Letters in Mathematical Physics **22** 321–333, 1991.

Failure of Saturated Ferromagnetism for the Hubbard Model with Two Holes

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(Received: 1 May 1991; revised version: 5 June 1991)

Abstract. We consider the Hubbard model on a finite set of sites with nonpositive hopping matrix elements and infinitely strong on-site repulsion. Nagaoka's theorem states that in this model the relative ground state in the sector with one unoccupied site is maximally ferromagnetic. We show that this phenomenon is a consequence of a combinatorial coincidence valid in the one-hole regime only. In the case of more than one hole there is no reason to expect maximally ferromagnetic ground states. We prove this claim for the case of two holes for models defined on a class of graphs which contains all tori that are not too small.

AMS subject classifications (1991). 81Q99, 81V70, 82B10.

1. Introduction

Let $\mathcal{V}=\{1,2,\ldots,V\}$ be a finite set and $(t_{a,b})_{(a,b)\in\mathcal{V}\times\mathcal{V}}$ a matrix satisfying

$$\begin{aligned} t_{a,b}&=t_{b,a}\geqslant 0, &&(\forall a,b\in\mathcal{V}),\\ t_{a,a}&=0, &&(\forall a\in\mathcal{V}). \end{aligned} \tag{1.1}$$

We consider the Hubbard model on the set of sites $\mathcal{V}$ with the (formal) Hamiltonian

$$H=-\tfrac{1}{2}\sum_{x,y\in\mathcal{V}}\sum_{\sigma=\uparrow\downarrow}t_{x,y}(c^{+}_{x\sigma}-c^{+}_{y\sigma})(c_{x\sigma}-c_{y\sigma})+\frac{U}{2}\sum_{x\in\mathcal{V}}n_x(1-n_x) \tag{1.2}$$

with infinitely strong on-site repulsion between the particles: $U=+\infty$. Notice the minus sign in front of the kinetic energy term, it is of crucial importance in the present setup. Its physical meaning is that the exchange integrals between the different sites $x,y\in\mathcal{V}$ are *negative*.

As the pair interaction is spin independent, the Hamiltonian conserves the number of spin-up and spin-down particles separately. Throughout this Letter h, m, n will denote a triplet of nonnegative integers with the sum $h+m+n=V$: m and n is the number of spin-up and spin-down particles, h is the number of holes (=unoccupied sites). (Due to the hard core repulsion, there are no doubly occupied

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sites.) We denote by $\mathscr{H}_{m,n}$ the sector (subspace) with m spin-up and n spin-down particles and by $H_{m,n}$ the restriction of H to $\mathscr{H}_{m,n}$. It is easy to see, that

$$[[m+n=m'+n'] \wedge [\max\{m,n\} \geqslant \max\{m',n'\}]] \Rightarrow [\operatorname{spec}(H_{m,n}) \subset \operatorname{spec}(H_{m',n'})]$$

since by a rotation in spin space one can lift isometrically $L: \mathscr{H}_{m,n} \to \mathscr{H}_{m',n'}$ changing the Hamiltonian canonically: $LH_{m,n} = H_{m',n'}L$. In particular, we always have

$$\varepsilon_{m+n,0} \geqslant \varepsilon_{m,n}, \tag{1.3}$$

where $\varepsilon_{m,n}$ stands for the ground-state energy of $H_{m,n}$.

Nagaoka's theorem (see [2, 4, 6]), stated in [5] in its most general form, says that under the conditions stated above

$$[m+n=V-1] \Rightarrow [\varepsilon_{m+n,0} = \varepsilon_{m,n}]. \tag{1.4}$$

and if some additional connectivity condition is satisfied (see, e.g., [5]), then the ground states $\varepsilon_{m,n}$, $m+n=V-1$ are nondegenerate. This means that in the $V-1$ particle (one hole) sector $\oplus_{m+n=V-1} \mathscr{H}_{m,n}$, the global ground state is *maximally ferromagnetic* and this ground state is unique up to the $(V-1)$-fold degeneracy due to rotation in spin space. The phenomenon was considered interesting, since it might have provided some insight into the mechanism of itinerant ferromagnetism.

In this Letter, we consider the same problem in the case of more than one hole. In the second section, we give a nonstandard, alternative representation of the Hamiltonians $H_{m,n}$ from which clearly emerges the *combinatorial reason* why Nagaoka's theorem holds for the case of one hole and why there is absolutely no reason whatsoever to expect a similar theorem to hold in the case of more than one hole. The last two sections are devoted to the case $h=2, m=1, n=V-3$. In Section 3 we give an upper bound on $\varepsilon_{1,V-3}$ in terms of some more easily handlable operator. Using this bound, in Section 4 we show that $\varepsilon_{1,V-3} < \varepsilon_{0,V-2}$ for the Hubbard Hamiltonian (1.2), defined on graphs of the form $\mathscr{T}_l \times \mathscr{R}$, where $\mathscr{T}_l$ is the one-dimensional torus of length $l \geqslant l_0$ and $\mathscr{R}$ is an *arbitrary* graph with first nonzero eigenvalue not less than the first nonzero eigenvalue of $\mathscr{T}_l$. Consequently, in these models the global ground state in the two-hole sector is *not* maximally ferromagnetic. Thus, we may conclude that Nagaoka's theorem is the consequence of a combinatorial coincidence valid in the one-hole regime only and it cannot provide a mechanism of itinerant ferromagnetism. However, let us mention here that an alternative mechanism of itinerant (anti-) ferromagnetism has been considered recently by Lieb in [3], where the results and ideas of [1] are further developed.

Some terminology: Given a finite set $\tilde{\mathscr{V}}$ and a matrix $(t_{a,b})_{(a,b) \in \mathscr{V} + \mathscr{V}}$ satisfying (1.1) we call the linear operator

$$\Delta: l_2(\tilde{\mathscr{V}}, \mathbb{C}) \to l_2(\tilde{V}, \mathbb{C}), \qquad -[\Delta f](x) = \sum_{y \in \mathscr{V}} t_{x,y}(f(x) - f(y)) \tag{1.5}$$

a *discrete Laplacian*. The reason for calling it so is that Δ is the generator of a continuous time random walk on $\mathscr{V}$, as the Laplacian is the generator of Brownian motion in continuous space and the operator Δ has very similar properties to the Laplacian. Discrete Laplacians defined on various sets $\mathscr{V}$ will emerge at a later stage. $-\Delta$ is always a positive operator. If unrestricted, its lowest eigenvalue is always 0, the corresponding eigenspace is $f(x) = \text{const}$. If the matrix $(t_{a,b})_{(a,b) \in \mathscr{V} \times \mathscr{V}}$ is the incidence matrix of a nonoriented graph $\mathscr{G} = (\mathscr{V}, \mathscr{E})$ with vertex set $\mathscr{V}$ and edge set $\mathscr{E}$, i.e.

$$t_{a,b} = \begin{cases} 1, & \text{if } (a, b) \in \mathscr{E}, \\ 0, & \text{otherwise}, \end{cases} \tag{1.6}$$

then we say that Δ is the discrete Laplacian of the graph $\mathscr{G}$. In the concrete examples of the last section, discrete Laplacians associated with different graphs will arise.

2. An Alternative Representation of the Hamiltonian

The natural representation of the sector with m spin-up and n spin-down fermions is

$$\begin{aligned} \mathscr{H}_{m,n} = \{ f \in l_2(\mathscr{V}^m \times \mathscr{V}^n, \mathbb{C}) \mid & \\ & [\forall \rho \in \mathscr{P}_m, \forall \sigma \in \mathscr{P}_n : f(\bar{x}_{\rho(i)} ; \bar{y}_{\sigma(j)}) = \text{sign}(\rho)\ \text{sign}(\sigma) f(\bar{x}_i ; \bar{y}_j)] \wedge \\ & \wedge [(\exists (i, j) \in \{1, \ldots, m\} \times \{1, \ldots, n\} : x_i = y_j) \Rightarrow f(\bar{x}_i ; \bar{y}_j) = 0] \} \end{aligned} \tag{2.1}$$

where $\mathscr{P}_r$ denotes the group of permutations of r indices $\{1, 2, \ldots, r\}$ and the shorthand notation $\bar{x}_i = (x_1, \ldots, x_m), \bar{y}_j = (y_1, \ldots, y_n)$, etc., has been used. The antisymmetry condition is due to the Fermi–Dirac statistics and the second, Dirichlet-type condition is the precise formulation of the hard core repulsion between the particles. The Hamiltonian acting on this sector is

$$\begin{aligned} [H_{m,n} f](\bar{x}_i ; \bar{y}_j) = - \prod_{i=1}^{m} \prod_{j=1}^{n} (1 - \delta_{x_i, y_j}) \times & \\ \times \Bigg(\sum_{i=1}^{m} \sum_{\xi \in \mathscr{V}} & t_{x_i, \xi} (f(x_1, \ldots, x_i, \ldots, x_m ; \bar{y}_j) - \\ & - f(x_1, \ldots, \xi, \ldots, x_m ; \bar{y}_j)) + \\ & + \sum_{j=1}^{n} \sum_{\eta \in \mathscr{V}} t_{y_j, \eta} (f(\bar{x}_i ; y_1, \ldots, y_j, \ldots, y_n) - \\ & - f(\bar{x}_i ; y_1, \ldots, \eta, \ldots, y_n)) \Bigg). \end{aligned} \tag{2.2}$$

We are going to define now another representation of the same sector and the Hamiltonian. This new representation might look less natural at the first glance but, hopefully, at the end of this section the reader will be convinced that the combinatorial aspects become more transparent.

Denote

$$\begin{aligned}\mathscr{V}_{h,m,n} = \{(\bar{z}_k, X, Y) \in \mathscr{V}^h \times P(\mathscr{V}, m) \times P(\mathscr{V}, n) \mid \\ [X \cap Y = \emptyset] \wedge [\forall k \in \{1, \dots, h\} : z_k \notin X \cup Y]\}\end{aligned} \tag{2.3}$$

where $P(\mathscr{V}, r)$ is the set of subsets of $\mathscr{V}$ with cardinality r. Let $\mathscr{K}_{h,m,n}$ be the following Hilbert space:

$$\mathscr{K}_{h,m,n} = \{\phi \in l_2(\mathscr{V}_{h,m,n}, \mathbb{C}) \mid (\forall \pi \in \mathscr{P}_h) : \phi(\bar{z}_{\pi(k)}, X, Y) = \operatorname{sign}(\pi)\phi(\tilde{z}_k, X, Y)\}. \tag{2.4}$$

Remark. Clearly, the notation is slightly redundant: it would be enough to keep only the $\bar{z}_k$ and X (or, alternatively, the $\bar{z}_k$ and Y) variables. However, for aesthetical reasons, we prefer to keep this notation for the moment. In the next section, we shall drop the notation of the third, redundant variable (e.g. $\mathscr{V}_{h,m,n}$ and $\mathscr{K}_{h,m,n}$ will be denoted by $\mathscr{V}_{h,m}$ and $\mathscr{K}_{h,m}$, etc.)

The dimensions of the spaces $\mathscr{H}_{m,n}$ and $\mathscr{K}_{h,m,n}$ are the same:

$$\dim(\mathscr{H}_{m,n}) = \dim(\mathscr{K}_{h,m,n}) = \frac{V!}{h!m!n!}.$$

Next we define a unitary mapping of $\mathscr{H}_{m,n}$ onto $\mathscr{K}_{h,m,n}$. Fix once and for all an ordering of the sites in $\mathscr{V}$, say $1, 2, \dots, V$, and define the function

$$s : \mathscr{V}^V \to \{-1, 0, 1\}, \quad s(\xi_1, \dots, \xi_V) = \sum_{\pi \in \mathscr{P}_V} \operatorname{sign}(\pi) \prod_{l=1}^{V} \delta_{\xi_l, \pi(l)}. \tag{2.5}$$

In plain words, $s(\xi_1, \dots, \xi_V)$ is zero if two different variables coincide, otherwise it is $+1$ or -1 according to the sign of the permutation of the elements of $\mathscr{V}$. Let the linear operator $U : \mathscr{H}_{m,n} \to \mathscr{K}_{h,m,n}$ be defined by

$$[Uf](\bar{z}_k, X, Y) = (h!)^{-1/2} s(\bar{z}_k, \bar{x}_i, \bar{y}_j) f(\bar{x}_i; \bar{y}_j), \tag{2.6}$$

where $\bar{x}_i = (x_1, \dots, x_m)$ and $\bar{y}_j = (y_1, \dots, y_n)$ are *arbitrary* orderings of the elements of the sets X, respectively Y. It is easy to check that U is an isometry and its adjoint is $U^* : \mathscr{K}_{h,m,n} \to \mathscr{H}_{m,n}$, defined by

$$[U^*g](\bar{x}_i; \bar{y}_j) = \begin{cases} (h!)^{1/2} s(\bar{z}_k, \bar{x}_i, \bar{y}_j) g(\bar{z}_k, X, Y), & \text{if } X \cap Y = \emptyset, \\ 0, & \text{if } X \cap Y \neq \emptyset, \end{cases} \tag{2.7}$$

where

$$X = \{x_1, \dots, x_m\}, \qquad Y = \{y_1, \dots, y_n\} \quad \text{and} \quad \bar{z}_k = (z_1, \dots, z_h)$$

is an *arbitrary* ordering of the elements of the set $Z = \mathscr{V} \setminus (X \cup Y)$. We want to find the new representation

$$\hat{H}_{h,m,n} = U H_{m,n} U^* \tag{2.8}$$

of the Hamiltonian.

Define the matrix $T\colon \mathscr{V}_{h,m,n} \times \mathscr{V}_{h,m,n} \to \mathbb{R}$ as follows:

$$T_{(\bar{z}_k, X, Y),(\bar{z}'_k, X', Y')} = \begin{cases} t_{a,b}, & \text{if } \mathbf{A} \wedge (\mathbf{B} \vee \mathbf{C} \vee \mathbf{D}), \\ 0, & \text{otherwise}, \end{cases} \tag{2.9}$$

where the conditions **A**, **B**, **C** and **D** are the following:

$$\mathbf{A} := (\exists k \in \{1, \ldots, h\}) : [z_k = a, z'_k = b] \wedge [(l \neq k) \Rightarrow (z_l = z'_l)],$$

$$\mathbf{B} := [X = X'] \wedge [Y \circ Y' = \{a, b\}],$$

$$\mathbf{C} := [Y = Y'] \wedge [X \circ X' = \{a, b\}],$$

$$\mathbf{D} := [X = X'] \wedge [Y = Y']$$

and the linear operator $\Delta_{h,m,n}$ on $\mathscr{K}_{h,m,n}$:

$$\begin{aligned} &-[\Delta_{h,m,n}\phi](\bar{z}_k, X, Y) \\ &\quad = \sum_{(\bar{z}'_k, X', Y') \in \mathscr{V}_{h,m,n}} T_{(\bar{z}_k, X, Y),(\bar{z}'_k, X' Y')}(\phi(\bar{z}_k, X, Y) - \phi(\bar{z}'_k, X', Y')). \end{aligned} \tag{2.10}$$

The operator $\Delta_{h,m,n}$ is actually defined on the whole $l_2(\mathscr{V}_{h,m,n}, \mathbb{C})$, and $\mathscr{K}_{h,m,n} \subset l_2(\mathscr{V}_{h,m,n}, \mathbb{C})$ is an invariant subspace of it. Further, let us denote by $I_{h,m,n}$ the identity in $\mathscr{K}_{h,m,n}$.

PROPOSITION 1.

$$\hat{H}_{h,m,n} = -\left(\sum_{a,b \in \mathscr{V}} t_{a,b}\right) I_{h,m,n} - \Delta_{h,m,n}. \tag{2.11}$$

We omit the lengthy but otherwise straightforward details of the proof of this proposition. However, we note that the basic ingredients of this are the identities

$$(h!)^{-1/2} s(\bar{z}_k, \bar{x}_i, \bar{y}_j)[U^* g](\bar{x}_i; \bar{y}_j) = g(\bar{z}_k, X, Y),$$

$$\begin{aligned} &(h!)^{-1/2} s(\bar{z}_k, \bar{x}_i, \bar{y}_j)[U^* g](x_1, \ldots, z_k, \ldots, x_m; \bar{y}_j) \\ &\quad = -g(z_1, \ldots, x_i, \ldots, z_h, X \circ \{x_i, z_k\}, Y), \end{aligned}$$

$$\begin{aligned} &(h!)^{-1/2} s(\bar{z}_k, \bar{x}_i, \bar{y}_j)[U^* g](\bar{x}_i; y_1, \ldots, z_k, \ldots, y_n) \\ &\quad = -g(z_1, \ldots, y_j, \ldots, z_h, X, Y \circ \{y_j, z_k\}), \end{aligned}$$

where

$$X = \{x_1, \ldots, x_m\}, \qquad Y = \{y_1, \ldots, y_n\},$$

in the second (third) equality on the left-hand side z_k replaces $x_i (y_j)$ and on the right-hand side $x_i (y_j)$ replaces z_k.

Remarks. (1) The first advantage of the representation (2.11) is principal: we clearly see from it why Nagaoka's theorem holds in the case of one hole and why there is no reason to expect a generalization of it for the case of more than one hole. Namely, in the case of one hole, the antisymmetry restriction on the $\bar{z}_k$ variables is void, i.e. $\mathscr{H}_{1,m,n} = l_2(\mathscr{V}_{1,m,n}, \mathbb{C})$, for all $m + n = V - 1$, and we know that in these cases the bottom of the spectrum for any one of the $-\Delta_{1,m,n}$ is 0 (this is true for any unrestricted discrete Laplacian). Thus, the ground state of the Hamiltonian in any one of the sectors $\mathscr{H}_{m,n}, m + n = V - 1$ has the same energy $-\Sigma_{a,b \in \mathscr{V}} t_{a,b}$. The nondegeneracy (up to rotation in spin space) of this ground state is a simple consequence of the connectivity condition formulated, e.g., in [5]. On the other hand, in the case of more than one hole, we have to compare the bottom of the spectra of the operators $-\Delta_{h,m,n}$ *restricted* to the proper subspaces $\mathscr{H}_{h,m,n} \subset l_2(\mathscr{V}_{h,m,n}, \mathbb{C})$. It is easy to see that

$$\mathrm{spec}(\Delta_{h,0,V-h}|_{\mathscr{H}_{h,0,V-h}}) \subset \mathrm{spec}(\Delta_{h,m,n}|_{\mathscr{H}_{h,m,n}}), \quad (\forall m, n): m + n = V - h$$

(see the lifting operator L defined in (3.15)), but we have no more reason for the coincidence of the bottom of the spectra. We also understand now why is the sign of the hopping matrix elements so crucial in Nagaoka's theorem: the bottom of the spectrum of $-\Delta$ is zero for any unrestricted discrete Laplacian, but there is no reason for coincidence of the top of the spectra.

(2) The technical advantage will become clear in the next section: in the case of few holes, the combinatorial aspects are more transparent in this representation.

3. $h = 2, m = 1, n = V - 3$: Preparation

The rest of this Letter is devoted to the case $h = 2, m = 1, n = V - 3$, i.e. two holes and total spin in the z-direction, one less than the possible maximum. More exactly, we want to find conditions under which the lowest eigenvalue of $-\Delta_{2,1,V-3}$ restricted to $\mathscr{H}_{2,1,V-3}$ is strictly less than the lowest eigenvalue of $-\Delta_{2,0,V-2}$ restricted to $\mathscr{H}_{2,0,V-2}$. At this stage, the introduction of a less general notation is convenient. Namely, as pointed out in the remark after (2.4), we are allowed to drop the notation of the third, redundant variable (Y).

As we are going to use a couple of different vector spaces and discrete Laplacians, let us define them from the start. The discrete sets on which the functions of a 'different level' are defined, are

$$\mathscr{V} = \{1, 2, \ldots, V\}, \tag{3.1}$$

$$\mathscr{V}_{2,0} = \{(z_1, z_2) \mid z_1, z_2 \in \mathscr{V}\}, \tag{3.2}$$

$$\mathscr{V}_{2,1} = \{(z_1, z_2 \mid x) \mid z_1, z_2, x \in \mathscr{V}, z_1 \neq x \neq z_2\}, \tag{3.3}$$

$$\mathscr{V}_{2\neq} = \{(z, x) \mid z, x \in \mathscr{V}, z \neq x\}. \tag{3.4}$$

The corresponding Hilbert spaces are

$$\mathscr{H} = l_2(\mathscr{V}, \mathbb{C}) \tag{3.5}$$

$$\mathscr{H}_{2,0} = \{\phi \in l_2(\mathscr{V}_{2,0}, \mathbb{C}) \mid (\forall (z_1, z_2) \in \mathscr{V}_{2,0}): \phi(z_1, z_2) = -\phi(z_2, z_1)\} \tag{3.6}$$

$$\mathscr{K}_{2,1} = \{\phi \in l_2(\mathscr{V}_{2,1}, \mathbb{C}) \mid \forall (z_1, z_2 \mid x) \in \mathscr{V}_{2,1}) : \phi(z_1, z_2 \mid x) = -\phi(z_2, z_1 \mid x)\} \tag{3.7}$$

$$\mathscr{K}_{2\neq} = \left\{ \varphi \in l_2(\mathscr{V}_{2\neq}, \mathbb{C}) \mid [(\forall (z, x) \in \mathscr{V}_{2\neq}) : \varphi(z, x) = \varphi(x, z)] \wedge \right. \\ \left. \wedge \left[(\forall z \in \mathscr{V}) : \sum_{x \in \mathscr{V} \setminus \{z\}} \varphi(z, x) = 0 \right] \right\} \tag{3.8}$$

The different discrete Laplacians

$$\Delta_{\#} : \mathscr{K}_{\#} \to \mathscr{K}_{\#},$$

where $\#$ stands for any one of the subscripts, are defined as follows:

$$[-\Delta f](z) = \sum_{\zeta \in \mathscr{V}} t_{z,\zeta}(f(z) - f(\zeta)), \tag{3.9}$$

$$[-\Delta_{2,0}\phi](z_1, z_2) = \sum_{\zeta \in \mathscr{V}} t_{z_1,\zeta}(\phi(z_1, z_2) - \phi(\zeta, z_2)) + \\ + \sum_{\zeta \in \mathscr{V}} t_{z_2,\zeta}(\phi(z_1, z_2) - \phi(z_1, \zeta)), \tag{3.10}$$

$$[-\Delta_{2,1}\phi](z_1, z_2 \mid x) = \sum_{\zeta \in \mathscr{V} \setminus \{x\}} t_{z_1,\zeta}(\phi(z_1, z_2 \mid x) - \phi(\zeta, z_2 \mid x)) + \\ + \sum_{\zeta \in \mathscr{V} \setminus \{x\}} t_{z_2,\zeta}(\phi(z_1, z_2 \mid x) - \phi(z_1, \zeta \mid x)) + \\ + t_{z_1,x}(\phi(z_1, z_2 \mid x) - \phi(x, z_2 \mid z_1)) + \\ + t_{z_2,x}(\phi(z_1, z_2 \mid x) - \phi(z_1, x \mid z_2)), \tag{3.11}$$

$$[-\Delta_{2\neq}\varphi](z, x) = \sum_{\zeta \in \mathscr{V} \setminus \{x\}} t_{z,\zeta}(\varphi(z, x) - \varphi(\zeta, x)) + \\ \sum_{\xi \in \mathscr{V} \setminus \{z\}} t_{x,\xi}(\varphi(z, x) - \varphi(z, \xi)). \tag{3.12}$$

Remark. The operators $\Delta_{\#}$ are actually defined on the whole $l_2(\mathscr{V}_{\#}, \mathbb{C})$ and $\mathscr{K}_{\#} \subset l_2(\mathscr{V}_{\#}, \mathbb{C})$ are invariant subspaces of $\Delta_{\#}$. It is clear that $\mathscr{K}_{2,0}$, $\mathscr{K}_{2,1}$, $\Delta_{2,0}$, and $\Delta_{2,1}$ are the same as $\mathscr{K}_{2,0,V-2}$, $\mathscr{K}_{2,1,V-3}$, $\Delta_{2,0,V-2}$, and $\Delta_{2,1,V-3}$ of the previous section.

The bottom of the spectrum of $-\Delta_{\#}$, $\# = (2, 0), (2, 1), (2\neq)$, is given by the variational formula

$$\lambda_{\#}^{*} = \inf_{\phi \in \mathscr{K}_{\#}} \frac{\langle \phi, -\Delta_{\#}\phi \rangle_{\#}}{\langle \phi, \phi \rangle_{\#}} \tag{3.13}$$

and we trivially have

$$\lambda_{2,0}^{*} = \lambda^{*} = \inf \left\{ \frac{\langle f, -\Delta f \rangle}{\langle f, f \rangle} \,\middle|\, f \in l_2(\mathscr{V}, \mathbb{C}), \sum_{z \in \mathscr{V}} f(z) = 0 \right\}. \tag{3.14}$$

There is a natural lifting of $\mathscr{H}_{2,0}$ to $\mathscr{H}_{2,1}$:

$$L: \mathscr{H}_{2,0} \to \mathscr{H}_{2,1}, \qquad [L\phi](z_1, z_2 \mid x) = \phi(z_1, z_2), \tag{3.15}$$

such that

$$L\Delta_{2,0} = \Delta_{2,1} L. \tag{3.16}$$

From this equality, it follows that the spectrum of $\Delta_{2,0}$ is contained in the spectrum of $\Delta_{2,1}$ and if we want to find an eigenvalue of $\Delta_{2,1}$ not belonging to the spectrum of $\Delta_{2,0}$, then we have to concentrate on the subspace

$$\operatorname{Ran}(L)^\perp = \left\{ \phi \in \mathscr{H}_{2,1} \mid (\forall z_1, z_2 \in \mathscr{V}): \sum_{x \in \mathscr{V} \setminus \{z_1, z_2\}} \phi(z_1, z_2 \mid x) = 0 \right\}. \tag{3.17}$$

On the other hand, knowing that the eigenfunction belonging to the lowest eigenvalue of $-\Delta_{2,0}$ is of the form $\phi(z_1, z_2) = \varphi(z_1) - \varphi(z_2)$, it is not completely out of the blue to try to minimize $\langle \phi, -\Delta_{2,1}\phi \rangle_{2,1} / \langle \phi, \phi \rangle_{2,1}$ on the subspace

$$\mathscr{S} = \{ \phi \in \mathscr{H}_{2,1} \mid \phi(z_1, z_2 \mid x) = \varphi(z_1, x) - \varphi(z_2, x) \}, \tag{3.18}$$

and, after some straightforward calculations, we find that the intersection of the subspaces $\operatorname{Ran}(L)^\perp$ and $\mathscr{S}$ is

$$\operatorname{Ran}(L)^\perp \cap \mathscr{S} = \operatorname{Ran}(M) \tag{3.19}$$

where M is the linear operator

$$M: \mathscr{H}_{2\neq} \to \mathscr{H}_{2,1}, \qquad [M\varphi](z_1, z_2 \mid x) = \varphi(z_1, x) - \varphi(z_2, x). \tag{3.20}$$

That is how the space $\mathscr{H}_{2\neq}$ arises. Next we minimize $\langle \phi, -\Delta_{2,1}\phi \rangle_{2,1} / \langle \phi, \phi \rangle_{2,1}$ on the subspace $\operatorname{Ran}(M)$. Straightforward calculations show that for $\varphi \in \mathscr{H}_{2\neq}$

$$\langle M\varphi, M\varphi \rangle_{2,1} = 2(V-1)\langle \varphi, \varphi \rangle_{2\neq} \tag{3.21}$$

and

$$\langle M\varphi, -\Delta_{2,1} M\varphi \rangle_{2,1} = V\langle \varphi, -\Delta_{2\neq}\varphi \rangle_{2\neq}. \tag{3.22}$$

So we may conclude this section with the following proposition.

PROPOSITION 2.

$$\lambda^*_{2,1} \leq \frac{V}{2(V-1)} \lambda^*_{2\neq}. \tag{3.23}$$

Remark. The subspace $\operatorname{Ran}(M)$ *in general is not* an invariant subspace of $\Delta_{2,1}$, so the right-hand side of (3.23) is not necessarily an eigenvalue of $-\Delta_{2,1}$, just an upper bound on the bottom of its spectrum. Clearly, $\Delta_{2\neq}$ is much easier to handle than $\Delta_{2,1}$.

Exploiting this bound, in the next section, we shall prove, for a collection of examples, that $\lambda^*_{2,1} < \lambda^*_{2,0}$ by showing that

$$\frac{V}{2(V-1)}\lambda^*_{2\neq} < \lambda^*.$$

4. $h = 2, m = 1, n = V - 3$: Concrete Examples

In our concrete examples, $(t_{a,b})_{(a,b) \in \mathscr{V} \times \mathscr{V}}$ will be the incidence matrix of a graph $\mathscr{G} = (\mathscr{V}, \mathscr{E})$ and, consequently, Δ will be the discrete Laplacian of $\mathscr{G}$. The graph $\mathscr{G}_{2\neq}$ is obtained from $\mathscr{G} \times \mathscr{G}$ by removing all its diagonal vertices and all the edges joining them to the rest of $\mathscr{G} \times \mathscr{G}$: $\mathscr{G}_{2\neq} = (\mathscr{V}_{2\neq}, \mathscr{E}_{2\neq})$, where $\mathscr{V}_{2\neq}$ is defined in (3.4) and

$$\begin{aligned}\mathscr{E}_{2\neq} = \{((x, z), (x', z')) \in \mathscr{V}_{2\neq} \times \mathscr{V}_{2\neq} \mid [x = x' \wedge (z, z') \in \mathscr{E}] \vee \\ \vee [z = z' \wedge (x, x') \in \mathscr{E}]\}.\end{aligned} \tag{4.1}$$

$\Delta_{2\neq}$ is the discrete Laplacian associated to this graph. $\mathscr{K}_{2\neq}$, as defined in (3.8), is an invariant subspace of $\Delta_{2\neq}$ and $\lambda^*_{2\neq}$ is the smallest eigenvalue of $\Delta_{2\neq}|_{\mathscr{K}_{2\neq}}$. We are going to prove

$$\frac{V}{2(V-1)}\lambda^*_{2\neq} < \lambda^*, \tag{4.2}$$

for a class of graphs which include, as a particular case, discrete tori in any dimensions.

Let $\mathscr{T}_l$ be the one-dimensional discrete torus of length l. Two vertices $x, y \in \{0, 1, \ldots, l-1\}$ are joined by an edge of $\mathscr{T}_l$ if $(|x - y| \bmod l) = 1, l - 1$. Our class of examples will consist of graphs of the form

$$\mathscr{G} = \mathscr{T}_l \times \mathscr{R},$$

where $\mathscr{R}$ is an arbitrary finite graph on r vertices. We prove the following proposition.

PROPOSITION 3. *There exists an $l_0 < \infty$ such that for any $l > l_0$ and any finite graph $\mathscr{R}$*

$$\frac{V}{2(V-1)}\lambda^*_{2\neq} < 2\left(1 - \frac{\cos 2\pi}{l}\right) = \lambda. \tag{4.3}$$

Remark. In (4.3) $V = lr$, of course, and the right-hand side is $\lambda = \lambda^*(\mathscr{T}_l)$. Clearly, $\lambda^*(\mathscr{G}) = \lambda^*(\mathscr{T}_l) \wedge \lambda^*(\mathscr{R})$, so if $\lambda^*(\mathscr{T}_l) \leqslant \lambda^*(\mathscr{R})$, then (4.3) is equivalent to (4.2), and our main claim is proved. In particular, discrete tori in any dimension with the longest side longer than l_0 are included. (Recall that $\lambda^*(\mathscr{G})$ denotes the smallest positive (nonzero) eigenvalue of $-\Delta$ associated to the graph $\mathscr{G}$.)

Proof. In the present proof we adopt the following notation: for $x, y \in \{0, 1, \ldots, l-1\}$ $x \pm y$ will be understood as $(x \pm y \bmod l)$. The (real valued) functions $f, g, \ldots$ will be defined on $\{1, \ldots, l-1\}$, their scalar product and norm are defined as

$$(f, g) = \sum_{z=1}^{l-1} f(z)g(z), \quad \|g\|^2 = (g, g). \tag{4.4}$$

Beware of the lower limit of the summation! Vertices of the graph $\mathscr{R}$ will be denoted by $\alpha, \beta, \ldots$

Denote

$$f\colon \{1, 2, \ldots, l-1\} \to \mathbb{R}, \quad f(z) = \cos\frac{2\pi}{l} z. \tag{4.5}$$

We minimize $\langle \phi, -\Delta_{2\neq}\phi \rangle_{2\neq} / \langle \phi, \phi \rangle_{2\neq}$ among trial functions of the form

$$\phi(x, \alpha; y, \beta) = \sqrt{\frac{2}{r^2 l}} \begin{cases} \cos\left(\frac{2\pi}{l}(x+y)\right) g(x-y), & \text{if } x \neq y, \\ -\frac{r}{r-1}(f, g), & \text{if } x = y \text{ and } \alpha \neq \beta, \end{cases} \tag{4.6}$$

where g is an even function on $\{1, 2, \ldots, 1-1\}$:

$$g(z) = g(l-z), \quad z \in \{1, 2, \ldots, l-1\}, \tag{4.7}$$

and in the case $r = 1$ (i.e. when $\mathscr{G} = \mathscr{T}_l$), the extra condition

$$(f, g) = \sum_{z=1}^{l-1} \cos\left(\frac{2\pi}{l} z\right) g(z) = 0 \tag{4.8}$$

is imposed. (Notice, that the $z = 0$ term is missing from the sum.)

One can easily check that the conditions (3.8) for $\phi \in \mathscr{H}_{2\neq}$ are satisfied. After some straightforward calculations, we find the $\mathscr{H}_{2\neq}$-norm of ϕ

$$\text{for } r > 1\colon \quad \|\phi\|_{2\neq}^2 = \left[\|g\|^2 + \frac{r}{r-1}(f, g)^2\right], \tag{4.9}$$

$$\text{for } r = 1\colon \quad \|\phi\|_{2\neq}^2 = \|g\|^2, \tag{4.9'}$$

and the Dirichlet form

for $r > 1$:

$$\begin{aligned} &\langle \phi, -\Delta_{2\neq}\phi \rangle_{2\neq} \\ &\quad = 2\left[(g, Sg) + \frac{2}{r(r-1)} \times \right. \\ &\quad \left. \times \left(r^2(f, g)^2 - 2r(r-1)\cos\left(\frac{2\pi}{l}\right)(f, g)g(1) + (r-1)^2 g^2(1)\right)\right] \end{aligned} \tag{4.10}$$

$$\text{for } r = 1\colon \quad \langle \phi, -\Delta_{2\neq}\phi \rangle_{2\neq} = 2(g, Sg), \tag{4.10'}$$

where S is the linear operator on $l_2(\{1, 2, \ldots, l-1\})$ defined below

$$[Sg](z) = \begin{cases} g(z) - \cos\left(\frac{2\pi}{l}\right)g(z+1), & \text{if } z = 1, \\ 2g(z) - \cos\left(\frac{2\pi}{l}\right)(g(z+1) + g(z-1)), & \text{if } z \neq 1, l-1, \\ g(z) - \cos\left(\frac{2\pi}{l}\right)g(z-1), & \text{if } z = l-1. \end{cases} \tag{4.11}$$

Let us first consider the case $r = 1$ (i.e. $\mathscr{G} = \mathscr{T}_l$). The smallest eigenvalue of S on the subspace of even $g-s$ satisfying (4.7) is found to be

$$\bar{\lambda} = 2\left(1 - \cos\frac{2\pi}{l}\cosh\theta\right), \tag{4.12}$$

where $\pm\theta$ are the only real solutions of the equation

$$e^{l\theta} = \frac{e^{\theta} - \cos\dfrac{2\pi}{l}}{\cos\dfrac{2\pi}{l} - e^{-\theta}}. \tag{4.13}$$

The corresponding eigenfunction of S is

$$\bar{g}(z) = \cosh\left[\theta\left(\frac{l}{2} - z\right)\right], \quad z \in \{1, 2, \ldots, l-1\} \tag{4.14}$$

and one can check that $\bar{g}$ satisfies (4.8).

For large values of l, the asymptotic behaviour of λ is

$$\lambda = 2\left(1 - \cos\frac{2\pi}{l}\right) = \frac{4\pi^2}{l^2} + o(l^{-3}) \tag{4.15}$$

and solving (4.13) up to the first three leading terms after some tedious, but straightforward calculations, we get

$$\theta = \frac{2\pi}{l^{3/2}} + \frac{\pi^2(\pi+3)}{3l^{5/2}} + o(l^{-5/2}) \tag{4.16}$$

and

$$\lambda - \bar{\lambda} = 2(\cosh\theta - 1)\cos\frac{2\pi}{l} = \frac{4\pi^2}{l^3} + \frac{4\pi^3(\pi+3)}{3l^4} + o(l^{-4}). \tag{4.17}$$

Using these asymptotic expansions and (4.9′), (4.10′), we finally get

$$(V-1)\lambda - \frac{V}{2}\frac{\langle\phi, -\Delta_{2\neq}\rangle_{2\neq}}{\langle\phi, \phi\rangle_{2\neq}} = l(\lambda - \bar{\lambda}) - \lambda = \frac{4\pi^3(\pi+3)}{3l^3} + o(l^{-3}). \tag{4.18}$$

This expression is positive for sufficiently large values of l, which proves our Proposition 3 for $r = 1$.

We turn now to the case $r > 1$. Choose

$$g = \bar{g} - c\mathbb{1} \tag{4.19}$$

where $\bar{g}$ is the eigenfunction of S defined in (4.14), c is a real number and $\mathbb{1}$ is the function identically one on $\{1, 2, \ldots, l-1\}$. With this choice formulae (4.9) and (4.10) become

$$\|\phi\|_{2\neq}^2 = \left[\|\bar{g}\|^2 - 2c(\bar{g}, \mathbb{1}) + c^2\left(l + \frac{1}{r-1}\right)\right], \tag{4.9''}$$

$$\begin{aligned}&\langle\phi, -\Delta_{2\neq}\phi\rangle_{2\neq}\\ &\quad = 2\left[\bar{\lambda}\|\bar{g}\|^2 - 2\bar{\lambda}c(\bar{g}, \mathbb{1}) + c^2(\mathbb{1}, S\mathbb{1}) + \frac{2}{r(r+1)} \times\right.\\ &\qquad \left.\times\left(r^2c^2 + 2\cos\left(\frac{2\pi}{l}\right)r(r-1)c(\bar{g}(1) + c) + (r-1)^2(\bar{g}(1) + c)^2\right)\right].\end{aligned} \tag{4.10''}$$

This last formula considerably simplifies with the choice

$$c = \frac{r-1}{2r-1}\bar{g}(1). \tag{4.20}$$

Noting that

$$(\mathbb{1}, S\mathbb{1}) = (l-2)\lambda, \tag{2.21}$$

we finally get

$$\langle\phi, -\Delta_{2\neq}\phi\rangle_{2\neq} = 2\left[\bar{\lambda}\|\bar{g}\|^2 - 2\bar{\lambda}c(\bar{g}, \mathbb{1}) + \lambda c^2\left(l + \frac{1}{r-1}\right)\right]. \tag{4.22}$$

Using the asymptotics (4.15), (4.17) (to first leading terms only) and the following straightforward expansions

$$\|\bar{g}\|^2 = l + o(l) = (\bar{g}, \mathbb{1}), \tag{4.23}$$

$$c = \frac{r-1}{2r-1} + o(1), \tag{4.24}$$

we finally get

$$\begin{aligned}&2(V-1)\lambda\langle\phi, \phi\rangle_{2\neq} - V\langle\phi, -\Delta_{2\neq}\Phi\rangle_{2\neq}\\ &\quad = [\langle\bar{g}\rangle^2 - 2c(\bar{g}, \mathbb{1})][lr(\lambda - \bar{\lambda}) - \lambda] - c^2\left(l + \frac{1}{r-1}\right)\lambda\\ &\quad = \frac{r(r-1)}{(2r-1)^2}\frac{4\pi^2}{l} + o(l^{-1}).\end{aligned} \tag{4.25}$$

Since the coefficient of the leading term in (4.25) is positive, this expression is eventually positive, which proves Proposition 3 for the cases $r > 1$.

Acknowledgements

It is a pleasure to thank Oliver Penrose for many illuminating discussions on the subject. During the preparation of this manuscript, I have learnt about Refs. [7, 8], where similar results are obtained by different methods. I wish to thank Elliott H. Lieb for drawing my attention to these papers and for other helpful comments.

This work was supported by the British Science and Engineering Research Council.

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