

The Ground State Energy per Particle for Infinite Particle Quantum Systems*

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Abstract. We give a simple proof that the ground state energy per particle for several interacting particle systems is monotone and bounded as the number of particles increases. Some of the systems for which the proof holds are anharmonic oscillator approximations to $|\phi|_d^4$ quantum fields, many body Schrödinger operators with nearest and next to nearest neighbor couplings, and systems whose energy is given by operators which are not restricted to being differential operators.

It is well known that if we pinch a vibrating system of particles, or clamp a vibrating membrane the fundamental frequencies increase. Similarly if we tear a vibrating membrane its fundamental frequency decreases. Some of the mathematical consequences of these observations, in classical physics, are that imposing Dirichlet or Neumann boundary conditions on $-\Delta$, (or finite difference approximations to $-\Delta$) along a curve in the interior of some bounded region, raises or lowers its eigenvalues [1].

Some of the mathematical consequences of these observations in quantum physics are described in this paper. We show in particular that the ground state energy per particle, for the sequence of coupled anharmonic oscillator Schrödinger operators with Dirichlet boundary conditions used in the “doubling algorithm” in [2] to numerically approximate the ϕ_2^4 quantum field theory, is monotone decreasing.

We next show that the ground state energy per particle, for the sequence of coupled anharmonic oscillator Schrödinger operators with Neumann Boundary conditions used in [2] to approximate the ϕ_2^4 theory, is monotone increasing.

We also show that the energy per particle is bounded from above and below in both of the preceding cases and hence it converges to a limit as the number of particles becomes infinite.

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We remark that our method of proof works for a larger class of coupled systems which includes spherically symmetric anharmonic oscillator approximations to $|\phi|_d^4$ quantum field theories. The method of proof also works for couplings between the oscillators which are not “nearest neighbors”. In fact, as is easily seen, the proof will work for a much larger class of interacting systems where the energy operator for each individual particle need not even be a differential operator.

We illustrate the proof in the simplest case, the n -oscillator approximation (with Dirichlet boundary conditions) to the ϕ_2^4 quantum field theory [2]. Let H_N denote the N -oscillator Schrödinger operator

$$H_N \equiv \sum_{j=1}^N A_j - \sum_{j=1}^{N-1} q_j q_{j+1}, \quad (1)$$

where for a, b, c , and d real numbers with $a > 0$

$$A_j \equiv \frac{1}{2} \left[-\frac{\partial^2}{\partial q_j^2} + a q_j^4 + b q_j^2 + c q_j + d \right]. \quad (2)$$

The operators H_N have a complete orthonormal set of eigenfunctions

$$\Omega_j^{(N)} = \Omega_j^{(N)}(q_1, q_2, \dots, q_N) \quad (3)$$

whose eigenvalues we denote by $E_j(N)$, where

$$E_0(N) < E_1(N) \leq E_2(N) \leq \dots \quad (4)$$

Theorem I. *If $E_0(N)$ denotes the lowest eigenvalue of the N -oscillator “Dirichlet” operator (1) then,*

- (i) $p(n) \equiv E_0(2^n)/2^n$, is monotone decreasing as n increases.
- (ii) $p(n)$ is bounded above and below for all n .
- (iii) The limit as $n \rightarrow \infty$ of $p(n)$ exists.

The proof of (i) would be trivial if the system was not interacting, i.e. if the “coupling” term $\sum q_j q_{j+1}$ was not present in (1) because then $E_0(N) = N E_0(1)$.

In the interacting or coupled case we use a variational calculation to prove monotonicity by showing that “pinching the system in the middle” raises its energy. We have that

$$E_0(2N) = \inf_{\psi \in L_2(\mathbb{R}^{2N})} \langle \psi, H_{2N} \psi \rangle \leq \langle \Omega, H_{2N} \Omega \rangle, \quad (5)$$

where we take

$$\Omega(q_1, \dots, q_N, q_{N+1}, \dots, q_{2N}) = \Omega_0^{(N)}(q_1 \dots q_N) \Omega_0^{(N)}(q_{N+1} \dots q_{2N}). \quad (6)$$

Observe that H_{2N} may be written as

$$H_{2N} = H_N^L + H_N^R - q_N q_{N+1}, \quad (7)$$

where

$$H_N^L \equiv \sum_{j=1}^N A_j - \sum_{j=1}^{N-1} q_j q_{j+1} \quad (8)$$

and

$$H_N^R = \sum_{j=N+1}^{2N} A_j - \sum_{j=N+1}^{2N-1} q_j q_{j+1}. \quad (9)$$

Thus from (5) and (6)

$$E_0(2N) \leq 2E_0(N) - Q_N Q_{N+1}, \quad (10)$$

where

$$\begin{aligned} Q_N &\equiv \langle \Omega_0^{(N)}(q_1 \dots q_N), q_N \Omega_0^{(N)}(q_1 \dots q_N) \rangle \\ Q_{N+1} &\equiv \langle \Omega_0^{(N)}(q_{N+1} \dots q_{2N}), q_{N+1} \Omega_0^{(N)}(q_{N+1} \dots q_{2N}) \rangle. \end{aligned} \quad (11)$$

We now use the facts that $E_0^{(N)}$ is non-degenerate, and H_N commutes with the unitary map R given by

$$R\psi(q_1 \dots q_N) = \psi(q_N \dots q_1) \quad (12)$$

to conclude that $Q_N = Q_{N+1}$.

Therefore

$$E_0(2N) \leq 2E_0(N) - Q_N^2 \leq 2E_0(N). \quad (13)$$

This inequality illustrates the fact that the ‘‘pinched’’ system [whose ground state energy is $2E_0(N)$] has higher energy than the original system. It follows from (13) that

$$\frac{E_0(2N)}{2N} \leq \frac{E_0(N)}{N} \quad (14)$$

and therefore the function $p(N) = E_0(2^N)/2^N$ is monotone decreasing as N increases.

We remark that the proof just given would hold if the q_j were replaced by vectors

$$\mathbf{q}_j = (q_j^1, q_j^2, \dots, q_j^m) \quad \text{and} \quad \frac{\partial^2}{\partial q_j^2} \text{ replaced by Laplacians } \sum_{k=1}^m (\partial/\partial q_j^k)^2$$

(the H_N 's would then be approximations to the $|\Phi\rangle_2^4$ theory). It is also clear that the proof would work if we took $A_j = -\partial^2/\partial q_j^2 + V(q_j)$ for a large class of functions V . In fact the A_j need not even be differential operators for the above proof to work.

We now prove that $p(n)$ is a bounded function of n by showing that $E_0(N)/N$ is bounded. As quadratic forms we have that

$$\frac{-q_j^2 - q_{j+1}^2}{2} \leq -q_j q_{j+1} \leq \frac{q_j^2 + q_{j+1}^2}{2} \quad (15)$$

and hence

$$\begin{aligned} &\sum_{j=2}^{N-1} A_j - q_j^2 + A_1 - \frac{q_1^2}{2} + A_N - \frac{q_N^2}{2} \\ &\leq H_N \leq \sum_{j=2}^{N-1} A_j + q_j^2 + A_1 + \frac{q_1^2}{2} + A_N + \frac{q_N^2}{2} \end{aligned} \quad (16)$$

which implies that

$$\sum_{j=1}^N A_j - q_j^2 \leq H_N \leq \sum_{j=1}^N A_j + q_j^2. \quad (17)$$

If we denote the lowest eigenvalues of $A_j \pm q_j^2$ by $E_0^\pm(1)$ then we have that

$$NE_0^-(1) \leq E_0(N) \leq NE_0^+(1) \quad (18)$$

from which it follows that

$$E_0^-(1) \leq \frac{E_0(N)}{N} \leq E_0^+(1) \quad (19)$$

proving the boundedness of $p(n)$. Part (iii) follows from (i) and (ii).

If instead of the ‘‘Dirichlet operators’’ we had used ‘‘Neumann operators’’ [2]

$$K_N \equiv \sum_{j=2}^{N-1} A_j + \left(\frac{A_1 - q_1^2}{2} \right) + \left(\frac{A_N - q_N^2}{2} \right) - \sum_{j=1}^{N-1} q_j q_{j+1}. \quad (20)$$

We have that

$$K_{2N} = K_N^L + K_N^R + \left(\frac{q_{N+1} - q_N}{2} \right)^2, \quad (21)$$

where

$$\begin{aligned} K_N^L &= \sum_{j=2}^{N-1} A_j + \left(\frac{A_1 - q_1^2}{2} \right) + \left(\frac{A_N - q_N^2}{2} \right) - \sum_{j=1}^{N-1} q_j q_{j+1} \\ K_N^R &= \sum_{j=N+1}^{2N-1} A_j + \left(\frac{A_{N+1} - q_{N+1}^2}{2} \right) + \left(\frac{A_{2N} - q_{2N}^2}{2} \right) - \sum_{j=N+1}^{2N-1} q_j q_{j+1}. \end{aligned} \quad (22)$$

Hence as quadratic forms

$$K_{2N} \geq K_N^L + K_N^R \quad (23)$$

which implies that the lowest eigenvalue $E_0^K(2N)$ of K_{2N} is larger than the lowest eigenvalue $2E_0^K(N)$ of the system ‘‘torn in the middle’’. Thus

$$\frac{E_0^K(2N)}{2N} \geq \frac{E_0^K(N)}{N} \quad (24)$$

which implies that $p^K(n) \equiv E_0^K(2^n)/2^n$ is an increasing function of n . The fact that $p^K(n)$ is bounded is proved as in the ‘‘Dirichlet’’ case. We have therefore proven

Theorem II. *If $E_0^K(N)$ denotes the lowest eigenvalue of the N -oscillator Neumann operator K_N (20) then*

- (i) $p^K(n) = E_0^K(2^n)/2^n$ is monotone increasing as n increases.
- (ii) $p^K(n)$ is bounded in n .
- (iii) The limit as $n \rightarrow \infty$ of $p^K(n)$ exists.

To illustrate the method of proof when the system has more than nearest neighbor interactions, we prove monotonicity of the ground state energy per particle for a system of oscillators with nearest and *next* nearest neighbor coupling

whose energy operator is

$$G_N = \sum_{j=1}^N B_j + \sum_{j=1}^{N-2} q_j q_{j+2} - \sum_{j=1}^{N-1} q_j q_{j+1}, \quad (25)$$

where, for example, we could take, for $a > 0$,

$$B_j \equiv -\frac{\partial^2}{\partial q_j^2} + a q_j^6 + b q_j^4 + c q_j^2 + \cos(q_j) + d. \quad (26)$$

Denote the lowest eigenvalue of G_N by $E_0^G(N)$ and its eigenfunction by $\Phi_0^{(N)}(q_1 \dots q_N)$. As in the proof of Theorem I we have that

$$E_0^G(2N) \leq \langle \Omega, G_{2N} \Omega \rangle, \quad (27)$$

where

$$\Omega = \Phi_0^{(N)}(q_1 \dots q_N) \Phi_0^{(N)}(q_{N+1} \dots q_{2N}) \quad (28)$$

and

$$G_{2N} = G_N^L + G_N^R - q_N q_{N+1} + q_{N-1} q_{N+1} + q_N q_{N+2}, \quad (29)$$

where

$$\begin{aligned} G_N^L &= \sum_{j=1}^N B_j - \sum_{j=1}^{N-1} q_j q_{j+1} + \sum_{j=1}^{N-2} q_j q_{j+2} \\ G_N^R &= \sum_{j=N+1}^{2N} B_j - \sum_{j=N+1}^{2N-1} q_j q_{j+1} + \sum_{j=N+1}^{2N-2} q_j q_{j+2}. \end{aligned} \quad (30)$$

From (27) and (29) it follows that

$$E_0^G(2N) \leq 2E_0^G(N) - Q_N Q_{N+1} + Q_{N-1} Q_{N+1} + Q_N Q_{N+2}, \quad (31)$$

where

$$\begin{aligned} Q_N &= \langle \Phi_0^{(N)}(q_1 \dots q_N), q_N \Phi_0^{(N)}(q_1 \dots q_N) \rangle \\ Q_{N+1} &= \langle \Phi_0^{(N)}(q_{N+1} \dots q_{2N}), q_{N+1} \Phi_0^{(N)}(q_{N+1} \dots q_{2N}) \rangle \\ Q_{N+2} &= \langle \Phi_0^{(N)}(q_{N+1} \dots q_{2N}), q_{N+2} \Phi_0^{(N)}(q_{N+1} \dots q_{2N}) \rangle. \end{aligned} \quad (32)$$

However $Q_N = Q_{N+1} = Q_{N+2} = 0$ here because G_N commutes with the unitary operator S which acts by

$$S\psi(q_1 \dots q_N) \equiv \psi(-q_1 \dots -q_N). \quad (33)$$

We have therefore shown that $p^G(n) \equiv E_0^G(2^n)/2^n$ is monotone decreasing as n increases.

The last system that we illustrate this method of proving monotonicity of the energy per particle is a Dirichlet anharmonic oscillator approximation to the ϕ_d^4 field theory, where for simplicity we choose $d=3$.

Let $H(M, N)$ be given by

$$\begin{aligned} H(M, N) &\equiv \sum_{j=1}^M \sum_{k=1}^N A_{j,k} - \sum_{j=1}^{M-1} \sum_{k=1}^N q_{j,k} q_{j+1,k} \\ &\quad - \sum_{j=1}^M \sum_{k=1}^{N-1} q_{j,k} q_{j,k+1}, \end{aligned} \quad (34)$$

where for $a > 0$

$$A_{j,k} \equiv \frac{1}{2} \left[-\frac{\partial^2}{\partial q_{j,k}^2} + aq_{j,k}^4 + bq_{j,k}^2 + cq_{j,k} + d \right]. \tag{35}$$

If we let $E_0(M, N)$ denote the lowest eigenvalue of $H(M, N)$ then we have

Theorem III

- (i) $p(n) \equiv E_0(2^n, 2^n)/2^{2n}$ is monotone decreasing as n increases.
- (ii) $p(n)$ is bounded.
- (iii) The limit as $n \rightarrow \infty$ of $p(n)$ exists.

We prove (i) by showing that

$$E_0(2N, 2N) \leq 2E_0(N, 2N) \tag{36}$$

and

$$E_0(N, 2N) \leq 2E_0(N, N) \tag{37}$$

thus

$$E_0(2N, 2N) \leq 4E_0(N, N) \tag{38}$$

which yields (i).

We prove (36) by comparing the ground state energy of $H(2N, 2N)$ to that of a system “pinched down the middle” i.e. we write

$$H(2N, 2N) = H^L(N, 2N) + H^R(N, 2N) - \sum_{k=1}^{2N} q_{N,k} q_{N+1,k}, \tag{39}$$

$$H^L(N, 2N) = \sum_{j=1}^N \sum_{k=1}^{2N} A_{j,k} - \sum_{j=1}^{N-1} \sum_{k=1}^{2N} q_{j,k} q_{j+1,k} - \sum_{j=1}^N \sum_{k=1}^{2N-1} q_{j,k} q_{j,k+1} \tag{40}$$

$$H^R(N, 2N) = \sum_{j=N+1}^{2N} \sum_{k=1}^{2N} A_{j,k} - \sum_{j=N+1}^{2N-1} \sum_{k=1}^{2N} q_{j,k} q_{j+1,k} - \sum_{j=N+1}^{2N} \sum_{k=1}^{2N-1} q_{j,k} q_{j,k+1}. \tag{40}$$

As in the proof of Theorem I we have that

$$E_0(2N, 2N) \leq 2E_0(N, 2N). \tag{41}$$

The inequality (37) is proven similarly by “pinching” $H^L(N, 2N)$ and $H^R(N, 2N)$ across their middles.

References

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