bethe ansatz" type. All the remaining states are then obtained by application of J^+, and $\widehat{J}^+$.

Many of the "Bethe Ansatz" results rely on a "string" hypothesis. Moreover, some assertions in [EKS], notably the linear independence of the solutions, rely on an appeal to some properties of Shastry's invariants that have not been verified. It is desirable to put these matters on a more rigorous basis.

The literature about this one-dimensional solution is vast and the above remarks do not reflect everything that is known about the subject.

3. Magnetism

A. One-Dimension.

It is convenient, now, to take an open chain instead of a ring. Then, by a general theorem of Lieb and Mattis [LM1], whose proof also works for lattice systems with nearest neighbors hopping and a *completely arbitrary* many-body potential, $E^N(S)$, the ground state energy of H, as a function of total spin $S\le\frac{1}{2}N$ and for N particles, satisfies

$$E^N(\tfrac{1}{2}N) > E^N(\tfrac{1}{2}N-1) > E^N(\tfrac{1}{2}N-2) > \ldots > E^N(0) \text{ or } E^N(\tfrac{1}{2}). \tag{3.1}$$

The numbers U_x are now totally arbitrary and not necessarily of one sign. [Note: The original theorem [LM1] uses a Perron-Frobenius positivity argument, which a-priori requires $t_{xy}>0$. However, any T can be reduced to this form in one-dimension by the simple unitary gauge transformation $c_{x\sigma}\to\exp[-i\theta(x)]c_{x\sigma}$, which carries t_{xy} into $\widehat{t}_{xy}:=t_{xy}\exp[i\theta(x)-i\theta(y)]$, where $\theta(x)$ is an arbitrary real number, selected so that $\widehat{t}_{xy}>0$ for all x and y.] Since we can then take T to be real, our H is then the (down-spin) hole-particle transform of some other $\widehat{H}$, in which U_x is replaced by $-U_x$. Assuming N to be even, (3.1) says that the ground state of H has $N_\uparrow=N_\downarrow=N/2$. The transformed $\widehat{H}$ system has $\widehat{N}_\uparrow=N_\uparrow$, $\widehat{N}_\downarrow=|\Lambda|-N_\downarrow$, whence $\widehat{S}^3=\frac{1}{2}(\widehat{N}_\uparrow-\widehat{N}_\downarrow)$ is the predetermined number $\frac{1}{2}(N-|\Lambda|)$. The $\widehat{H}$ system also satisfies (3.1) since it is one-dimensional, and the spin of the ground state of the $\widehat{H}$ system is therefore

$$\widehat{S}=\tfrac{1}{2}\big|N-|\Lambda|\big|.$$

This number, $\widehat{S}$, is *the pseudospin of our ground state* — a curious result whose physical significance is not entirely obvious. (Note the logic here. Both systems, H and $\widehat{H}$ must be in their respective ground states, consistent with the given conditions on each; for H it is $N_\uparrow+N_\downarrow=N$ and for $\widehat{H}$ it is $N_\uparrow-N_\downarrow=N-|\Lambda|$.)

This theorem was extended many years later by Aizenman and Lieb [AL] to positive temperatures. The main theorem, applicable to any many-body potential in a one-dimensional system, expresses the fact that the free energy is a monotone increasing function of the spin. This is done in terms of total spin S or 3-component s, as follows; neither inequality implies the other.

Classify the eigenstates by the 3-component of spin, $J^3=s=\frac{1}{2}(N_\uparrow-N_\downarrow)$, and by S, the total spin angular momentum (recall $\mathbf{J}^2=S(S+1)$). For a given N and inverse temperature β, let $Z_3(s)=\mathrm{Tr}_s e^{-\beta H}$ be the partition function in which only states of a given s value are included. Likewise, let $Z_J(S)=\mathrm{Tr}_S e^{-\beta H}$ be the partition function for a given S. We have the relation $Z_3(S)-Z_3(S+1)=(2S+1)^{-1}Z_J(S)$, which is obvious from the theory of angular momentum. Correspondingly, we have the combinatorial quantities $Y_3(s):=\binom{N}{\frac{N}{2}+s}$ and $Y_J(S):=(2S+1)[Y_3(S)-Y_3(S+1)]$, which are essentially the partition functions of free particles with $H=0$, and which serve to normalize the Z's. The two theorems are then that

$$\frac{Z_3(s)}{Y_3(s)} \quad \textit{and} \quad \frac{Z_J(S)}{Y_J(S)}$$

are *both strictly monotone decreasing functions of their arguments* (s or S). A corollary of this is that the magnetization is less than its value in the **atomic limit** (or what I prefer to call the pure paramagnetic value). I.e., for all β and magnetic field h

$$M(\beta,h)=\frac{1}{\beta}\frac{\mathrm{d}}{\mathrm{d}h}\ln Z(h)<N\tanh(\beta h). \tag{3.2}$$

Here $Z(h)=\sum_{s=-N/2}^{N/2}Z_3(s)\exp[2\beta sh]$ is the total partition function (recall that the g-factor of an electron is 2).

It is noteworthy that all this holds for *completely arbitrary*, Hermitian t_{xy} and (real) U_x. Indeed, it holds even if we add an arbitrary real one body potential

$$V=\sum_{x\in\Lambda}V_x(n_{x\uparrow}+n_{x\downarrow}).$$

An amusing fact about one-dimension concerns the $U=+\infty$ case. For an open chain the ground state is highly degenerate—indeed, it can have any value of S. For a closed chain the situation is quite different and the S of the ground state depends on the sign of the t_{xy}'s and whether N is even or odd; S can be $N/2$ in some cases [AL]. The situation is discussed in detail by Mielke [Mi2] who finds that the "average" S is $\sqrt{N}$. Some interesting facts about the closed one-dimensional chain with $U = 0$, but with a magnetic field, can be found in [LL2]. The $U \neq 0$ case is discussed by Fujimoto and Kawakami [FK1].

B. Half-Filled Band.

The hole-particle symmetry notwithstanding, the repulsive case (all $U_x \geq 0$) and the attractive case (all $U_x \leq 0$) are quite different, even for a bipartite lattice. The physical spin of one is the pseudospin of the other.

In the limit $U \to +\infty$ (by which I mean all $U_x \to +\infty$), the energy and wave functions have nice limits. The electrons become hard-core particles. When $N = |\Lambda|$ we just have one electron per site and, since motion is impossible, each electron can be, independently, spin-up or spin-down. This gives us the atomic limit whose partition function is Y_3 or Y_J given above. First order perturbation theory in t/U vanishes, but in second order we have to diagonalize our H among all the $2^{|\Lambda|}$ degenerate ground states just described. This yields an effective Hamiltonian H' that can be written in terms of the three Pauli spin operators $\mathbf{S}$ at each site. It turns out [AP] that for any graph

$$H' = \sum_{x,y\in\Lambda} J_{xy}(\mathbf{S}_x \cdot \mathbf{S}_y - \tfrac{1}{4}) \tag{3.3}$$

with $J_{xy} = |t_{xy}|^2(U_x^{-1} + U_y^{-1})$. This is the spin 1/2 antiferromagnetic Heisenberg Hamiltonian and it is known [LE1, LM2] that its ground state has total spin

$$S = \big||A| - |B|\big| \tag{3.4}$$

on a bipartite graph. It is also known [DLS, KLS] that in the **translation invariant case** (i.e., our graph is a D-dimensional hypercube with periodic boundary conditions and $t_{xy} =$ constant $= t$ and $U_{xy} =$ constant $= U$) there is long range order when $D \geq 3$.

The obvious question is whether the results just stated (i.e., (3.4) and the long range order) hold non-perturbatively in the repulsive case. One would also guess that in the attractive case the total spin should be zero in the ground state because when $U_x = -\infty$ for all x the ground state consists simply of bound pairs of electrons sitting on selected sites. These questions about the spin are answered in the following [LE1].

Theorem 1: *Assume t_{xy} is real for all $x, y \in \Lambda$. If $U_x < 0$ for all x, the ground state on any connected graph is unique and has spin $S = 0$* for any even electron number, N, not just $N = |\Lambda|$. *If $U_x > 0$ for all x, if Λ is connected and bipartite and if $N = |\Lambda|$ is even, the ground state is unique (except for the $(2S+1)$-fold degeneracy) and has spin $S = \frac{1}{2}\big||A| - |B|\big|$.*

We can easily have $|A| - |B|$ of the order of $|\Lambda|$ itself. As an example, take a square lattice and add a site at the center of each bond of this square lattice. The original sites are then B sites and the new sites are A sites. Then $|A| = 2|B|$ and the ground state has a bulk magnetization per site of 1/3. This is really more like ferrimagnetism than ferromagnetism but, in any case, it is one of the few examples known in which the system has a bulk magnetization without an external magnetic field.

There is an interesting corollary of this theorem if Λ is bipartite and if $|A| \geq |B|$. Suppose we ask for the absolute minimum energy, without fixing N. Starting with $U_x > 0$ we find that an optimum N is $N = |\Lambda|$ (by the $SU(2) \times SU(2)$ symmetry mentioned in Sec. 1). But $J^3 = (N_\uparrow - N_\downarrow)/2$ can be anywhere in the interval $(|B|-|A|)/2$ to $(|A|-|B|)/2$ since $S = (|A|-|B|)/2$. Now using hole-particle symmetry to obtain the $U_x < 0$ model, we find that the optimum N is any integer satisfying $2|B| \leq N \leq 2|A|$. (E.g., starting with $N_\uparrow = |A|, N_\downarrow = |B|$, the transformed values are $N_\uparrow = |A|, N_\downarrow = |\Lambda| - |B|$, which yields $N = 2|A|$.) Thus, *there can be a large degeneracy in the attractive case!* (For $U = 0$ this is easily seen from the remark that T has at least $|A| - |B|$ zero eigenvalues.)

This theorem was extended to positive temperature by Kubo and Kishi [KK] who found upper bounds on certain two-point functions. They discuss only the translation invariant case on a hypercubic lattice with $U_x = U =$ constant, but their method easily extends to the general case. For $U < 0$ they bound the spin susceptibility at wave vector q by

$$\chi_q \leq \frac{1}{4|U|} \tag{3.5}$$

for all temperatures and all filling fraction $N/|\Lambda|$ (more precisely, they use the grand canonical ensemble and prove (3.5) for all chemical potentials μ). This result precludes magnetic long range order. In the repulsive case $U > 0$, and with μ adjusted to the half-filled band case $N = |\Lambda|$, namely $\mu = 0$, they bound the charge susceptibility as

$$(\delta\widehat{n}_q, \delta\widehat{n}_{-q}) \leq (\beta U)^{-1} \tag{3.6}$$

and the pairing susceptibility as

$$(\widehat{p}_q, \widehat{p}_{-q}) \leq (\beta U)^{-1}. \tag{3.7}$$

Here (A, B) is the Duhamel two-point function $(A, B) = \int_0^1 \mathrm{Tr}[A^\dagger e^{t\beta H} B e^{(1-t)\beta H}]\, dt$ and $\delta\widehat{n}_q = \widehat{n}_q - \langle \widehat{n}_q \rangle$ and $p_x = c^\dagger_{x\uparrow} c_{x\downarrow}$ and $\widehat{\ }$ denotes spatial Fourier transform. Charge long range order is precluded by (3.6) while Cooper pairing is precluded by (3.7).

Although I am restricting this review to the Hubbard model, I cannot resist the temptation to mention that Theorem 1 has recently been extended [FL2] to another model—the Holstein model—in which electrons interact with a quantized phonon field instead of with each other. Again, the finite system ground state for any even number of electrons is unique and has zero spin. The method of proof of Theorem 1 has also been used by Ueda, Tsunetsugu and Sigrist [UTS] to show that the periodic Anderson model at half-filling has a singlet ground state.

This close connection between the half-filled band, repulsive Hubbard model and the antiferromagnetic Heisenberg model points to the first of our spin problems. The antiferromagnetic Heisenberg model on a hypercubic lattice, in the thermodynamic limit, has no long range order (LRO) at positive temperature in dimensions $D = 1$ or 2. This is a consequence of the Hohenberg-Mermin-Wagner theorem. The same is true for the Hubbard model as first shown by Walker and Ruijgrok [WR], then by Ghosh [GD]. Later, Koma and Tasaki [KT]proved it by a different method—that of McBryan and Spencer [MS]. As far as the ground state is concerned, the Heisenberg model has LRO for $D = 2$ and spin 1 or more per site [KLS] (i.e. $|\mathbf{S}_x|^2 = S(S+1)$ and $S \geq 1$) and it is believed to have LRO also when $S = 1/2$, which is the case of interest for us. The $D = 1$ case is believed to have no LRO in the ground state. For $D \geq 3$ there is LRO in the ground state for all $S \geq 1/2$ [KLS] and at positive temperature [DLS, KLS] for $S \geq 1$ (presumably, also for all $S \geq 1/2$). The obvious conjecture is the following.

Problem 1: *Prove that there is antiferromagnetic LRO in the half-filled band, repulsive Hubbard model on the hypercubic lattice (with $t_{xy} = 1$ for $|x - y| = 1$ and $U_x =$ positive, finite constant) in the ground state when $D = 2$ and for positive temperature when $D \geq 3$. For which values of N will the attractive model have LRO?*

The Falicov-Kimball [FK2] model poses an analogous problem that *can be solved* affirmatively. In this model, one kinetic energy term, $K_\downarrow$, is omitted from the Hamiltonian. Although the down spins are not dynamic their locations are left arbitrary. After "integrating out" the movable particles (up-spins), an effective interaction among the fixed particles (down-spins) is left. This, then, is a classical lattice gas with a complicated interaction. It resembles an Ising (not Heisenberg) model when U is large and it can be shown [KL] to have long range order at low temperatures (and no long range order at high temperatures) in two or more dimensions—as does the Ising model.

C. The Surprising Hole.

In the previous subsection we considered the half-filled band and showed a strong tendency to antiferromagnetism. The only important requirement on T was that it was real (i.e., no magnetic field acts on the orbital motion). Nagaoka [NY] made a surprising discovery about the case $U = +\infty$, but *with one hole* (i.e., $N = |\Lambda| - 1$). Thouless [TD] had a similar result a bit earlier (cf. note 7 in [NY] and the discussion on p. 47 in [LE2]) but there is little doubt that Nagaoka's presentation of this particular result is clearer, more precise and applicable to certain non-bipartite lattices such as *bcc* and *fcc*. The Thouless approach uses a Perron-Frobenius argument that appears to be restricted to bipartite lattices; for such lattices it is true that fermions behave like bosons when $U = +\infty$ and there is one hole. Nagaoka, on the other hand seems to require a regular Bravais lattice, but this is not really necessary provided *all* t_{xy} are nonpositive. The fully general result with a considerably simplified proof, was given by Tasaki [TH1].

It is usually assumed in the condensed matter literature that the t_{xy}'s are nonnegative, but there seems to be neither a compelling reason for this assumption nor many examples in which it can be verified (S. Kivelson, private communication). (For a bipartite lattice, however, one can have either sign with the help of the unitary operator $(-1)^x$ applied to *both* spin $\uparrow$ and $\downarrow$.) Notice that $t_{xy} > 0$ puts the lowest kinetic energy at one point, namely $k = 0$, in Fourier space. The condition $t_{xy} < 0$ puts it at the edge of the Brillouin zone, and thus the lowest kinetic energy can be highly degenerate. The physical intuition is then quite different in the two cases—a fact that should not be lost sight of because of the hole-particle symmetry that holds for bipartite graphs. The proof in [TH1] shows that negative, not positive t_{xy} is the *natural mathematical assumption* for this theorem. If this upsets anyone's physical proclivity, that is a pity.

Theorem 2: *If $N = |\Lambda| - 1$, if $U_x = +\infty$ for all $x \epsilon \Lambda$, and if $t_{xy} \leq 0$ for all x, y, then the ground state has total spin $S = N/2$. This state is unique up to the trivial $(N+1)$–fold degeneracy if Λ satisfies a certain connectivity condition [TH1].*

The connectivity condition mentioned above is not stringent and it holds for all regular lattices in dimension greater than one (see also [AL]). Essentially it means that there are loops that permit nontrivial permutations of the particles.

In the case that Λ is completely translation invariant, i.e., that all vertices of Λ are equivalent, as is the case on a hypercubic lattice on a torus, a different proof of the theorem, very similar to Nagaoka's, was given by Tian [TG1] and by Trugman [TS].

The obvious next question to ask is this: *If there is more than one hole ($N < |\Lambda| - 1$) and $U = +\infty$, is the ground state totally ferromagnetic, i.e., is $S = N/2$?* There can be no simple general theorem because numerical calculation on small systems show that the answer seems to be "no" and, at the same time, no simple pattern seems to emerge. Yet there are a few theoretical results, as follows.

(i) The Nagaoka-Tian-Trugman method can be generalized for $\Lambda =$ the D-dimensional hypercubic lattice with periodic boundary conditions and with $t_{xy} = t =$ nonpositive constant to show [TG2, TG3, TS, SQT] that the completely magnetized state energy, $E(S = N/2; \Lambda)$, when compared to the actual ground state energy, $E(\Lambda)$, satisfies

$$\lim_{\Lambda \to \infty} E(S = N/2; \Lambda) - E(\Lambda) = 0 \tag{3.8}$$

in the thermodynamic limit, $\Lambda \to \infty$, when the number of holes $N_h = |\Lambda| - N$ is not too large. The best result is by Shen, Qiu and Tian [SQT], which gives (3.8) when $N_h < |\Lambda|^\alpha$ with $0 < \alpha < 2/(D + 2)$. Note that we do not divide by $|\Lambda|$ in (3.8), which thus truly represents the vanishing of a gap. The proof here is elegant and simple. However, one would expect (3.8) to hold as long as $N_h/|\Lambda| \to 0$ as $|\Lambda| \to 0$.

(ii) If there are many holes, $N_h/|\Lambda| > 0.49$ for the $D = 2$ or $N_h/|\Lambda| > 0.32$ for the $D = 3$ hypercubic lattices, and $\Lambda \to \infty$ as in (i) then

$$E(S = N/2; \Lambda) - E(S = N/2 - 1; \Lambda) \not\to 0. \tag{3.9}$$

There really is an instability of the $S = N/2$ state with respect to one spin flip. This was proved by Shastry, Krishnamurthy and Anderson [SKA]; see also [SA1]. The estimate was improved to $N_h/|\Lambda| > 0.29$ by von der Linden and Edwards [LvE]; Hanisch and Müller-Hartmann [HM] simplified the calculation (but not the estimate of 0.29).

(iii) Several authors [DW, FRDS, SA1, TB] were able to prove, for a translation invariant hypercubic lattice model, that when there are two holes the ground state energies satisfy $E(S = N/2-1; \Lambda) < E(S = N/2; \Lambda)$. However, assumptions have to be made about the relative lengths of the sides. Sütő [SA1] extended this to $2, \ldots, 6$ holes for a bcc lattice.

(iv) Sütő [SA2] shows, as expected, that the energy splitting needed for demagnetization is, in any case, negligible. He proves that $M(\beta, h, \rho)$, the magnetization per site in field h at density $\rho = N/|\Lambda|$ satisfies (in the thermodynamic limit) $M(\beta, h, \rho) \to \tanh(\beta h)$ as $\rho \to 1$.

The results in (ii) and (iii) are achieved with a variational calculation. The value of $E(S = N/2; \Lambda)$ is easy to find exactly because it equals the energy of spinless electrons, i.e.,

$$E(S = N/2; \Lambda) = \sum_{j=1}^{N} \lambda_j(T) \tag{3.10}$$

for any Λ and hopping matrix, T, and in which $\lambda_1(T) \le \lambda_2(T) \le \cdots$ are the eigenvalues of T. Thus, the hard problem is to find a good variational function with $S = N/2 - 1$, and this appears to be extraordinarily difficult. Why? No one seems to know! And why is it so difficult to treat $S = N/2 - 2$?

These results, (i)–(iii), show that one cannot expect $S = N/2$ except when $N = |\Lambda| - 1$, but one can ask the following.

Problem 2: *With $U = +\infty$, for which $\rho := N/|\Lambda|$ is it true that some (if there is more than one) ground state has $S/|\Lambda| > 0$ in the thermodynamic limit $\Lambda \to \infty$?*

This brings us to two more open problems about the $U = +\infty$ case; the first is a corollary of the second. We take a large Λ and N particles and suppose that the thermodynamic limit $\Lambda \to \infty$ with $\rho = N/|\Lambda|$ fixed is well defined. We set $S =$ spin of the ground state (the maximum such spin if there is more than one ground state) and we set $S_{\max} = N/2$. We also assume that $t_{xy} \ge 0$ for all x and y. Then

Problem 3: *Prove or disprove that*

$$\lim_{\rho \to 0} \lim_{\Lambda \to \infty} \quad S/S_{\max} = 0. \tag{3.11}$$

Problem 4: *Does there exist some number $\rho_c > 0$ such that*

$$\lim_{\Lambda \to \infty} S/S_{\max} = 0 \quad \textit{for all } \rho < \rho_c\,? \tag{3.12}$$

The requirement that $t_{xy} \ge 0$ is important. As we shall see in Sect. D, Mielke's work shows that there can be nice, periodic lattices in any dimension (such as the kagome lattice in two-dimensions) for which $S = S_{\max}$ for all $\rho < \rho_c$ with $\rho_c > 0$, thereby contradicting (3.11) and (3.12). To achieve this, however, one needs $t_{xy} \le 0$. Perhaps (3.11) and (3.12) hold in the case $t_{xy} \le 0$ if we replace "maximum such spin" by "average of such spins", because Mielke's and Tasaki's examples have highly degenerate ground states with spins ranging from 0 to $N/2$.

Closely related in spirit to Theorem 2, but with an interesting, different proof, is the result of Chakravarty, Chayes and Kivelson [CCK]. They start with a half-filled band, $N = |\Lambda|$, and U large. Then they add or subtract one or two particles, and define $E_n := E(N = |\Lambda| + n)$ for $-2 \le n \le +2$. They then define

$$\Delta_e = 2E_1 - E_2 - E_0$$

$$\Delta_h = 2E_{-1} - E_{-2} - E_0. \tag{3.13}$$

The interpretation of Δ_e is as a 2-particle binding energy, while that of Δ_h is as a 2-hole binding energy. The picture of Δ_e, for example, is that given two very large systems at half-filling, and given two extra electrons, is it energetically favorable to add the two electrons to one system ($\Delta_e > 0$), or is it favorable to add one electron to each system ($\Delta_e < 0$)? The former, $\Delta_e > 0$, connotes **pair binding**.

It is pointed out in [CCK] that $\Delta_e \le 0$ and $\Delta_h \le 0$ when $U = 0$, but they quote numerical studies showing that $\Delta_e > 0$ and $\Delta_h > 0$ for some U and some Λ. They prove, however, that in the limit $U \to \infty$, $\Delta_e \le 0$ if all t_{xy} are nonnegative and $\Delta_h \le 0$ if all t_{xy} are nonpositive. For a bipartite graph the sign does not matter (as long as all t_{xy} are positive or all are negative), and thus $\Delta_e \le 0$ and $\Delta_h \le 0$ in this case. They interpret this result to mean that the numerical positive binding results are only an intermediate U phenomenon but, strictly speaking, the (unlikely) alternatives $\Delta_e = 0$ and $\Delta_h = 0$ in their theorems would first have to be eliminated.

D. Another Path to Ferromagnetism.

The one-hole, $U = +\infty$ model is not the only one known to have *saturated* ferromagnetism (i.e., $S = N/2$). Mielke [Mi1] and later Tasaki [TH2] and then both [MT] found interesting, but very special models with this property.

The basic idea is to find a graph Λ and a hopping matrix T such that the lowest eigenvalue of T (call it λ_0) is highly degenerate; in fact we want the degeneracy to be at least N and, to be interesting, we want that to be of the order of $|\Lambda|$. Let N_0 denote the degeneracy of this lowest eigenvalue and denote the space of these eigenfunctions by $\mathcal{H}_0$. If $U_x \ge 0$ for all $x \in \Lambda$, it is easy to see that if $N = N_0$ then

(i) There is a ground state having $S = N_0/2$.

(ii) The state is simply a determinant formed from the N_0 vectors in $\mathcal{H}_0$ and its energy is $N_0\lambda_0$.

(iii) The ground state is unique if certain additional conditions (known to be optimal) are met [Mi1].

If $N < N_0$ the ground state manifold will contain at least one state with $S = N/2$, but perhaps others as well (see [Mi1]).

A comparison with Theorem 1 is interesting, but it is not clear whether or not it is misleading. Note that the $S = \big||A| - |B|\big|/2$ result there for a bipartite graph and a half-filled band was somehow related to the $\big||A| - |B|\big|$-fold degeneracy of the zero-mode of T. Thus, a common feature is degeneracy, and it is often said that itinerant ferromagnetism is associated with atomic or kinetic energy degeneracy. But there are also important differences:

(i) The spin in Theorem 1, while it might be proportional to $|\Lambda|$, is not $N/2 = |\Lambda|/2$.

(ii) No fine tuning of T or of Λ was needed for Theorem 1. All that was needed was the bipartite structure, the positivity of the U_x's and the reality of the t_{xy}'s.

Mielke's way of achieving the degeneracy N_0 is to start with some graph G and then to set $\Lambda = L(G)$, the **line graph of G**, which is defined as follows. Make a mark in the center of every edge of G; those marks will be the sites of $L(G)$. Two sites are connected by an edge in $L(G)$ if the two edges of G on which they reside have a G-site in common. Note that $L(G)$ is never bipartite, except for the trivial case of a ring. A well known example of a line graph is the kagome lattice. (Incidentally, kagome is not a person—it is a pattern of woven bamboo.)

The hopping matrix T is defined to be $-t < 0$ on every edge of $\Lambda = L(G)$. Not only is there a restriction on the magnitude of t_{xy} but we see, once again, that negative t_{xy} is the natural sign—as it is for Theorem 2.

Of course, as Mielke and Tasaki note, and as is also true in Theorem 2, one can convert positive t_{xy} into negative t_{xy} by a hole-particle transformation on both spin $\uparrow$ and spin $\downarrow$. This does not alter the interaction or the total spin, S, but it changes N into $N' = 2|\Lambda| - N$. For positive, t_{xy}, then, we can transform to the negative t_{xy} situation and conclude that $S = N'/2$ when $N' \leq N_0$. This translates into $S = |\Lambda| - N/2$ when $N \geq 2|\Lambda| - N_0$ (and not $\leq$). This construction would yield saturated ferromagnetism, $S = N/2$, only at $N = |\Lambda|$ (half-filled band), provided it were possible to achieve $N_0 \geq |\Lambda|$; this is clearly impossible (unless $T = 0$), so the positive t_{xy} choice does *not* yield the desired saturated ferromagnetism. However, it is still possible to have unsaturated ferromagnetism, i.e. $1 > 2S/N \neq 0$ in the thermodynamic limit. By taking $N = 2|\Lambda| - N_0$ and $S = |\Lambda| - N/2$ we have $2S/N = N_0/(2|\Lambda| - N_0)$. (One *can* reasonably argue, however, that the condition $S = |\Lambda| - N/2$ *is indeed* saturated ferromagnetism because this value of the spin is the maximum possible one when $N > |\Lambda|$, given the constraints of the sytem and given the Pauli principle. The system is constrained by allowing only a limited number of states for the electrons, i.e., two per site. I leave the semantic resolution to the reader.)

The homology of G determines $\mathcal{H}_0$ in a simple way. Pick any closed, self avoiding path in G of even length. This path corresponds, in an obvious way, to a closed path, P, of the same length in $L(G)$. If, now, we take the vector $\phi(x) = 0$ for x not a vertex of P and $\phi(x) =$ alternately $+1$ and -1 as we traverse the vertices of P, we see at once that ϕ is an eigenvector with eigenvalue $-2t$. It is also not hard to prove that $-2t$ cannot be improved, i.e., $\lambda_0 = -2t$. Moreover, this construction yields all of $\mathcal{H}_0$.

In [TH2, MT] essentially the same result as Mielke's (with similar requirements on T) is achieved, but with certain decorated lattices with next nearest neighbor hoppings. The ferromagnetism of [TH2, MT] is shown to be stable under small change of the electron density, by using a "grand canonical ensemble" with a fixed electron density. It is also proved that there is a transition to a paramagnetic phase as one decreases the electron density. Thus (3.11) and (3.12) (with S replaced by its grand canonical average) are proved for these special graphs.

In all cases, the eigenvectors in $\mathcal{H}_0$ can all be taken to have compact support, i.e., each $\phi(x)$ vanishes except on a finite set of sites of Λ, and each such set is independent of Λ once Λ is large enough to include the set. This property leads to the result [MT] that the effective Hamiltonian, in a suitable subspace of states that includes the ground states, can be written exactly as a Heisenberg Hamiltonian.

4. The Flux Phase Problem

Very little seems to be known rigorously about the effect of a magnetic field on the orbital motion, that is, if we set

$$t_{xy} = |t_{xy}| \exp[i\theta_{xy}], \qquad \theta_{xy} = \int_x^y A \cdot ds \tag{4.1}$$

for some vector potential A. The spin of the ground state might well change. The known proofs of Theorems 1 and 2 fail when $A \neq 0$. If, indeed, the spin of the ground state changes then we have a new kind of "magnetic field—spin" interaction, brought about by the Pauli exclusion principle. Indeed, something similar is discussed in the one-dimensional context in [FK1].

The energy certainly does change, and it is by now well known that when $U = 0$ the zero flux state does *not* give the lowest ground state energy. When Λ is a square lattice and when $N = |\Lambda|$, it is conjectured that the *maximum* (!) possible flux, namely π in each square ($t_{12}t_{23}t_{34}t_{41} = -1$ around a square), is optimum. (For a survey of this question and for some rigorous results about it see [LL2].) The same conjecture has been made for $U \neq 0$.

Problem 5: *Solve the flux phase problem for $U \neq 0$ (or even for $U = 0$) for a half-filled band on a square lattice.*

The moral of this story is that the Pauli exclusion principle can really upset our ideas about diamagnetism. For one solitary electron, the imposition of a magnetic field raises the ground state energy. For many electrons it can and does lower the energy. It is trivially true, for example, that when $U = +\infty$ and $N = |\Lambda|$, or $U =$ anything and $N = 2|\Lambda|$, a magnetic field has absolutely no effect on the energy.

5. Uniform Density Theorem

The hole-particle transformation has remarkable consequences for the Hubbard model on a bipartite graph with a half-filled band, $N = |\Lambda|$. The ideas given below are well known to chemists—less so to physicists. They go back to Coulson and Rushbrooke [CR] for the $U = 0$ case, and to MacLachlan [MA] who generalized them to many interacting models—including the Hubbard model as a special case. A simplified proof together with an extension to models involving explicity spin-spin interactions (such as the $t - J$ model), and to the Falicov-Kimball model, is given in [LLM].

The results apply equally to three cases: (a) The canonical Gibbs state with $N = |\Lambda|$; (b) The grand-canonical Gibbs state with zero chemical potential; (c) The ground state with $N = |\Lambda|$ and which is defined, in case of degeneracy, to be the $\beta \to \infty$ limit of the canonical Gibbs state. The one-body density matrix $\rho_\sigma(x, y)$ is the expectation value of $c^\dagger_{x\sigma} c_{y\sigma}$ in the state in question.

Theorem 4: *For a half-filled band on a bipartite lattice, the one-body density matrix for each of the above states satisfies (for each $\sigma =\uparrow$ or $\downarrow$).*

$$\rho_\sigma(x, y) = \tfrac{1}{2}\delta_{xy} \qquad \textit{if } x, y \epsilon A \textit{ or } x, y \epsilon B. \tag{5.1}$$

If $x \epsilon A$ and $y \epsilon B$, nothing simple can be said. Note that the theorem does *not* require T to be real, and is thus one of the few theorems that applies to complex t_{xy}. However, a true, physical magnetic field would also act on the electron spins and thereby vitiate the hole-particle symmetry needed for the proof.

The complex case is a bit subtle, for it uses more than just a hole-particle transformation (call it W). It also utilizes the nonlinear antiunitary map J that maps a vector ψ, considered as a polynomial in the $c^\dagger_{x\sigma}$'s applied to the vacuum, into the vector ψ^* corresponding to the polynomial with complex conjugate coefficients. While J is nonlinear, JKJ is linear when K is any linear operator, and $TrJKJ = (TrK)^*$. The antiunitary $Y = JW$ satisfies $Y = JW = WJ$ (and hence $Y^2 = \mathbf{1}$) and $Yc_{x\sigma}Y = Wc_{x\sigma}W$. Most important is the invariance of the Hamiltonian, $YHY = H$, which replaces the hole particle invariance, $WHW = H$, which fails for complex T.

What is the significance of this result? It seems to contradict the conjecture in Problem 1 that there can be antiferromagnetic, i.e., staggered, LRO. Such an ordering can occur only in the thermodynamic limit and it has the property that for every state with ordering $\uparrow\downarrow\uparrow\downarrow \cdots$ there is a state with ordering $\downarrow\uparrow\downarrow\uparrow \cdots$. The point about Theorem 4, applied to the thermodynamic limit, is that for every state with ordering there is an equally good state (obtained by changing boundary conditions) with the opposite ordering, and on the average each site will have the same density for each spin value. In other words, *there is no way to adjust the potentials U_x or the hopping matrix t_{xy} in a clever way so as to enhance the occupation of certain sites* — in a manner independent of boundary conditions. This stability is remarkable and, although it is not true for real materials, the theorem hints at some kind of remnant stability that might transcend the overly idealized assumptions needed for its proof.

Problem 6: *Is there any residue of (5.1) when $N \neq |\Lambda|$?*

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