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The Ground State Energy of a Bose Gas with Coulomb Interaction II*

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Abstract. Let H_N be the quantum mechanical Hamiltonian for a neutral system of $2N$ charged particles, each of unit charge. The Hamiltonian H_N is assumed to act on wave functions ψ in $L^2(\mathbb{R}^{6N})$ which satisfy Bose statistics. It is shown that if the kinetic energy of ψ is sufficiently small, then $\langle\psi|H_N|\psi\rangle \geqq -CN^{7/5}$ for some universal constant C.

1. Introduction

In this paper we are concerned with a Hamiltonian acting on a system of $2N$ particles which interact via a Coulomb potential. We assume that N of these particles are negative with charge -1 and located at positions $x_1,\dots,x_N\in\mathbb{R}^3$. The other particles are positive with charge $+1$ and located at $x_{N+1},\dots,x_{2N}\in\mathbb{R}^3$. We may write the quantum mechanical Hamiltonian for the system as H_N, where

$$H_N=\sum_{i=1}^{2N}(-\Delta_i)+\sum_{i<j=1}^{N}|x_i-x_j|^{-1}+\sum_{i<j=1}^{N}|x_{i+N}-x_{j+N}|^{-1}-\sum_{i,j=1}^{N}|x_i-x_{j+N}|^{-1}. \tag{1.1}$$

Here Δ_i denotes the Laplacian in the variable x_i, $1\leqq i\leqq 2N$.

We consider H_N acting on wave functions $\psi(x_1,\dots,x_{2N})$ in $L^2(\mathbb{R}^{6N})$ which are in the domain of the unique self-adjoint operator corresponding to H_N. We shall assume that these wave functions satisfy Bose statistics, and hence that ψ is invariant under permutations of the sets $(x_1,\dots,x_N)$ and $(x_{N+1},\dots,x_{2N})$. Our result is the following:

Theorem 1.1. *Let Λ be a cube in $\mathbb{R}^3$ and suppose that $\psi(x_1,\dots,x_{2N})$ is infinitely differentiable with compact support in Λ^{2N}. Let γ_ψ be defined by*

$$\frac{N\gamma_\psi^2}{L^2}=\sum_{i=1}^{2N}\langle\psi,-\Delta_i\psi\rangle, \tag{1.2}$$

where L is the length of a side of Λ. Then if $\gamma_\psi\leqq N^{1/3}$ there is the estimate

$$\langle\psi,H_N\psi\rangle\geqq -CN^{7/5}, \tag{1.3}$$

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and C is a universal constant.

We shall prove Theorem 1.1 by using the techniques developed in [1]. In fact one has just to note some straightforward extensions of the estimates of [1] to obtain our theorem. However this paper is written so that it can be read independent of [1].

Theorem 1.1 is in some sense the natural result one can expect to obtain from the methods of [1]. The basic assumption of the theory developed there was that most particles are in low momentum states and that the creation and annihilation operators corresponding to these states can be approximated by multiplication operators. By definition of γ_ψ one can say that in the wave function ψ most particles are concentrated in momentum states k with $|k| \leqq \gamma_\psi$. The number of such states is about γ_ψ^3, and hence if $\gamma_\psi \ll N^{1/3}$ there are on average many particles in each k state. Thus the creation and annihilation operators for these states can be approximated by scalar multiplication operators.

We show how the main theorem of [1] can be obtained from Theorem 1.1 above. Let us assume ψ is a product wave function:

$$\psi(x_1, \dots, x_{2N}) = \Psi(x_1, \dots, x_N)\Psi(x_{N+1}, \dots, x_{2N}), \tag{1.4}$$

and that Ψ has constant density on the box Λ. Then there is a well-known lower bound on the potential energy, P.E.,

$$\text{P.E.} \geqq -CN^{4/3}/L, \tag{1.5}$$

where C is a universal constant. Now if $\gamma_\psi < N^{1/3}$ then Theorem 1.1 implies the result of [1] that (1.3) holds. Otherwise we have a lower bound on the kinetic energy, K.E.,

$$\text{K.E.} \geqq \frac{N^{5/3}}{L^2}. \tag{1.6}$$

Taking (1.5) and (1.6) together implies that (1.3) continues to hold provided we make the constant density assumption of [1].

The motivation in obtaining Theorem 1.1 was to prove (1.3) independent of restrictions on ψ. The idea was that in the case when $\gamma_\psi > N^{1/3}$ one should decompose the cube Λ into smaller cubes and then apply the Fourier analysis methods of [1] to these smaller cubes. In order to do this one would need to be able to prove the analogue of Theorem 1.1 in the case when ψ satisfies Neumann boundary conditions. However the methodology of [1] breaks down when the boundary conditions on ψ are changed.

2. Proof of Theorem 1.1

Here we shall show how the proof of Theorem 1.1 follows from some lemmas. In the next section we shall give the proofs of these lemmas.

Our first task as in Sect. 3 of [1] is to approximate the Coulomb potential $1/|x|$ by a potential $\phi_p(x)$ which is periodic on a cube Q_Λ containing Λ. The cube Q_Λ is concentric with Λ but with side which has 4 times the length of a side of Λ. Let us define $\phi_\alpha(x)$ by

$$\phi_\alpha(x) = \int_0^{N^{1/5}/L} e^{-u|x|}\,du, \tag{2.1}$$

where L from now on is the length of a side of Q_Λ. We consider the Hamiltonian $H_{N,\alpha}$ which is defined like H_N in (1.1) but with the Coulomb potential $1/|x|$ replaced by $\phi_\alpha(x)$. It is easy to see then that

$$\langle \psi, H_{N,\alpha}\psi \rangle \geqq \frac{CN}{L^2} - \frac{2N^{6/5}}{L} \geqq -C'N^{7/5}, \tag{2.2}$$

where C and C' are constants. We may therefore replace the Coulomb potential in our future considerations by the potential $1/|x| - \phi_\alpha(x)$.

Next we state a lemma which is analogous to Lemma 3.7 of [1].

Lemma 2.1. *For $x \in Q_\Lambda$ with $|x| < L/2$, the potential $1/|x| - \phi_\alpha(x)$ may be expanded in a Fourier series*

$$1/|x| - \phi_\alpha(x) = \sum_{k \in Z^3} v_\alpha(k) e^{2\pi i k \cdot x/L}, \tag{2.3}$$

where $v_\alpha(k)$ satisfies the inequality

$$0 \leqq v_\alpha(k) \leqq 1/\pi L(|k|^2 + 1). \tag{2.4}$$

Now we wish to represent the expected value (1.1) with the Coulomb potential replaced by (2.3) in the second quantised form. Let a_k be the Boson annihilation operator which acts on the variables $(x_1, \ldots, x_N)$ and corresponds to the normalised wave function $L^{-3/2} \exp[2\pi i k \cdot x/L]$ on $L^2(Q_\Lambda)$. Similarly let b_k be the operator acting on the variables $(x_{N+1}, \ldots, x_{2N})$. The $2N$ particle kinetic energy K_N is then given by

$$K_N = \frac{4\pi^2}{L^2} \sum_{k \in Z^3} k^2 [a_k^* a_k + b_k^* b_k]. \tag{2.5}$$

Let A_k be the operator

$$A_k = \sum_{n \in Z^3} [a_{n+k}^* a_n - b_{n+k}^* b_n]. \tag{2.6}$$

Then if $H_{N,\beta}$ denotes the Hamiltonian H_N of (1.1) with the Coulomb potential replaced by (2.3) we have for the wave functions ψ in Theorem 1.1 the representation

$$\langle \psi, H_{N,\beta}\psi \rangle = \langle \psi, K_N \psi \rangle + \sum_{k \in Z^3} v_\alpha(k) [\langle \psi | A_k^* A_k | \psi \rangle - 2N]. \tag{2.7}$$

Let $k \in Z^3$ and $m = (n, \pm 1)$ be in $Z^3 \times Z_2$. We define the norm of m as $|m| = |n|$ and operators $S_{k,m}$, $T_{k,m}$ for $|m| \leqq |k|/4$ by

$$S_{k,m} = \begin{array}{ll} a_n^* a_{n+k} & \text{if} \quad m = (n, 1), \\ -b_n^* b_{n+k} & \text{if} \quad m = (n, -1), \end{array}$$

$$T_{k,m} = \begin{array}{ll} a_n^* a_{n-k} & \text{if} \quad m = (n, 1) \\ -b_n^* b_{n-k} & \text{if} \quad m = (n, -1). \end{array} \tag{2.8}$$

It is evident from (2.6) that

$$A_k = \sum_{|m| \leqq |k|/4} [S_{k,m}^* + T_{k,m}] + B_k, \tag{2.9}$$

where the operator B_k contains only products $a_p^* a_q$, $b_p^* b_q$, where both $|p|$ and $|q|$ exceed $|k|/4$.

We obtain a lower bound on the kinetic energy of ψ which is analogous to the inequality (2.10) of [1]. We have the following lemma:

Lemma 2.2. *Let $\delta > 0$ and γ be a positive number with $1 \leqq \gamma \leqq N^{1/3}$. For $k \in R^3$ let $C_k(\psi)$ be defined by*

$$C_k(\psi) = \sum_{r=0}^{\infty} \frac{1}{2^{r(3+\delta)}} \sum_{(2^r-1)\gamma \leqq |m| < (2^{r+1}-1)\gamma} \langle \psi | S^*_{k,m} S_{k,m} + T^*_{k,m} T_{k,m} | \psi \rangle. \tag{2.10}$$

Then there is the inequality

$$\langle \psi | K_N | \psi \rangle \geqq \frac{C_\delta}{NL^2} \sum_{|k| > 4\gamma} k^2 C_k(\psi), \tag{2.11}$$

where C_δ is a positive constant depending only on $\delta > 0$.

We define a function $I_k(\varepsilon, \gamma)$ similar to (4.17) of [1] by

$$I_k(\varepsilon, \gamma) = \varepsilon C_k(\psi) + \langle \psi | A^*{}_k A_k | \psi \rangle - 2N. \tag{2.12}$$

Then we have

$$\langle \psi, H_{N,\beta} \psi \rangle \geqq -2N \sum_{|k| \leqq 4\gamma} v_\alpha(k) + \sum_{|k| > 4\gamma} v_\alpha(k) I_k(C_\delta k^2/NL^2 v_\alpha(k), \gamma). \tag{2.13}$$

From Lemma 2.1 we have

$$2N \sum_{|k| \leqq 4\gamma} v_\alpha(k) \leqq CN\gamma/L, \tag{2.14}$$

for some constant C. From now on we take $\gamma = \gamma_\psi$ as defined in Theorem 1.1. Since it is evident that

$$N\gamma^2/L^2 - CN\gamma/L \geqq -C'N, \tag{2.15}$$

for some constant C', it is only necessary for us to find a lower bound on the second sum in (2.13) in order to complete the proof of Theorem 1.1.

We define $N(u)$ by

$$N(u) = \sum_{|n| > u} \langle \psi | a^*_n a_n + b^*_n b_n | \psi \rangle. \tag{2.16}$$

The following lemma is analogous to Lemma 4.1 of [1].

Lemma 2.3. *For $m \in Z^3 \times Z_2$*, let

$$N_m = \begin{bmatrix} \langle \psi | a^*_n a_n | \psi \rangle & \text{if} \quad m = (n, +1), \\ \langle \psi | b^*_n b_n | \psi \rangle & \text{if} \quad m = (n, -1). \end{bmatrix} \tag{2.17}$$

Let α_m, $|m| \leqq |k|/4$, be the positive roots of the polynomial in μ,

$$\sum_{r=0}^{\infty} \sum_{(2^r-1)\gamma \leqq |m| < (2^{r+1}-1)\gamma} \left[\frac{N_m}{\varepsilon N_m / 2^{r(3+\delta)} - \mu} + \frac{N_m}{\varepsilon N_m / 2^{r(3+\delta)} + \mu} \right] + 1 = 0, \tag{2.18}$$

where the double sum in (2.18) is only over m with $|m| \leqq |k|/4$. Then $I_k(\varepsilon, \gamma)$ satisfies the inequality

$$I_k(\varepsilon, \gamma) \geqq \sum_{r=0}^{\infty} \sum_{(2^r-1)\gamma \leqq |m| < (2^{r+1}-1)\gamma} \left[\alpha_m - \left(1 + \frac{\varepsilon}{2^{r(3+\delta)}} \right) N_m \right] - 3N(|k|/4) \tag{2.19}$$

Now we have by definition of γ.

$$N(u) \leqq N\gamma^2/u^2, \quad \text{and hence} \tag{2.20}$$

$$\sum_{|k|>4\gamma} v_\alpha(k) N(|k|/4) \leqq CN\gamma/L, \tag{2.21}$$

for some constant C. In view of (2.15) it is sufficient for us to bound below appropriately the sum in (2.19). This is accomplished by the following lemma.

Lemma 2.4. *Let $J_k(\varepsilon, \gamma)$ denote the sum on the right in (2.19). Then J_k satisfied the inequalities*

$$J_k(\varepsilon, \gamma) \geqq -2N, \tag{2.22}$$

$$J_k(\varepsilon, \gamma) \geqq -C_\delta N(\gamma^3/\varepsilon)^{1/(3+\delta/2)}, \quad \varepsilon > \gamma^3, \tag{2.23}$$

where C_δ is a constant depending only on $\delta > 0$.

Lemma 2.4 is analogous to Lemma 4.2 of [1], but is a weaker estimate for large ε. However this estimate is still sufficient to prove Theorem 1.1. We need only to estimate

$$\sum_{|k|>4\gamma} v_\alpha(k) J_k(C_\delta k^2/NL^2 v_\alpha(k), \gamma). \tag{2.24}$$

and by (2.23) this is bounded below by

$$-C_\delta N^{5/4}(\gamma/L)^{3/4}, \tag{2.25}$$

where C_δ is a constant depending on δ. Now since

$$N(\gamma/L)^2 - C_\delta N^{5/4}(\gamma/L)^{3/4} \geqq -C'_\delta N^{7/5}, \tag{2.26}$$

for some constant C'_δ depending only on δ, we have completed the proof of Theorem 1.1.

3. Proof of Lemmas

Here we turn to the proof of Lemmas 2.1 to 2.4.

Proof of Lemma 2.1. For $u > 0$ and $\xi \in \mathbb{R}^3$ let

$$I(u, \xi) = \int_0^{L/2} \frac{e^{-u|x|}}{|x|} e^{i\xi \cdot x} dx. \tag{3.1}$$

It is easy to see that I is given by the formula

$$I(u, \xi) = \frac{4\pi}{|\xi|^2 + u^2} \left\{ 1 - e^{-uL/2} \left[\cos|\xi|L/2 + (uL)\frac{\sin|\xi|L/2}{|\xi|L/2} \right] \right\}. \tag{3.2}$$

The coefficient $v_\alpha(k)$ in (2.3) is given by

$$v_\alpha(k) = \frac{1}{L^3} I\left(\frac{N^{1/5}}{L}, \frac{2\pi k}{L} \right), \tag{3.3}$$

and it is easy to see from (3.2) and (3.3) that the inequality (2.4) holds. Q.E.D.

Proof of Lemma 2.2. First note that the sum in (2.10) is finite since $S_{k,m}$ and $T_{k,m}$ are defined only for $|m| \leqq |k|/4$. We have

$$\begin{aligned}\langle\psi|K_N|\psi\rangle &= \frac{4\pi^2}{L^2}\langle\psi|\sum_{k\in Z^3} k^2[a_k^* a_k + b_k^* b_k]|\psi\rangle \\ &= \frac{4\pi^2}{L^2 N}\left[\langle\psi|\sum_{m,k} a_m^* a_m k^2 a_k^* a_k|\psi\rangle + \langle\psi|\sum_{m,k} b_m^* b_m k^2 b_k^* b_k|\psi\rangle\right]. \end{aligned}\tag{3.4}$$

Now we have

$$\begin{aligned}\sum_{m,k} a_m^* a_m k^2 a_k^* a_k &= \sum_{m,k} a_m^* a_m (m+k)^2 a_{m+k}^* a_{m+k} \geqq \sum_k \frac{|k|^2}{4}\sum_{|m|\leqq|k|/4} a_m^* a_m a_{m+k}^* a_{m+k} \\ &\geqq \sum_k \frac{|k|^2}{4}\sum_{|m|\leqq|k|/4}\frac{1}{2^{(3+\delta)r(m)}} a_m^* a_m a_{m+k}^* a_{m+k} \\ &= \sum_k \frac{|k|^2}{4}\sum_{|m|\leqq|k|/4}\frac{1}{2^{(3+\delta)r(m)}}[S_{k,m}^* S_{k,m} - a_{m+k}^* a_{m+k}], \end{aligned}\tag{3.5}$$

where

$$r(m) = r \quad \text{if} \quad (2^r - 1)\gamma \leqq |m| < (2^{r+1}-1)\gamma. \tag{3.6}$$

The last expression in (3.5) gives an inequality for the kinetic energy of the desired form except for the terms in $a_{m+k}^* a_{m+k}$. These are negligible since $\gamma^3 \leqq N$. This follows since

$$\sum_k \frac{|k|^2}{4}\sum_{|m|\leqq|k|/4}\frac{1}{2^{(3+\delta)r(m)}} a_{m+k}^* a_{m+k} \leqq \sum_t \sum_{|m|\leqq|t|/2}\frac{1}{2^{(3+\delta)r(m)}}|t|^2 a_t^* a_t, \tag{3.7}$$

and from (3.6) it is evident that

$$\sum_m \frac{1}{2^{(3+\delta)r(m)}} \leqq C_\delta \gamma^3, \tag{3.8}$$

for some constant C_δ depending only on $\delta > 0$.

By similar argument we therefore obtain an inequality

$$\langle\psi|K_N|\psi\rangle \geqq \frac{\pi^2}{2NL^2}\sum_{|k|>4\gamma} k^2 C_k(\psi) - \frac{C_\delta \gamma^3}{N}\langle\psi|K_N|\psi\rangle, \tag{3.9}$$

where C_δ is a positive constant depending only on $\delta > 0$. The inequality (2.11) clearly follows from (3.9). Q.E.D.

Proof of Lemma 2.3. We apply a Bogoliubov transformation to the operators $S_{k,m}, T_{k,m}$ with $|m| \leqq |k|/4$. Let M be a matrix which is in the block form

$$M = \begin{bmatrix} V & W \\ W & V \end{bmatrix}, \tag{3.10}$$

and satisfies the matrix identity

$$M'\begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} M = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}, \tag{3.11}$$

where I is the identify matrix. The matrices M, V, W are assumed to be real with adjoints denoted by M', V', W'. One can see that (3.11) holds if and only if

$$V'V - W'W = I, \quad V'W = W'V. \tag{3.12}$$

Further, it is clear that M^{-1} is given by the formula

$$M^{-1} = \begin{bmatrix} V' & -W' \\ -W' & V' \end{bmatrix}. \tag{3.13}$$

From (3.13) it follows that, as well as (3.12), one has

$$VV' - WW' = I, \quad VW' = WV'. \tag{3.14}$$

Now let V, W be matrices with the same dimension d as the number of elements m with $|m| \leqq |k|/4$. We write I_k in (2.12) as

$$\begin{aligned} I_k(\varepsilon, \gamma) = \langle \psi | & \sum_{|m| \leqq d} \varepsilon_m [S_m^* S_m + T_m^* T_m] \\ & + \left(\sum_{|m| \leqq d} [S_m^* + T_m] + B \right)^* \left(\sum_{|m| \leqq d} [S_m^* + T_m] + B \right) | \psi \rangle - 2N, \end{aligned} \tag{3.15}$$

where the S_m and T_m denote $S_{k,m}$ and $T_{k,m}$ as defined by (2.8). Now let us denote by σ the sum,

$$\sigma = \sum_{|m| \leqq d} \frac{1}{\varepsilon_m}, \tag{3.16}$$

and λ_m, $|m| \leqq d$, be arbitrary positive numbers. We make a transformation on the S_m, T_m, by

$$S_m = \lambda_m F_m - B^*/\varepsilon_m(1 + 2\sigma), \quad T_m = \lambda_m G_m - B/\varepsilon_m(1 + 2\sigma). \tag{3.17}$$

Then (3.15) becomes

$$\begin{aligned} I_k(\varepsilon, \gamma) = \langle \psi | & \sum_{|m| \leqq d} \varepsilon_m \lambda_m^2 [F_m^* F_m + G_m^* G_m] \\ & + \left(\sum_{|m| \leqq d} \lambda_m [F_m^* + G_m] \right)^* \left(\sum_{|m| \leqq d} \lambda_m [F_m^* + G_m] \right) | \psi \rangle - 2N \\ & + \frac{1}{(1 + 2\sigma)^2} \langle \psi | (1 + \sigma) B^* B + \sigma B B^* | \psi \rangle \\ & + \frac{1}{(1 + 2\sigma)} \langle \psi | \sum_{|m| \leqq d} [B^*, \lambda_m F_m^*] + [\lambda_m F_m, B] | \psi \rangle. \end{aligned} \tag{3.18}$$

We obtain a lower bound on the last term in (3.18). Indeed it is the same as

$$\frac{1}{1 + 2\sigma} \langle \psi | \sum_{|m| \leqq d} [B^*, S_m^*] + [S_m, B] | \psi \rangle + \langle \psi | \frac{2\sigma}{(1 + 2\sigma)^2} [B^*, B] | \psi \rangle, \tag{3.19}$$

and since the first expression in (3.19) is identically zero this is the same as

$$\frac{2\sigma}{(1+2\sigma)^2}\langle\psi|[B^*,B]|\psi\rangle. \tag{3.20}$$

It is easy to see that

$$\langle\psi|[B^*,B]|\psi\rangle \geqq -N(|k|/4), \tag{3.21}$$

and this yields the lower bound on the third term in (3.18).

The second expression in (3.18) is evidently positive and so we are reduced to estimating the first expression which we shall write as

$$\begin{aligned} J_k(\varepsilon,\gamma) = \langle\psi| &\sum_{|m|\leqq d} \varepsilon_m\lambda_m^2[F_m^*F_m + G_m^*G_m] \\ &+\left(\sum_{|m|\leqq d}\lambda_m[F_m^*+G_m]\right)^*\left(\sum_{|m|\leqq d}\lambda_m[F_m^*+G_m]\right)|\psi\rangle - 2N. \end{aligned} \tag{3.22}$$

Our next goal is to find an accurate lower bound on J_k by using Bogoliubov transformations. To do this we write J_k in matrix form as

$$J_k(\varepsilon,\gamma) = \langle\psi|\begin{bmatrix} F \\ G^* \end{bmatrix}'\begin{bmatrix} C+D & C \\ C & C+D \end{bmatrix}\begin{bmatrix} F^* \\ G \end{bmatrix} - \sum_{|m|\leqq d}\varepsilon_m\lambda_m^2[F_m,F_m^*]|\psi\rangle - 2N, \tag{3.23}$$

where F and G are vectors with entries F_m and G_m, $|m|\leqq d$, respectively. The matrices C and D are given by

$$C = (\lambda_m\lambda_n), \quad D = (\varepsilon_n\lambda_n^2\delta_{n,m}). \tag{3.24}$$

Next we choose a Bogoliubov transformation M given by (3.10) which diagonalizes the matrix in (3.23). Thus

$$M'\begin{bmatrix} C+D & C \\ C & C+D \end{bmatrix} M = \begin{bmatrix} \alpha_0 & & & \\ & \ddots & & \\ & & \alpha_0 & \\ & & & \ddots \end{bmatrix}. \tag{3.25}$$

Hence if we define the transformation

$$\begin{bmatrix} F^* \\ G \end{bmatrix} = M\begin{bmatrix} \eta^* \\ \zeta \end{bmatrix}, \tag{3.26}$$

we have $J_k(\varepsilon,\gamma)$ given by

$$J_k(\varepsilon,\gamma) = \langle\psi|\sum_{|m|\leqq d}\alpha_m[\eta_m\eta_m^* + \zeta_m^*\zeta_m] - \sum_{|m|\leqq d}\varepsilon_m\lambda_m^2[F_m,F_m^*]|\psi\rangle - 2N. \tag{3.27}$$

We conclude therefore that

$$J_k(\varepsilon,\gamma) \geqq \langle\psi|\sum_{|m|\leqq d}\alpha_m[\eta_m,\eta_m^*] - \varepsilon_m\lambda_m^2[F_m,F_m^*]|\psi\rangle - 2N. \tag{3.28}$$

We need to estimate the commutators in (3.28). To do this we see from (3.13) that

$$\eta = V'F - W'G^*, \quad \zeta = -W'F^* + V'G, \tag{3.29}$$

and hence we have

$$\eta_m = \sum_n V_{n,m} F_n - W_{n,m} G_n^* = \sum_n \lambda_n^{-1} [V_{n,m} S_n - W_{n,m} T_n^*]$$
$$+ \frac{B^*}{(1+2\sigma)} \sum_n \frac{1}{\lambda_n \varepsilon_n} (V_{n,m} - W_{n,m}). \tag{3.30}$$

Thus the right-hand side of (3.28) is

$$\langle \psi | \sum_{|m| \leq d} \alpha_m \left[\sum_n \lambda_n^{-1} (V_{n,m} S_n - W_{n,m} T_n^*), \sum_n \lambda_n^{-1} (V_{n,m} S_n^* - W_{n,m} T_n) \right] - \sum_m \varepsilon_m [S_m, S_m^*] | \psi \rangle$$
$$- 2N + \langle \psi | B^*, B] | \psi \rangle \left[\frac{-\sigma}{(1+2\sigma)^2} + \frac{1}{(1+2\sigma)^2} \sum_{|m| \leq d} \alpha_m \left[\sum_n \frac{1}{\lambda_n \varepsilon_n} (V_{n,m} - W_{n,m}) \right]^2 \right]. \tag{3.31}$$

We wish to bound below the last expression in (3.31). The last sum in (3.31) can be written in matrix form as

$$h'(V-W) \begin{bmatrix} \alpha_0 & & \\ & \alpha_1 & \\ & & \ddots \end{bmatrix} (V-W)'h, \tag{3.32}$$

where h is the vector with entries h_m given by $h_m = 1/\lambda_m \varepsilon_m$. The expression (3.32) is clearly bounded in absolute value by

$$2h' \left\{ V \begin{bmatrix} \alpha_0 & & \\ & \alpha_1 & \\ & & \ddots \end{bmatrix} V' + W \begin{bmatrix} \alpha_0 & & \\ & \alpha_1 & \\ & & \ddots \end{bmatrix} W' \right\} h. \tag{3.33}$$

One can see from (3.25) that

$$V \begin{bmatrix} \alpha_0 & & \\ & \alpha_1 & \\ & & \ddots \end{bmatrix} V' + W \begin{bmatrix} \alpha_0 & & \\ & \alpha_1 & \\ & & \ddots \end{bmatrix} W' = C + D. \tag{3.34}$$

Thus (3.33) is

$$2[h'Ch + h'Dh] = 2[\sigma^2 + \sigma]. \tag{3.35}$$

It follows then that the coefficient of $\langle \psi | B^*, B] | \psi \rangle$ in (3.31) is bounded in absolute value by 1/2.

We need now to consider the expression

$$H_k(\varepsilon, \gamma) = \langle \psi | \sum_{|m| \leq d} \alpha_m \left[\sum_n \lambda_n^{-1} (V_{n,m} S_n - W_{n,m} T_n^*), \right.$$
$$\left. \sum_n \lambda_n^{-1} (V_{n,m} S_n^* - W_{n,m} T_n) \right] - \sum_m \varepsilon_m [S_m, S_m^*] | \psi \rangle - 2N. \tag{3.36}$$

This is the same as

$$H_k(\varepsilon,\gamma)=\langle\psi|\sum_{|m|\leq d}\alpha_m\left[\sum_n\lambda_n^{-2}(V_{n,m})^2[S_n,S_n^*]-\lambda_n^{-2}(W_{n,m})^2[T_n,T_n^*]\right]$$
$$-\sum_n\varepsilon_m[S_m,S_m^*]|\psi\rangle-2N. \tag{3.37}$$

To proceed further we need to explicitly compute the commutators involved in (3.37). First we introduce a slight change of notation from the definition (2.8) for the S_m and T_m. Let $m\in Z^3\times Z_2$ and $m=(n,\alpha)$, $\alpha=\pm 1$. Then if $k\in Z^3$ we define $m+k$ by $m+k=(n+k,\alpha)$. For $m=(n,\alpha)$ we define a_m by

$$\begin{aligned} a_m &= a_n \quad \text{if} \quad \alpha=1,\\ &= b_n \quad \text{if} \quad \alpha=-1. \end{aligned} \tag{3.38}$$

Thus from (2.8) we have

$$S_{k,m}=\alpha a_m^* a_{m+k},\quad T_{k,m}=\alpha a_m^* a_{m-k},\quad \text{if}\quad m=(n,\alpha). \tag{3.39}$$

From (3.39) it is easy to calculate the commutators involved in (3.37) as

$$[S_{k,m},S_{k,m}^*]=a_m^*a_m-a_{m+k}^*a_{m+k},\quad [T_{k,m},T_{k,m}^*]=a_m^*a_m-a_{m-k}^*a_{m-k}. \tag{3.40}$$

Thus (3.37) is the same as

$$H_k(\varepsilon,\gamma)=\langle\psi|\sum_{|m|\leq d}\alpha_m\left[\sum_n\lambda_n^{-2}\{(V_{n,m})^2-(W_{n,m})^2\}a_n^*a_n\right]$$
$$-\sum_m(1+\varepsilon_m)a_m^*a_m|\psi\rangle-N(|k|/4)+P_k(\varepsilon,\gamma), \tag{3.41}$$

where

$$P_k(\varepsilon,\gamma)=\sum_{|n|\leq|k|/4}\langle\psi|a_{n+k}^*a_{n+k}|\psi\rangle\left[\varepsilon_n-\sum_m\alpha_m\lambda_n^{-2}(V_{n,m})^2\right]$$
$$+\sum_{|n|\leq|k|/4}\langle\psi|a_{n-k}^*a_{n-k}|\psi\rangle\sum_m\alpha_m\lambda_n^{-2}(W_{n,m})^2. \tag{3.42}$$

From the matrix identity (3.34) it is clear that

$$\sum_m\alpha_m(V_{n,m})^2\leqq\lambda_n^2(1+\varepsilon_n). \tag{3.43}$$

It follows therefore that

$$P_k(\varepsilon,\gamma)\geqq -N(|k|/4). \tag{3.44}$$

Finally we consider the first expression in (3.41). If we let $\lambda_n\to\langle\psi|a_n^*a_n|\psi\rangle=N_n$ and use the identity (3.14), it is clear that this expression converges to

$$\sum_m[\alpha_m-(1+\varepsilon_m)N_m], \tag{3.45}$$

and this is exactly the sum on the right in (2.19). Equation (2.18) which determines the roots α_m is just the characteristic polynomial for the matrix diagonalization problem (3.11), (3.25). The polynomial is explicitly computed in [1]. The lemma now follows easily from the estimates we have made. Q.E.D.

Proof of Lemma 2.4. The inequality (2.22) follows since the α_m can be arranged such that

$$\alpha_m \geqq \varepsilon N_m/2^{r(m)(3+\delta)}. \tag{3.46}$$

Now define $n_r, r = 0, 1, 2, \ldots$, by

$$n_r = \sum_{(2^r-1)\gamma \leqq |m| < (2^{r+1}-1)\gamma} N_m, \tag{3.47}$$

and let β_r, $r = 0, 1, 2, \ldots$, be the positive roots of the equation

$$\sum_{r=0}^{\infty} \left[\frac{n_r}{C\varepsilon n_r/2^{r(6+\delta)}\gamma^3 - \mu} + \frac{n_r}{C\varepsilon n_r/2^{r(6+\delta)}\gamma^3 + \mu} \right] + 1 = 0, \tag{3.48}$$

where C is any positive constant which satisfies

$$\sum_{(2^r-1)\gamma \leqq |m| < (2^{r+1}-1)\gamma} 1 \geqq C 2^{3r}\gamma^3. \tag{3.49}$$

Then we see by the argument of Lemma 4.2 of [1] that

$$J_k(\varepsilon, \gamma) \geqq \sum_{r=0}^{\infty} \left[\alpha_r - \left(1 + \frac{C\varepsilon}{2^{r(6+\delta)}\gamma^3} \right) n_r \right]. \tag{3.50}$$

By definition of γ we have

$$n_r \leqq C' N/2^{2r}, \tag{3.51}$$

for some universal constant C'. Thus if we define η_r, ν by

$$\eta_r = C'/2^{2r}, \nu = \varepsilon/\gamma^3, \tag{3.52}$$

we have $J_k(\varepsilon, \gamma)$ bounded below as

$$J_k(\varepsilon, \gamma) \geqq N \sum_{r=0}^{\infty} \left[\beta'_r - \left(1 + \frac{C\nu}{2^{r(6+\delta)}} \right) \eta_r \right], \tag{3.53}$$

where β'_r are the positive roots of the polynomial equation

$$\sum_{r=0}^{\infty} \left[\frac{\eta_r}{C\nu\eta_r/2^{r(6+\delta)} - \mu} + \frac{\eta_r}{C\nu\eta_r/2^{r(6+\delta)} + \mu} \right] + 1 = 0. \tag{3.54}$$

Now let β'_r be the root of (3.54) which lies in the region

$$\frac{C\nu\eta_{r-1}}{2^{(r-1)(6+\delta)}} > \beta'_r > \frac{C\nu\eta_r}{2^{r(6+\delta)}}. \tag{3.55}$$

We bound β'_r below by

$$\beta'_r \geqq \frac{C\nu\eta_r}{2^{r(6+\delta)}} \quad \text{if} \quad \frac{\nu}{2^{r(6+\delta)}} \leqq 1. \tag{3.56}$$

If the restriction on ν in (3.56) is violated we proceed differently. Consider a particular β'_r such that $\nu > 2^{r(6+\delta)}$. Then it is clear that

$$\sum_{m=0}^{\infty} \frac{\eta_m}{C\nu\eta_m/2^{m(6+\delta)} + \beta'_r} \leqq \sum_{m \leqq r} \frac{2^{m(6+\delta)}}{C\nu} + \sum_{m>r} \frac{\eta_m}{\beta'_r} \leqq C' \frac{2^{r(6+\delta)}}{\nu}, \tag{3.57}$$

for some universal constant C'. Similarly it is easy to see that

$$\sum_{m=0}^{r-2} \frac{\eta_m}{C\nu\eta_m/2^{m(6+\delta)} - \beta'_r} \leqq C' \frac{2^{r(6+\delta)}}{\nu}, \tag{3.58}$$

for some constant C'. Thus there is a positive constant C' such that β'_r satisfies the inequality

$$\frac{\eta_{r-1}}{C\nu\eta_{r-1}/2^{(r-1)(6+\delta)} - \beta'_r} + \frac{\eta_r}{C\nu\eta_r/2^{r(6+\delta)} - \beta'_r} + \frac{C'2^{r(6+\delta)}}{\nu} + 1 \geqq 0. \tag{3.59}$$

The inequality (3.59) is a quadratic inequality in β'_r, and it is not difficult to see that as a consequence we must have

$$\beta'_r \geqq \frac{C\nu\eta_r}{2^{r(6+\delta)}} + \left[1 + \frac{C'2^{r(6+\delta)}}{\nu}\right]^{-1} \eta_r, \tag{3.60}$$

for some constant C' (which may differ from the constant in (3.59)). From (3.60) we obtain a lower bound on β'_r if $\nu > 2^{r(6+\delta)}$ as

$$\beta'_r \geqq \frac{C\nu\eta_r}{2^{r(6+\delta)}} + \eta_r - \frac{C'2^{r(6+\delta)}}{\nu}\eta_r. \tag{3.61}$$

We shall find a lower bound on J_k in (3.53) by using the estimates (3.56) and (3.61) on the β'_r. We have

$$\begin{aligned} J_k(\varepsilon, \gamma) &\geqq N \sum_{\nu \leqq 2^{r(6+\delta)}} + N \sum_{\nu > 2^{r(6+\delta)}} \geqq N \sum_{\nu \leqq 2^{r(6+\delta)}} -\eta_r + N \sum_{\nu > 2^{r(6+\delta)}} -\frac{C'2^{r(6+\delta)}}{\nu}\eta_r \\ &\geqq -C'N/\nu^{1/(3+\delta/2)}, \end{aligned} \tag{3.62}$$

for some constant C'.

The inequality (3.62) completes the proof of the lemma. Q.E.D.

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