Preprint UC Davis Math 1999-30

A continuum approximation for the excitations of the $(1, 1, \ldots, 1)$ interface in the quantum Heisenberg model

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Abstract: It is shown that, with an appropriate scaling, the energy of low-lying excitations of the $(1, 1, \ldots, 1)$ interface in the d-dimensional quantum Heisenberg model are given by the spectrum of the $d-1$-dimensional Laplacian on an suitable domain.

Keywords: Anisotropic Heisenberg ferromagnet, XXZ model, interface excitations, 111 interface.

MCS2000 numbers: 82B10, 82B24, 82D40

1 Introduction and main results

We consider the spin 1/2 XXZ Heisenberg model on the d-dimensional lattice $\mathbb{Z}^d$. For any finite volume $\Lambda \subset \mathbb{Z}^d$, the Hamiltonian is given by

$$H_\Lambda = - \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} \Delta^{-1}(S_x^{(1)}S_y^{(1)} + S_x^{(2)}S_y^{(2)}) + S_x^{(3)}S_y^{(3)}, \tag{1.1}$$

where $\Delta > 1$ is the anisotropy. We refer to the next section for more precise definitions. By adding an appropriate boundary term one can insure that the ground states of this model describe an interface in the $(1, 1, \dots, 1)$ direction between two domains with opposite magnetization. For a particular choice of boundary term, the model has exactly one ground state ψ_n for each fixed number of down spins, n. We call these the canonical ground states. In analogy with statistical mechanics of particle systems one can introduce the grand canonical ground states of the form

$$\Psi = \sum_n z^n \psi_n$$

It turns out that these states are inhomogeneous product states [3]. In this paper, we consider a class of perturbations of these product states, of which we calculate the energy. By the variational principle this leads to bounds for the energy of the first excited state of the model. As the excitation spectrum above the interface states is gapless [4, 5], this bound should vanish as the volume tends to infinity. This is indeed the case (see (1.2)).

The perturbations we consider are in correspondence with functions $f : \Lambda \to \mathbb{C}$. Furthermore, we consider functions which are slowly-varying in all directions perpendicular to $(1, 1, \dots, 1)$ though they may have discrete jumps parallel to this direction. In other words $\|\nabla f \cdot v\|_\infty \ll \|f\|_\infty$ for all $v \perp (1, 1, \dots, 1)$. We consider general perturbations of this type and conclude that the optimal perturbations, in the sense of minimizing energy, are localized near the interface. With this restriction, the Hamiltonian, projected to and restricted to the appropriate subspace, is just the Laplacian

This result may be compared to the recent bound of [2]. The main difference is that there we considered a canonical ensemble, for which there were a fixed number of down-spins (hence a fixed number of up-spins). We developed a version of equivalence of ensembles whereby we estimated the canonical expectation of a gauge invariant observable by a grand canonical expectation, provided that the interfaces of the canonical and grand canonical states occupied the same position.

In the present paper, we begin with the grand canonical ensemble, so that we make no reference to equivalence of ensembles. Specifically, we consider a cylindrical region of total height $L+1$ and whose cross-section is a region Ω_R with linear size R. Then a class of excitations is parametrized by smooth functions Φ on a fixed domain $\Omega = R^{-1}\Omega_R$.

Main Result: *Excitations on Λ have a normalized energy*

$$\frac{\langle \psi^f | \, H \, | \psi^f \rangle}{\langle \psi^f | \psi^f \rangle} \approx \frac{1}{2\Delta R^2} \cdot \frac{\|\nabla \Phi\|^2_{L^2(\Omega)}}{\|\Phi\|^2_{L^2(\Omega)}} \cdot g(\Delta, \mu) \tag{1.2}$$

where

$$g(\Delta, \mu) = \frac{\sum_{l=-L/2}^{L/2-1} \operatorname{sech}(\alpha[l-\mu]) \operatorname{sech}(\alpha[l+1-\mu])}{\sum_{l=-L/2}^{L/2} \operatorname{sech}(\alpha[l-\mu]) \operatorname{sech}(\alpha[l-\mu])}.$$

Here, μ is a real parameter of the grand canonical ground state describing the location of the interface between the regions of homogeneous up and down spins. As $\mu \to -\infty$, the ground state has all spins up, and for $\mu \to \infty$, all spins are down. For all $\mu \in \mathbb{R}$, and sufficiently large L, g satisfies the bounds

$$\frac{1}{2\Delta} \le \Delta - \sqrt{\Delta^2 - 1} \le g(\Delta, \mu) \le 1$$

Remark: The normalized energy of (1.2) is exactly the same as that for the Laplacian. Equating the first variation to zero, we see that the local extrema of the normalized energy are precisely the solutions of $\nabla^2 \Phi = -\lambda \Phi$ (here ∇^2 is the Laplacian), and $\lambda = \|\nabla \Phi\|^2_{L^2(\Omega)} / \|\Phi\|^2_{L^2(\Omega)}$. The space of excitations we consider does not form an invariant subspace of H, so that the eigenvectors of the Laplacian are not truly eigenvectors of H. But, using the variational inequality, we see that the spectral gap of H is bounded thus:

$$\gamma_1 \le \frac{\lambda_1}{2\Delta R^2} \cdot g(\Delta, \mu)(1 + O(\frac{1}{R^2})),$$

where λ_1 is the first positive eigenvalue of $-\nabla^2$ with Dirichlet boundary conditions on the domain Ω.

2 The Spin-$\frac{1}{2}$ Heisenberg XXZ Ferromagnet

A quantum spin model, such as the Heisenberg XXZ ferromagnet, is defined in terms of a family of local Hamiltonians H_Λ, acting as self-adjoint linear operators on a Hilbert space $\mathcal{H}_\Lambda$. This family is parametrized by finite subsets $\Lambda \subset \mathbb{Z}^d$.

We choose Λ to be "cylindrical" in the following sense: Let $\{e_j\}_{j=1}^d$ be the set of coordinate unit vectors and define the vector $e_* = \sum_{j=1}^d e_j = (1, 1, \ldots, 1)$, which is the axial direction for the cylinder. Define the functional $l(x) = x \cdot e_* = \sum_{j=1}^d x^j$, where $x = \sum_{j=1}^d x^j e_j$. Observe that the kernel of l in $\mathbb{Z}^3$ is a $(d-1)$-dimensional sublattice perpendicular to the axial direction. Take for the base of Λ a finite subset of this $(d-1)$-dimensional sublattice, and call it Γ. A discrete approximation to the line of all scalar mutliples of e_* is the *one-dimensional stick* Σ. Σ is a bi-infinite sequence of points $\{x_n\}_{n=-\infty}^{\infty}$ such that $x_0 = 0$ and all other points x_n are specified by the relation $x_n - x_{n-1} = e_{n \bmod d}$. So

$$\begin{aligned} \Sigma \;=\; & \{\ldots, -(e_d + e_{d-1} + \cdots + e_1 + e_d), -(e_d + e_{d-1} + \cdots + e_1), \ldots, -e_d, \\ & 0, e_1, (e_1 + e_2), \ldots, (e_1 + e_2 + \cdots + e_d), (e_1 + e_2 + \cdots + e_d + e_1), \ldots\}. \end{aligned}$$

A finite stick of length $L+1$, where L is even, is $\Sigma_L = \{x \in \Sigma : -L/2 \leq l(x) \leq L/2\}$. Now define Λ to be the translates of Γ along Σ_L, i.e.

$$\Lambda = \Gamma + \Sigma_L = \{x + y : x \in \Gamma, y \in \Sigma_L\}. \tag{2.1}$$

Let us now define *nearest neighbors* to be points $x, y \in \mathbb{Z}^d$ such that $|l(x) - l(y)| = 1$ and $\|x - y\|_{l^1} = 1$. Also, we define oriented bonds between nearest neighbors as ordered pairs (x, y) satisfying $l(y) = l(x) + 1$ and $\|x - y\|_{l^1} = 1$. Hence $\{(x, x + e_j)\}_{j=1}^d$ is the set of all oriented bonds with lower point x. The collection of all oriented bonds with both points in Λ, will be called $B(\Lambda)$.

The local Hilbert spaces are $\mathcal{H}_\Lambda = (\mathbb{C}^2)^{\otimes|\Lambda|}$. Each copy of $\mathbb{C}^2$ comes with an ordered basis $(|\uparrow\rangle, |\downarrow\rangle)$ and a spin-$\frac{1}{2}$ representation of $SU(2)$ defined by the Pauli matrices:

$$S^{(1)} = \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix}, \quad S^{(2)} = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix}, \quad S^{(3)} = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \tag{2.2}$$

(So, for example, $S^{(3)}\left|\uparrow\right\rangle = \frac{1}{2}\left|\uparrow\right\rangle$ and $S^{(3)}\left|\downarrow\right\rangle = -\frac{1}{2}\left|\downarrow\right\rangle$.) We consider a family of Hamiltonians parametrized by a real number $\Delta \geq 1$. In order to define the total Hamiltonian, we first define local Hamiltonians h_{xy} for each oriented bond (x, y):

$$h_{x,y} = -\Delta^{-1}(S_x^{(1)}S_y^{(1)} + S_x^{(2)}S_y^{(2)}) - S_x^{(3)}S_y^{(3)} + \frac{1}{4} + \frac{1}{4}A(\Delta)(S_y^{(3)} - S_x^{(3)}), \quad (2.3)$$

where $A(\Delta) = \frac{1}{2}\sqrt{1 - 1/\Delta^2}$. The total Hamiltonian is

$$H_\Lambda = \sum_{(x,y)\in B(\Lambda)} h_{x,y}^q. \quad (2.4)$$

Δ parametrizes "anisotropic coupling". The case $\Delta = 1$ is the isotropic model, also known as the Heisenberg XXX ferromagnet, which exhibits $SU(2)$ symmetry (because H_Λ commutes with S^1, S^2 and S^3).

We find it convenient to introduce a positive constant α, which solves $\Delta = \cosh(\alpha)$. We note that the nearest neighbor interaction h_{xy} is an orthogonal projection

$$h_{xy} = \left|\xi_{xy}\right\rangle\left\langle\xi_{xy}\right| \otimes \mathbb{1}_{\Lambda\setminus(\mathrm{x,y})}, \quad (2.5)$$

where

$$\xi_{xy} = \frac{e^{-\alpha/2}\left|\downarrow\uparrow\right\rangle - e^{\alpha/2}\left|\uparrow\downarrow\right\rangle}{\sqrt{2\cosh(\alpha)}}. \quad (2.6)$$

This also shows that each h_{xy} is a nonnegative self-adjoint operator, hence H_Λ is, as well. To simplify the notation we will often drop the subscript Λ when the volume is obvious from the context.

3 Ground States and a Perturbation

The ground states of the XXZ ferromagnet can be calculated exactly [1]. We will choose a particular ground state and construct an orthogonal subspace (but not the entire orthogonal complement) which is parametrized by H^1-functions on a compact domain $\Omega_0 \subset \mathbb{R}^{d-1}$. The inner product becomes approximately the L^2 inner-product and the orthogonal projection of the Hamiltonian is approximately the Laplacian.

The lowest eigenvalue for H, which is zero, has a $(|\Lambda|+1)$-fold degeneracy in the eigenspace. This space of ground states is spanned by the simple tensor ground states, which we will call grand canonical states. Specifically, let z be any complex number, and $\mu = \mathrm{Re}(z)$. Define the vector

$$v_x(z) = \frac{e^{\alpha(l_x - z)/2}\,|{\uparrow}\rangle + e^{-\alpha(l_x - z)/2}\,|{\downarrow}\rangle}{\sqrt{2\cosh(\alpha[l_x - \mu])}}, \tag{3.1}$$

for each site $x \in \Lambda$. We define the product of these vectors

$$\psi_0(z) = \bigotimes_{x\in\Lambda} v_x(z), \tag{3.2}$$

and we may quickly establish that it is a ground state. Indeed, the oriented bonds are defined between points x and y with $l(y) = l(x) + 1$, from which we see

$$\langle{\uparrow\downarrow}\,|v_x(z) \otimes v_y(z)\rangle = e^{\alpha}\langle{\downarrow\uparrow}\,|v_x(z) \otimes v_y(z)\rangle. \tag{3.3}$$

This implies $v_x(z) \otimes v_y(z)$ is orthogonal to ξ_{xy}, for each $(x, y) \in B(\Lambda)$, which proves that $\psi_0(z)$ is a ground state. As we have said, the states $\psi_0(z)$ span the entire ground state space, as z ranges over all the complex numbers [3]. (More than this can be said. The simple tensor ground states are parametrized by elements of $\mathbb{C}P^1$, so that the submanifold of all such states in $\mathcal{H}$ is topologically a sphere. But to obtain the north and south poles of the sphere, it is necessary to take the limits $z \to \infty$ and $z \to -\infty$.)

Let us now fix z, and for simplicity we will just write ψ_0 and v_x without explicit reference to z. For each site x we define a vector orthogonal to v_x,

$$w_x = \frac{e^{-\alpha(l_x - \bar{z})/2}\,|{\uparrow}\rangle - e^{\alpha(l_x - \bar{z}/2}\,|{\downarrow}\rangle}{\sqrt{2\cosh(\alpha[l_x - \mu])}}. \tag{3.4}$$

We will make use of w_x to define an orthonormal system of states

$$\psi^x = w_x \otimes \bigotimes_{y\in\Lambda\backslash x} v_y, \tag{3.5}$$

where x ranges over Λ. Each of these states is also orthogonal to ψ_0, let us call their span V. An arbitrary state in V is characterized by a function $f : \Lambda \to \mathbb{C}$. Explicitly, $\psi^f = \sum_{x\in\Lambda} f(x)\psi^x$. It is then clear that $\langle\psi^f|\psi^g\rangle = \sum_{x\in\Lambda} \overline{f(x)}g(x)$.

Our interest is the case that $\Lambda \nearrow \mathbb{Z}^d$, i.e. the thermodynamic limit. In terms of v_x and w_x, we see that the local interaction h_{xy} describes a nearest-neighbor interaction. It may be interpreted as a bilinear form, which is a first order finite-difference operator in each variable. To be clear, a straightforward calculation gives

$$\begin{aligned}\langle\psi^f|\, h_{xy}\,|\psi^g\rangle &= \frac{1}{2}\operatorname{sech}(\alpha)\operatorname{sech}(\alpha[l_x-\mu])\operatorname{sech}(\alpha[l_y-\mu])\\ &\quad\times\big(\cosh(\alpha[l_y-\mu])\overline{f(y)}-\cosh(\alpha[l_x-\mu])\overline{f(x)}\big)\\ &\quad\times\big(\cosh(\alpha[l_y-\mu])g(y)-\cosh(\alpha[l_x-\mu])g(x)\big). \quad (3.6)\end{aligned}$$

Recall that $\mu = \operatorname{Re}(z))$ and the energy is

$$\langle\psi^f|\, H\,|\psi^g\rangle = \sum_{l=-L/2}^{L/2-1}\sum_{x\in\Gamma_l}\sum_{j=1}^{d}\langle\psi^f|\, h_{x,x+e_j}\,|\psi^g\rangle\,, \quad (3.7)$$

where Γ_l refers to the set of points $x\in\Lambda$ with $l(x)=l$. In the thermodynamic limit, we may scale the plane $e_*^\perp = \{v\in\mathbb{R}^d : v\cdot e_* = 0\}$ so that H becomes, to first order, a differential operator with respect to each direction of the plane. However, the inhomogeneity in the e_* direction admits no such scaling for that coordinate, so that H is genuinely a finite-difference operator even in the thermodynamic limit.

This intuitive description of the last paragraph is made precise, now. Let Ω be a bounded, open subset of $e_*^\perp$ with a C^1 boundary. Let Ω_R be the dilation $R\cdot\Omega = \{Rx : x\in\Omega\}$, and let $\Gamma = \Omega_R\cap\mathbb{Z}^d$ be the discrete approximation to Ω_R. As before, Γ is the base of Λ. Now we choose a smooth, complex-valued function Φ on Ω, and extend it to the infinite cylinder $\Omega\times\mathbb{R}e_*$ so that $\nabla\Phi\cdot e_* = 0$. (In other words, Φ is constant along the direction e_*.) Let $\phi(x) = \Phi(x/R)$, which is defined on $\Omega_R\times\mathbb{R}e_*$ with the property that $\nabla\phi\cdot e_* = 0$. Finally, let $f(x) = F(l_x)\phi(x)$, where F is a sequence $F(-L/2),\dots,F(L/2)$. Note that f is not the most general form possible for a function on Λ, most notably because it is the product of functions which vary on perpendicular subspaces. However, the span of such functions does correspond to all of V for a fixed value of L and R.

Next we consider the norm and energy for such a state. We will introduce estimates for these quantities, but we will postpone the actual error terms until the next section. First we replace the sum over Γ with the integral over Ω, and thus obtain an expression for the norm:

$$\langle\psi^f|\psi^f\rangle = \sum_{l=-L/2}^{L/2}\sum_{x\in\Gamma_l}|f(x)|^2$$

$$\begin{aligned} &\approx |\Gamma| \sum_{l=-L/2}^{L/2} |F(l)|^2 \cdot \frac{1}{m(\Omega_R)} \int_{\Omega_R} |\phi(x)|^2\, dx \\ &= |\Gamma| \sum_{l=-L/2}^{L/2} |F(l)|^2 \cdot \frac{1}{m(\Omega)} \int_{\Omega} |\Phi(x)|^2\, dx. \end{aligned} \tag{3.8}$$

To obtain an approximation for $\langle \psi^f | \, H \, | \psi^f \rangle$, we decompose a step of f along a coordinate direction into a step parallel to e_* and a step perpendicular to e_*,

$$\begin{aligned} f(x+e_j) &= F(l_x+1)\phi(x+e_j) \\ &\approx F(l_x+1)\phi(x) + F(l_x+1)\nabla\phi(x)\cdot e_j. \end{aligned}$$

Then using the fact that

$$\sum_{j=1}^{d} \nabla\phi(x)\cdot e_j = \nabla\phi(x)\cdot e_* = 0,$$

and referring to (3.6) and (3.7) we have the apparently cumbersome expression

$$\begin{aligned} \langle \psi^f | \, H \, | \psi^f \rangle \approx\ & \frac{3|\Gamma|}{2\cosh(\alpha)} \cdot \frac{1}{m(\Omega)} \int_\Omega |\Phi(x)|^2 dx \\ & \times \sum_{l=-L/2}^{L/2} \Big[\operatorname{sech}(\alpha[l-\mu]) \operatorname{sech}(\alpha[l+1-\mu]) \\ & \qquad |\cosh(\alpha[l+1-\mu])F(l+1) - \cosh(\alpha[l-\mu])F(l)|^2 \Big] \\ & + \frac{|\Gamma|}{2R^2\cosh(\alpha)} \cdot \frac{1}{m(\Omega)} \int_\Omega |\nabla\Phi(x)|^2 dx \\ & \times \sum_{l=-L/2}^{L/2} \operatorname{sech}(\alpha[l-\mu]) \cosh(\alpha[l+1-\mu]) |F(l+1)|^2. \end{aligned}$$

We notice that the first summand is order 1, while the second summand is order $1/R^2$. We wish to minimize the energy in the limit $R \to \infty$, so it seems sensible to eliminate the order 1 summand. This is accomplished by letting $F(l) = \frac{1}{2}\operatorname{sech}(\alpha[l-\mu])$, or any constant multiple thereof. One point of interest is that the perturbation takes place primarily in a neighborhood of the interface. The expression for the energy is

$$\begin{aligned}\left\langle\psi^f\right| H\left|\psi^f\right\rangle &\approx \frac{|\Gamma|}{8R^2\cosh(\alpha)}\cdot\frac{1}{m(\Omega)}\int_\Omega|\nabla\Phi(x)|^2dx\\ &\times\sum_{l=-L/2}^{L/2-1}\operatorname{sech}(\alpha[l-\mu])\operatorname{sech}(\alpha[l+1-\mu]). \quad (3.9)\end{aligned}$$

Similarly, (3.8) may be rewritten as

$$\langle\psi^f|\psi^f\rangle \approx \frac{|\Gamma|}{4}\cdot\frac{1}{m(\Omega)}\int_\Omega|\Phi(x)|^2dx\cdot\sum_{l=-L/2}^{L/2}\operatorname{sech}^2(\alpha[l-\mu]). \quad (3.10)$$

Taking the ratio, we arrive at a normalized energy

$$\begin{aligned}\frac{\left\langle\psi^f\right| H\left|\psi^f\right\rangle}{\langle\psi^f|\psi^f\rangle} &\approx \frac{\operatorname{sech}(\alpha)}{2R^2}\cdot\frac{\|\nabla\Phi\|^2_{L^2(\Omega)}}{\|\Phi\|^2_{L^2(\Omega)}}\\ &\times\frac{\sum_{l=-L/2}^{L/2-1}\operatorname{sech}(\alpha[l-\mu])\operatorname{sech}(\alpha[l+1-\mu])}{\sum_{l=-L/2}^{L/2}\operatorname{sech}(\alpha[l-\mu])\operatorname{sech}(\alpha[l-\mu])}. \quad (3.11)\end{aligned}$$

Let P be the orthogonal projection to the subspace of perturbations considered so far, i.e. the span of ψ^f, where $f(x)=\frac{1}{2}\operatorname{sech}(\alpha[l_x-\mu])\phi(x)$. Then the projection of H to this subspace is PHP. We have determined that $PHP\psi^f=\psi^g$ where g has in place of Φ

$$\Psi=-\frac{\operatorname{sech}(\alpha)}{2R^2}\cdot\frac{\sum_{l=-L/2}^{L/2-1}\operatorname{sech}(\alpha[l-\mu])\operatorname{sech}(\alpha[l+1-\mu])}{\sum_{l=-L/2}^{L/2}\operatorname{sech}(\alpha[l-\mu])\operatorname{sech}(\alpha[l-\mu])}\nabla^2\Phi. \quad (3.12)$$

(We write ∇^2 for the Laplacian. The symbol Δ is reserved for the anisotropy.) We should note that it really is necessary to consider PHP instead of H. The reason for this is that

$$\xi_{xy}=\frac{-2\cosh(\alpha[l_x-\mu])w_x\otimes v_y+2\cosh(\alpha[l_y-\mu])v_x\otimes w_y+2\sinh(\alpha)w_x\otimes w_y}{\sqrt{2\cosh(\alpha[l_x-\mu])\cdot 2\cosh(\alpha[l_y-\mu])\cdot 2\cosh(\alpha)}}, \quad (3.13)$$

which means that H does not preserve the total number of v_x's or w_x's. Thus the perturbations we have considered (those with a single w_x) do not form an invariant subspace of H.

4 Error Terms

We now come to the task of tying-up some loose ends, in order that non-rigorous approximations can be replaced by rigorous bounds. We start with a simple lemma.

Lemma 4.1 *Let Γ be a finite subset of a lattice L. Let Ω be the Voronoi domain of Γ with respect to L, and let Ω_0 be the Voronoi domain for the single site $0 \in L$. Then, for a smooth function $\phi : \Omega \to \mathbb{C}$,*

$$\Big|\frac{1}{|\Gamma|}\sum_{x\in\Gamma} u(x) - \frac{1}{m(\Omega)}\int_\Omega \phi(x)\,dx\Big| < \|\partial^2\phi\|_{op,\infty}\cdot\frac{1}{m(\Omega_0)}\int_{\Omega_0}\frac{|x|^2}{2}dx, \quad (4.14)$$

where $\partial^2\phi$ is the second-derivative matrix and

$$\|\partial^2\phi\|_{op,\infty} = \sup_{x\in\Omega}\ \sup_{v\in\mathbb{R}^d\setminus 0}\frac{v\cdot\partial^2 u(x)v}{v\cdot v}. \quad (4.15)$$

Note that the second moment $m(\Omega_0)^{-1}\int |x|^2\,dx$ is bounded by the radius of the Voronoi domain, which is in turn bounded by the distance of nearest neighbors of L.

Proof: For the Voronoi domain Ω_0 of 0, we observe that

$$\begin{aligned}
\frac{1}{m(\Omega_0)}\int_{\Omega_0}\phi(x)\,dx - \phi(0) &= \frac{1}{m(\Omega_0)}\int_{\Omega_0}[\phi(x)-\phi(0)]\,dx \\
&= \frac{1}{m(\Omega_0)}\int_{\Omega_0}\int_0^1 \nabla\phi(tx)\cdot x\,dt\,dx \\
&= \frac{1}{m(\Omega_0)}\int_{\Omega_0}\int_0^1\int_0^t x\cdot\nabla^2\phi(sx)x\,ds\,dt\,dx \\
&\quad +\frac{1}{m(\Omega_0)}\int_{\Omega_0}\nabla\phi(0)\cdot x\,dx \\
&= \frac{1}{m(\Omega_0)}\int_{\Omega_0}\int_0^1(1-s)x\cdot\partial^2\phi(sx)x\,ds\,dx \\
&\quad +\nabla\phi(0)\cdot\frac{1}{m(\Omega_0)}\int_{\Omega_0}x\,dx.
\end{aligned}$$

But the centroid of Ω_0 is 0. Thus

$$\Big|\frac{1}{m(\Omega_0)}\int_{\Omega_0}\phi(x)\,dx - \phi(0)\Big| \le \frac{1}{m(\Omega_0)}\int_{\Omega_0}\frac{|x|^2}{2}dx\times\|\partial^2\phi\|_{op,\infty}. \quad (4.16)$$

The lemma follows by decomposing Ω into the $|\Gamma|$ affine copies of Ω_0, one for each site, and adding the inequalities obtained from (4.16). ∎

Using the result of this lemma, we make rigorous the approximation of (3.8). Thus

$$\langle \psi^f | \psi^f \rangle = |\Gamma| \sum_{l=-L/2}^{L/2} |F(l)|^2 \cdot \left(\frac{1}{m(\Omega)} \int_\Omega |\Phi(x)|^2 \, dx + \epsilon_1 \right), \tag{4.17}$$

where

$$|\epsilon_1| \leq \frac{1}{R^2} \| \partial^2 |\Phi|^2 \|_{op,\infty}. \tag{4.18}$$

(We have used the fact that the distance between nearest-neighbors for Γ is $\sqrt{2}$.) In order to fix the approximation of (3.9), we begin with the elementary bound $|\phi(x + e_j) - \phi(x) - \nabla\phi(x) \cdot e_j| < \frac{1}{2} \|\partial^2 \phi\|_{op,\infty}$ and its natural successor

$$\Big| \sum_{j=1}^{d} |\phi(x + e_j) - \phi(x)|^2 - \|\nabla\phi(x)\|^2 \Big| < d\Big(\|\nabla\phi\|_\infty + \frac{1}{4} \|\partial^2\phi\|_{op,\infty} \Big) \|\partial^2 \phi\|_{op,\infty}. \tag{4.19}$$

Using this estimate, as well as the lemma, we may replace (3.9) with

$$\begin{aligned} \langle \psi^f | \, H \, | \psi^f \rangle \;\; \approx \;\; & \frac{|\Gamma|}{8R^2 \cosh(\alpha)} \sum_{l=-L/2}^{L/2} \operatorname{sech}(\alpha[l - \mu]) \sec(\alpha[l + 1 - \mu]) \\ & \left(\frac{1}{m(\Omega)} \int_\Omega |\nabla\Phi(x)|^2 dx + \epsilon_2 + \epsilon_3 \right), \end{aligned} \tag{4.20}$$

where

$$|\epsilon_2| \leq \frac{d}{R} \Big(\|\nabla\Phi\|_\infty + \frac{1}{4R} \|\partial^2\Phi\|_{op,\infty} \Big) \|\partial^2\Phi\|_{op,\infty}, \tag{4.21}$$

and

$$|\epsilon_3| \leq \frac{1}{R^2} \|\partial^2 |\nabla\Phi|^2 \|_{op,\infty}. \tag{4.22}$$

Acknowledgements

O.B. was supported by Fapesp under grant 97/14430-2. B.N. was partially supported by the National Science Foundation under grant # DMS-9706599.

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