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A class of lower bounds for Hamiltonian operators†

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Abstract. A method for deriving lower bounds to the ground states of nonrelativistic quantum Hamiltonians is developed and illustrated with examples. The bound depends on a trial function and can be made arbitrarily close to the true value, except for systems of fermions. For one-dimensional and spherically symmetric systems bounds for the excited states may also be derived. From the bound another one as found by Barnsley may be derived.

1. Introduction

Bargmann (1972) derived integral inequalities which can be used to give a lower bound for the kinetic energy of a wavefunction in terms of expectation values of r^n. Sachrajda *et al* (1978) observed that one may use functions other than just r^n and proposed to use these bounds for a variational principle. Although their statement about 'localised minima' to provide general lower bounds is incorrect (we give an explicit counter-example, example 1), their approach can be extended to arbitrary dimensions and made fruitful in a rather unexpected way.

A slightly extended version of the formal arguments of Sachrajda *et al* is given in § 2 and discussed rigorously in § 3. Section 4 contains the new results and § 5 some applications.

2. The formal arguments

Throughout this paper we set $\hbar^2/2m = 1$ and consider Hamiltonians $H = K + V$, $K = -\Delta$ in n space dimensions. We take $\mathscr{H} = \mathscr{L}^2(\mathbb{R}^n)$. The Schwarz inequality in $C^n \otimes \mathscr{H}$ tells us

$$\langle \nabla\psi, \nabla\psi\rangle\langle g\psi, g\psi\rangle \geq |\langle\nabla\psi, g\psi\rangle|^2 \tag{1}$$

where g is an n-component vector function. Suppose g is real. By partial integration

$$2\,\mathrm{Re}\langle\nabla\psi, g\psi\rangle = -\langle\psi, (\nabla\,.\,g)\psi\rangle, \tag{2}$$

and, since the modulus squared is not smaller than the real part squared,

$$\langle\psi, K\psi\rangle = \langle\nabla\psi, \nabla\psi\rangle \geq \langle\psi, (\nabla\,.\,g)\psi\rangle^2/4\langle\psi, g^2\psi\rangle. \tag{3}$$

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This may be looked upon as a quasiclassical term, for it does not really use the wavefunction ψ, but only the measure $d\mu(x) = |\psi(x)|^2 \, dx$ which it determines. We may therefore write

$$E(g, \mu) := \frac{(\mu(\nabla \cdot g))^2}{4\mu(g^2)} + \mu(V), \tag{4}$$

$$\inf_{\|\psi\|=1} \langle \psi, H\psi \rangle \geqslant \inf_{\|\mu\|=1, \mu \geqslant 0} E(g, \mu). \tag{5}$$

Suppose you could apply variational calculus in this situation. Take E as the Lagrangian multiplier for the condition $\|\mu\| = 1$. Then you would have to evaluate the equation

$$\frac{\delta}{\delta\mu(x)}\left(E(g, \mu) - E \int d\mu\right) = 0$$

for those x where $d\mu(x) \neq 0$ (i.e. $x \in \operatorname{supp}(\mu)$) and the inequality

$$\frac{\delta}{\delta \, d\mu(x)}\left(E(g, \mu) - E \int d\mu\right) \geqslant 0$$

where $d\mu(x) = 0$. You get

$$(\alpha(\mu)(\nabla \cdot g)(x) - \alpha^2(\mu) g^2(x) + V(x) - E)\chi_\mu(x) = 0 \tag{6a}$$

$$(\alpha(\mu)(\nabla \cdot g)(x) - \alpha^2(\mu) g^2(x) + V(x) - E)(1 - \chi_\mu(x)) \geqslant 0 \tag{6b}$$

as the condition for $E(g, \mu) = \inf E(g, \mu)$, where we have set

$$\alpha(\mu) := \mu(\nabla \cdot g)/2\mu(g^2) \tag{6c}$$

$$\chi_\mu(x) := \begin{cases} 1 & \text{if } x \in \operatorname{supp}(\mu) \\ 0 & \text{if } x \notin \operatorname{supp}(\mu). \end{cases} \tag{6d}$$

In generic situations, $\nabla \cdot g$, g^2 and V will be transversal, which means that (6a) can only hold for $\operatorname{supp}(\mu)$ being some $n-1$-dimensional hypersurface. Actually the situation is much more favourable.

3. Conditions for the admissibility of g

To be specific, we consider three types of situation.

(A) V is a sum of Coulomb pair potentials for $(\frac{1}{3})n$ particles.

(B) $V = V_1 + V_2$, $V_1 \in \mathscr{L}^\infty(\mathbb{R}^n)$, $V_2 \in \mathscr{L}^2(\mathbb{R}^n \backslash \{0\})_{\mathrm{loc}}$, $V_2(x) \geqslant -n(n-4)/4|x|^2$.

(C) $n = 1$, $K = -\partial^2/\partial x^2$ on the interval $[-l, +l]$ with Dirichlet boundary conditions $|V| \leqslant aK + b$, $a < 1$.

A further condition on V for all three cases is imposed below in condition 4.

In order to know what conditions g has to fulfil so that part 2 makes sense, one has first to decide which class of ψ's should be admitted. A maximal choice (with respect to equation (1)) would be the form domain $Q(K)$ of the kinetic energy. Then one had to ensure that $Q(g^2) \supset Q(K)$, which would be too restrictive for practical purposes. A reasonable choice is to let ψ vary in a form core $\mathscr{C}(H)$ of the Hamiltonian. That will ensure that $\inf \langle \psi, H\psi \rangle$ is the same as if all ψ's of the domain of H, $\mathscr{D}(H)$, were admitted.

As form cores we may choose:

(A) $C_0^\infty(\mathbb{R}^n)$ (theorem X 16 of Reed and Simon (1972));

(B) $C_0^\infty(\mathbb{R}^n\backslash\{0\})$ (theorem X 30 of Reed and Simon);
(C) $\{\psi \in C_0^\infty[-l, +l] : \psi(-l) = \psi(+l) = 0\}$. This is an operator core for K and a form core for H by the KLNM theorem (Reed and Simon, theorem X 17).

In all three cases we have to demand the following conditions.

Condition 1. The components g_i are locally $\mathscr{L}^2$, that is, $\int g^2$ is finite on all compact sets, except those for which, in case B, $0 \in K$, in case C, $-l$ or $+l \in K$. $g_i(x)$ may grow A without restriction for $x \to \infty$, B without restriction for $x \to \infty$ and $x \to 0$ and C not stronger than $(x \pm l)^{-3/2+\epsilon}$, $\epsilon > 0$.

One could argue that the infimum of $\langle\psi, H\psi\rangle$ is needed only for real ψ's. With this restriction one could admit complex g's and would get instead of (3):

$$\langle\psi, K\psi\rangle \geq |\langle\psi|(\nabla \cdot g)\psi\rangle|^2/\langle\psi||g|^2\psi\rangle \qquad |g|^2 = \sum |g_i|^2. \tag{7}$$

That does not seem to be any advantage, so we further assume condition 2.

Condition 2. g is real.

For $\psi \in C_0^\infty$ one also has $|\psi|^2 \in C_0^\infty$ and $\partial_i\psi \in C_0^\infty$. We may view g_i as a continuous linear functional on C_0^∞ and define $(\nabla \cdot g)$ as the weak derivative: $(\partial_i g_i)[f] = -g_i[\partial_i f]$. The derivation of equation (2) then takes the form

$$(-\partial_i g_i)[\psi\bar{\psi}] = g_i[\bar{\psi}\partial_i\psi] + g_i[\psi\partial_i\bar{\psi}] = 2 \operatorname{Re} g_i[\psi\partial_i\bar{\psi}]. \tag{8}$$

An example is in one dimension: $g(x) = (\theta(x) - \frac{1}{2})$, $g'(x) = \delta(x)$. Equation (3) becomes

$$\langle\psi, K\psi\rangle \geq |\psi(0)|^4/\|\psi\|^2. \tag{9}$$

This can be used to bound the wavefunction by the kinetic energy, but we will not follow this line here.

Since one wants equation (4) to be defined for a class of measures which contains 'almost all' point measures, one has to ensure that $\nabla \cdot g$, g^2 and V are rather tame functions.

Condition 3. The closure of the set of points where $\nabla \cdot g$, g^2 or V is discontinuous has Lebesgue measure zero.

Definition. We denote the union of this closed set with $\{x, g(x) = 0\}$ by S.

In order to be able to divide by $\langle\psi, g^2\psi\rangle$ we must have:

Condition 4. The Lebesgue measure of $\{x, g(x) = 0\}$ is zero.

4. The main results

In all that follows, ψ means any of the normalised elements of the appropriate form core, the 'allowed set' is $\mathbb{R}^n\backslash S$ or $[-l, +l]\backslash S$, respectively. A 'δ measure' is a positive normalised measure, the support of which is one point of the allowed set. A convex combination is a linear combination with real coefficients λ_i that satisfy $\lambda_i \geq 0$, $\Sigma\, \lambda_i = 1$.

Theorem 1. The set of 3-tuples $(\langle\psi, V\psi\rangle, \langle\psi, g^2\psi\rangle, \langle\psi, \nabla \cdot g\psi\rangle)$ is contained in the closure of $\{(\mu(V), \mu(g^2), \mu(\nabla \cdot g))\}$, where each μ is a convex combination of four δ measures.

Proof. For a given ψ, consider μ_K:

$$\mu_K(f) := \left(\int_K |\psi(x)|^2 \, \mathrm{d}^n x\right)^{-1} \int_K f(x)|\psi(x)|^2 \, \mathrm{d}^n x \tag{10}$$

where K is a compact subset of the allowed set. We write $f = (f_1, f_2, f_3) = (V, g^2, \nabla \cdot g)$. For every $\epsilon > 0$ there is a K such that $|\langle\psi, f_j\psi\rangle - \mu_K(f_j)| \leq \epsilon$, $j = 1, 2, 3$. Each μ_K defines a positive, normed continuous linear functional, a 'state' of $C(K)$. By the Krein–Milman theorem it is contained in the closure of the convex hull of the extreme states which are the δ measures on K. Therefore $\mu_K(f)$ is in the closure of the convex hull CH_K of $f(K) = \{f(x), x \in K\} \subset \mathbb{R}^3$. Since $f(K)$ is compact, CH_K is already closed. By the theorem of Caratheodory every point in CH_K is already a convex combination of four points of $f(K)$ (Roberts and Varberg 1973). Now let $\epsilon \searrow 0$.

Theorem 2. For each ψ, define μ_ψ by $\mu_\psi(f) = \int f|\psi|^2 \, \mathrm{d}^n x$. Consider $E(g, \mu)$ as given in equation (4). The closure of $\{E(g, \mu_\psi)\}$ (g fixed, ψ variable) equals the closure of $\{E(g, \mu)\}$, where each μ is a convex combination of three δ measures.

Proof. Consider μ_K as above. $\overline{\{E(g, \mu_\psi)\}} \subset \overline{\{E(g, \mu_K)\}}$. We show that for each μ_K there is a convex combination of three δ measures yielding the same value of E. By theorem 1, μ_K defines a point in a three-dimensional simplex T with vertices given by $\delta_x(f)$. The function $E = (a^2/4b) + c$ is monotonous in c (also in b). Therefore, there is on the topological boundary of T on one side a point with a lower (or equal) value of E, on the other side one with a bigger (or equal) value. Since the boundary of T is connected, and E is continuous on each $f(K)$, there is also a point on the boundary with the same value for E as given by $E(g, \mu_K)$. But every point on the boundary of T is already a convex combination of three $\delta_x(f)$. That proves one direction. Conversely, any δ measure may be approximated by elements of C_0^∞ in the w^* topology of $C(K)'$.

Corollary. In the case that one of $g^2, \nabla \cdot g, V$ is a constant, or $g^2 = V$, or $g^2 = \nabla \cdot g$, then it suffices to consider convex combinations of two δ measures.

Proof. The proofs of theorems 1 and 2 also hold in one less dimension, because at least one parameter, b or c, is left for the monotonicity argument.

The proofs also show that in the cases where $\inf E(g, \mu)$ is not obtained for some μ, it has to be approximated by convex combinations of δ-measures δ_{x_i}, where some subsequence of the $\{x_i\}$ tends out of the allowed region. If one can disprove this possibility in a special case, equations $6(a)$–(d) may be used to gain further information on where to search for the minimum (example 1). It is now easy to justify these equations. Suppose

$$\inf_{\mu, \mu \geq 0, \|\mu\| = 1} E(g, \mu) = E(g, \mu_0) \tag{11}$$

with

$$\mu_0 = \sum_{i=1}^{3} \lambda_i^0 \delta_{x_i} \qquad \lambda_i^0 \geq 0 \qquad \sum \lambda_i^0 = 1. \tag{12}$$

Take any $x_4 \notin \{x_1, x_2, x_3\}$ and consider the four-dimensional Euclidian space

$\{\Sigma_{i=1}^4 \lambda_i \delta_{x_i}\}$, where the λ_i are the Cartesian coordinates. Now you have to search for the minimum of

$$F(\lambda_1 \ldots \lambda_4) = \frac{(\Sigma \lambda_i (\nabla \cdot g)(x_i))^2}{\Sigma \lambda_i g^2(x_i)} + \sum \lambda_i V(x_i) - E(\sum \lambda_i - 1) \tag{13}$$

in the cone $\{\lambda_i \geqslant 0\}$.

The conditions that $F(\lambda_1^0 \ldots \lambda_4^0 = 0)$ is minimal are for the λ_i^0 not equal to zero:

$$\frac{\partial}{\partial \lambda_i} F(\lambda_1 \ldots \lambda_4)|_{\lambda_i = \lambda_i^0} = 0, \tag{14}$$

and this gives equation 6(a).

For the $\lambda_i^0 = 0$ (e.g. λ_4)

$$\frac{\partial}{\partial \lambda_i} F(\lambda_1 \ldots \lambda_4)|_{\lambda_i = \lambda_i^0} \geqslant 0, \tag{15}$$

and this gives equation 6(b).

There are cases, of course, where the minimising μ is not unique. This situation occurs, for example, if you choose $g = -\nabla\psi/\psi$, where ψ is the solution of Schrödinger's equation which turns out to be equivalent to

$$(\nabla \cdot g)(x) - g^2(x) + V(x) - E = 0. \tag{16}$$

In that case the lower bound is optimal. Use (16) to substitute for $\nabla \cdot g$ in equation (4):

$$E(g, \mu) = \frac{1}{4}\left(\frac{(\mu(V) - E)^2}{\mu(g^2)} + \mu(g^2)\right) + \frac{\mu(V) + E}{2} \geqslant \max\{\mu(V), E\} \geqslant E. \tag{17}$$

Therefore

$$\inf_{\mu} E(\nabla\psi/\psi, \mu) = E. \tag{18}$$

If we do not have to consider Fermi statistics, the wavefunction of the ground state may be chosen positive and $g = \nabla\psi/\psi$ is admissible. So one may hope to derive reasonable lower bounds by making a good guess for ψ (or rather for $\nabla\psi/\psi$: see example 2).

For a particle in one space dimension we can use the node theorem to derive lower bounds for any excited state. The zeros of the eigenfunction ψ_n corresponding to the $(1+n)$th eigenvalue E_n divides $\mathbb{R}$ into $n+1$ intervals I_K. In any other partition of $\mathbb{R}$ into $n+1$ intervals J_K there exists at least one K and a l such that $J_l \supset I_K$. Define

$$\phi_K(x) = \begin{cases} \psi_n(x) & x \in I_K \\ 0 & x \notin I_K \end{cases} \tag{19}$$

and let H_J be the Hamiltonian $K + V$ with Dirichlet boundary conditions on the n endpoints of the J_K. ϕ_K is in the domain of H_J and therefore

$$\inf \frac{1}{\|\phi\|^2}\langle\phi|H_J\phi\rangle \leqslant \frac{1}{\|\phi_K\|^2}\langle\phi_K|H_J\phi_K\rangle = E_n. \tag{20}$$

To use the Dirichlet boundary condition effectively, one has to choose a g with appropriate singularities at n points. The same kind of reasoning applies to the radial equation in spherically symmetric systems.

In one space dimension, Fermi statistics can also be taken into account: the eigenvalues of H on the space of antisymmetric functions $\psi(x_1 \ldots x_n)$ are the same as for H with Dirichlet boundary conditions on the hyperplane $x_i = x_j$.

5. Some simple examples

Example 1. The square well

$H = -\partial^2/\partial x^2$ on $[-l, +l]$ with Dirichlet boundary conditions. Take $g(x) = e^{\kappa x}$ to obtain

$$E_0 \geq \kappa^2 \langle e^{\kappa x}\rangle^2 / 4\langle e^{2\kappa x}\rangle. \tag{21}$$

You see immediately that it is not enough to consider the measures with only one point as support. That would lead to the paradoxical result $E_0 \geq \frac{1}{4}\kappa^2$, where κ is any real number! Apply instead the equations (6): $\alpha(\mu) = \kappa\langle e^{\kappa x}\rangle / 2\langle e^{2\kappa x}\rangle$ is certainly positive. The first factor of 6(a) and 6(b) is $f(x) = \alpha\kappa\, e^{\kappa x} - \alpha^2\, e^{2\kappa x} - E$, which has one maximum and goes continuously down on both sides of it. Since f has to be positive on $[-l, +l]$, except on supp(μ), the support of the minimising measure has to be the endpoints, $-l$ and $+l$. It remains only to determine their relative weight. One arrives at

$$E_0 \geq \frac{\kappa^2}{2 + e^{2l\kappa} + e^{-2l\kappa}}, \tag{22}$$

which is, however, numerically poor.

The best choice for g in this case, yielding the exact ground-state energy, is $\tan(\pi x/2l)$. This may serve as a guide as to how to deal with Dirichlet boundary conditions in general: the appropriate singularity of g is like $1/x$. We will use this in the last example.

Example 2. $V = -1/r^\nu$ in three dimensions, $0 < \nu < 1$

Take $g(x) = x/r$, $r = |x|$:

$$E_0 \geq \inf[\langle r^{-1}\rangle^2 - \langle r^{-\nu}\rangle] \geq \inf[\langle r^{-1}\rangle^2 - \langle r^{-1}\rangle^\nu] = (\tfrac{1}{2}\nu)^{\nu/(2-\nu)}(\tfrac{1}{2}\nu - 1). \tag{23}$$

Here we have used that z^ν is concave in z, which implies $\langle z^\nu\rangle \leq \langle z\rangle^\nu$. The bound is exact for $\nu = 1$ and $\nu = 0$. Of course, $g = \nabla\psi/\psi$, $\psi = e^{-|x|}$, which is the ground state of the Coulomb problem. A seemingly innocent change in ψ may change the quality of the lower bound drastically: try to use $\psi = e^{-x^2}$, which gives $g = x$ and

$$E_0 \geq \inf(4\langle r^2\rangle)^{-1} - \langle r^{-\nu}\rangle = -\infty.$$

Example 3. $V = \lambda r^{2\nu}$ in n dimensions, $\nu > 1$

Take $g = x$ and use the convexity of z^ν in z, $z = r^2$:

$$E_0 \geq \inf\left[\frac{n^2}{4\langle r^2\rangle} + \lambda\langle r^{2\nu}\rangle\right] \geq \inf\left[\frac{n^2}{4\langle r^2\rangle} + \lambda\langle r^2\rangle^\nu\right] = (1 + \nu^{-1})(\lambda\nu)^{1/(\nu+1)}(\tfrac{1}{4}n^2)^{\nu/(\nu+1)}. \tag{24}$$

The bound is exact for the harmonic oscillator ($\nu = 1$).

Example 4. $V = 1 - \cos x$ *in one dimension*

Writing the (unnormalised) ground-state function as $\psi = 1 + \Sigma\, a_k \cos kx$ and minimising $\|\psi\|^{-2}\langle\psi, H\psi\rangle$ by varying $a_1 \ldots a_3$ gives as the upper bound

$$E_0 \leqslant 0{\cdot}622, \tag{25}$$

which is obtained for $a_1 = 0{\cdot}759$, $a_2 = 0{\cdot}087$, $a_3 = 0{\cdot}004$. The best g ought to be

$$\frac{\Sigma\, k a_k \sin k_x}{1 + \Sigma\, a_k \cos kx}.$$

We take a crude approximation, $g = \sin x$, which yields

$$E_0 \geqslant \inf\left\{\frac{\langle\cos x\rangle^2}{4\langle\sin^2 x\rangle} + 1 - \langle\cos x\rangle\right\}. \tag{26}$$

In the spirit of the proof of theorem 2, we examine the convex hull of $\{(\sin^2 x, \cos x, \cos x)\} = f(\mathbb{R})$. It is the interior of a piece of the parabola $\{(1 - a^2, a, a)\}$ and E takes its lowest values on that part of the boundary which is $f(\mathbb{R})$. Therefore

$$E_0 \geqslant \inf\{\tfrac{1}{4}\cot^2 x + 1 - \cos x\} = 0{\cdot}53. \tag{27}$$

Example 5. One-dimensional 'helium atom'

Two particles, $V(x, y) = 2|x| + 2|y| - |x - y|$. To obtain a lower bound for the ground state with Fermi statistics we impose Dirichlet boundary conditions on the line $x = y$ and choose

$$g = \begin{pmatrix} -1 \\ +1 \end{pmatrix} |x - y|^{-1}.$$

$$E_{0,\mathrm{F}} \geqslant \inf\{\tfrac{1}{2}\langle (x-y)^{-2}\rangle + \langle 2|x| + 2|y| - |x - y|\rangle\}. \tag{28}$$

Set $a = 2|x| + 2|y| - |x - y|$, $b = (x - y)^{-2}$; then

$$E_{0,\mathrm{F}} \geqslant \inf\{\tfrac{1}{2}\langle b\rangle + \langle a\rangle\},$$

$\{(a(x, y), b(x, y))\} = \{(a, b = \gamma/a^2), \gamma \geqslant 1\}$. This set is already convex. The minimum is attained for $\gamma = 1$:

$$E_{0,\mathrm{F}} \geqslant \inf\{\tfrac{1}{2}a^{-2} + a\} = \tfrac{3}{2}. \tag{29}$$

This is actually higher than a simple upper bound for the ground state without statistics, obtained with Gaussian functions:

$$E_0 \leqslant 0{\cdot}9.$$

Example 6. Gravitating bosons

$$H = -\sum_{i=1}^{N} \Delta_i - \kappa \sum_{i<j} |x_i - x_j|^{-1}.$$

The trial function g has to be a $3N$-component vector. We write $g = (g_1 \ldots g_N)$, where each g_i is a three-vector which we choose as

$$g_i = \sum_{j \neq i} \frac{x_i - x_j}{|x_i - x_j|}.$$

This yields

$$(\nabla \cdot g) = 4 \sum_{i<j} |x_i - x_j|^{-1}$$

$$g^2 = \sum_i \sum_{j \neq i} \sum_{k \neq i} \frac{(x_i - x_j)(x_i - x_k)}{|x_i - x_j|\,|x_i - x_k|} \leqslant N(N-1)^2$$

and

$$E_0 \geqslant \inf \frac{4}{N(N-1)^2} \langle \sum_{i<j} |x_i - x_j|^{-1} \rangle^2 - \kappa \langle \sum_{i<j} |x_i - x_j|^{-1} \rangle = -\tfrac{1}{16} N(N-1)^2 \kappa^2. \tag{30}$$

This is the same bound as that one which is implicit in Thirring (1974b, §1.2).

6. Other bounds

Starting with equations (4) and (5) we can derive other lower bounds. Substitute $(\nabla \cdot g - g^2) + g^2$ for $\nabla \cdot g$ in equation (4):

$$E(g, \mu) = \frac{1}{4}\left(\frac{(\mu(\nabla \cdot g - g^2))^2}{\mu(g^2)} + \mu(g^2) + 2\mu(\nabla \cdot g - g^2) \right) + \mu(V)$$
$$\geqslant \tfrac{1}{2}(|\mu(\nabla \cdot g - g^2)| + \mu(\nabla \cdot g - g^2)) + \mu(V). \tag{31}$$

Therefore

$$E_0 \geqslant \inf_{\mu} \mu(\nabla \cdot g - g^2)\theta(\mu(\nabla \cdot g - g^2)) + \mu(V). \tag{32}$$

θ is the step function:

$$\theta(a) = \begin{cases} 1 & a \geqslant 0 \\ 0 & a < 0. \end{cases}$$

Applying the same kind of arguments used to prove theorems 1 and 2, one can show that it suffices to consider those μ which are convex combinations of two δ measures.

Up to this point the lower bounds for the kinetic energy have always been non-negative. This is no longer true in the next step, where we leave out the θ function:

$$E_0 \geqslant \inf_{\mu} \mu(\nabla \cdot g - g^2) + \mu(V) = \inf_{x} (\nabla \cdot g(x) - g^2(x) + V(x). \tag{33}$$

The infimum has to be taken over all x in the allowed set. This yields Barnsley's (1978) bound: set $g = -\nabla\psi/\psi$; then the RHS of equation (33) reads

$$\inf_{x} [(H\psi)(x)/\psi(x)].$$

7. Discussion

The examples of § 5 were not meant to demonstrate numerical efficiency but to show how the method may be applied in various circumstances. A quantitative test and comparison with other well known methods (Löwdin 1965, Bazley and Fox 1963, Thirring 1974a) would necessitate extensive computer studies. The numerical search for the infimum of $E(g, \mu)$ should present no difficulties in situations where not too many coordinates are involved.

One thing remains to be done: to find a systematic approximation procedure for the best g. Certainly it is not sufficient in general to have a sequence $g_\alpha = \nabla\psi_\alpha/\psi_\alpha$, with ψ_α converging to the ground state in the $\mathscr{L}^2$ norm. By examining example 2, it is easy to find counterexamples. It may be that a method similar to that of Bartlett (1955) leads to useful trial functions.

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