A New Estimate for the Ground State Energy of Schrödinger Operators

Asao Arai

Series #382. May 1997

HOKKAIDO UNIVERSITY
PREPRINT SERIES IN MATHEMATICS

#358 N. Hayashi, P.I. Naumkin and T. Ozawa, Scattering theory for the Hartree equation, 14 pages. 1996.

#359 I. Tsuda and K. Tadaki, A logic-based dynamical theory for a genesis of biological threshold, 49 pages. 1996.

#360 I. Tsuda and A. Yamaguchi, Singular-continuous nowhere-differentiable attractors in neural systems, 40 pages. 1996.

#361 M. Nakamura and T. Ozawa, Low energy scattering for nonlinear Schrödinger equations in fractional order Sobolev spaces, 17 pages. 1996.

#362 I. Nakamura, Hilbert schemes and simple singularities E_6, E_7 and E_8, 21 pages. 1996.

#363 T. Mikami, Equivalent conditions on the central limit theorem for a sequence of probability measures on R, 7 pages. 1996.

#364 S. Izumiya and T. Sano, Generic affine differential geometry of space curves, 23 pages. 1996.

#365 T. Tsukada, Stability of reticular optical caustics, 12 pages. 1996.

#366 A. Arai and M. Hirokawa, On the existence and uniqueness of ground states of a generalized spin-boson model, 40 pages. 1996.

#367 A. Arai, A class of representations of the *-algebra of the canonical commutation relations over a Hilbert space and instability of embedded eigenvalues in quantum field models, 12 pages. 1996.

#368 K. Ito, BV-solutions of a hyperbolic-elliptic system for a radiating gas, 33 pages. 1997.

#369 M. Nakamura and T. Ozawa, Nonlinear Schrödinger equations in the Sobolev space of critical order, 20 pages. 1997.

#370 N.H. Bingham and A. Inoue, An Abel-Tauber theorem for Hankel transforms, 8 pages. 1997.

#371 T. Nakazi and H. Sawada, The commutator ideal in Toeplitz algebras for uniform algebras and the analytic structure, 9 pages. 1997.

#372 M.-H. Giga and Y. Giga, Stability for evolving graphs by nonlocal weighted curvature, 70 pages. 1997.

#373 T. Nakazi, Brown-Halmos type theorems of weighted Toeplitz operators, 14 pages. 1997.

#374 J. Inoue and S.-E. Takahashi, On characterizations of the image of Gelfand transform of commutative Banach algebras, 30 pages. 1997.

#375 L. Solomon and H. Terao, The double coxeter arrangement, 21 pages. 1997.

#376 G. Ishikawa and T. Morimoto, Solution surfaces of Monge-Ampère equations, 15 pages. 1997.

#377 G. Ishikawa, A relative transversality theorem and its applications, 16 pages. 1997.

#378 J. Inoue and T. Nakazi, On the zeroes of solutions of an extremal problem in H^1, 14 pages. 1997.

#379 Y. Giga and K. Ito, On pintching of curves moved by surface diffusion, 12 pages. 1997.

#380 F. Hiroshima, Weak coupling limit removing an ultraviolet cut-off for a Hamiltonian of particles interacting with a scalar field, 39 pages. 1997.

#381 Y. Giga, S. Matsui and Y. Shimizu, On estimates in Hardy spaces for the Stokes flow in a half space, 13 pages. 1997.

A New Estimate for the Ground State Energy of Schrödinger Operators

ASAO ARAI *

Department of Mathematics, Hokkaido University
Sapporo 060, Japan

to be published in *Letters in Mathematical Physics*

Abstract

A new estimate for the ground state energy of Schrödinger operators on $L^2(\mathbf{R}^n)$ $(n \geq 1)$ is presented. As a corollary, it is shown that the ground state energy of the Schrödinger operator with a scalar potential V is more than the classical lower bound $\mathrm{ess.inf}_{x\in\mathbf{R}^n} V(x)$ if V is essentially bounded from below in a certain manner (enhancement of the ground state energy due to quantization). As an application, it is proven that the ground state energy of the Hamiltonian of the hydrogen-like atom is enhanced under a class of perturbations given by scalar potentials (vanishing at infinity).

AMS Mathematics Subject Classification(1991). 81Q10, 47N50

1 Introduction and the main results

In this Letter we present a new estimate for the ground state energy of Schrödinger operators and its applications. The method is based on a remarkable structure of a class of symmetric operators on an L^2 space [1] (see Theorem 2.2 in Section 2 below).

Let $x = (x_1, \cdots, x_n) \in \mathbf{R}^n$ $(n \in \mathbf{N})$ and $a(x) = (a_{ij}(x))_{i,j=1,\cdots,n}$ be an $n \times n$ real, positive semi-definite matrix of the form

$$a(x) = b(x)^* b(x), \tag{1.1}$$

*Work supported by the Grant-In-Aid No.08454021 for science research from the Ministry of Education, Japan.

where $b(x) = (b_{ij}(x))_{i,j=1,\cdots,n}$ is an $n \times n$ complex matrix. We assume that each function $b_{ij} : x \to b_{ij}(x)$ is continuously differentiable on $\mathbf{R}^n$.

We denote by D_j the generalized partial differential operator in the j-th variable x_j. We define a symmetric operator H_0 on $L^2(\mathbf{R}^n)$ by

$$H_0 := -\sum_{j,k=1}^{n} D_j a_{jk} D_k \tag{1.2}$$

with $D(H_0) := \{f \in L^2(\mathbf{R}^n) | f \in D(D_j), a_{jk}D_k f \in D(D_j), j,k = 1,\cdots,n\}$, where $D(\cdot)$ denotes operator domain. It follows that $H_0 \geq 0$.

For $p \geq 1$ (resp. $p = \infty$), we denote by $L^p_{\text{loc}}(\mathbf{R}^n)$ the set of functions f on $\mathbf{R}^n$ such that for all compact sets K of $\mathbf{R}^n$, $\int_K |f(x)|^p dx < \infty$ (resp. $\text{ess.sup}_{x\in\mathbf{R}^n}|f(x)| < \infty$), where ess.sup denotes essential supremum. Let V be a real-valued measurable function on $\mathbf{R}^n$ such that

$$V \in L^2_{\text{loc}}(\mathbf{R}^n). \tag{1.3}$$

We denote the multiplication operator defined by the function V on $L^2(\mathbf{R}^n)$ by the same symbol V. It follows that V is self-adjoint with $D(V) \supset C_0^\infty(\mathbf{R}^n)$.

We consider a symmetric operator of the form

$$H_{a,V} := H_0 + V \tag{1.4}$$

on $L^2(\mathbf{R}^n)$ with $D(H_{a,V}) = C_0^\infty(\mathbf{R}^n)$. The ground state energy (the lower bound) of $H_{a,V}$ is defined by

$$E_0(H_{a,V}) := \inf_{u\in C_0^\infty(\mathbf{R}^n), \|u\|_{L^2(\mathbf{R}^n)}=1} (u, H_{a,V}u)_{L^2(\mathbf{R}^n)}, \tag{1.5}$$

provided that $H_{a,V}$ is bounded from below, where $(\cdot,\cdot)_{L^2(\mathbf{R}^n)}$ and $\|\cdot\|_{L^2(\mathbf{R}^n)}$ denote the inner product and the norm of $L^2(\mathbf{R}^n)$ respectively.

If $H_{a,V}$ is essentially self-adjoint and bounded from below, then $E_0(H_{a,V}) = \inf \sigma(\overline{H}_{a,V})$, the infimum of the spectrum of $\overline{H}_{a,V}$ (the closure of $H_{a,V}$). For the main theorems stated below, however, we do not need assume that $H_{a,V}$ is essentially self-adjoint.

The operator $H_{a,V}$ with $a(x) = (\delta_{ij})_{i,j=1,\cdots,n}$ is the Schödinger operator with the scalar potential V:

$$H_V := -\Delta + V, \tag{1.6}$$

where $\Delta := \sum_{j=1}^n D_j^2$ is the Laplacian on $L^2(\mathbf{R}^n)$.

The function space

$$\begin{aligned} W(\mathbf{R}^n) := \{f \in L^\infty_{\text{loc}}(\mathbf{R}^n) \;\; | \;\; & f \text{ is real-valued}, D_j f \in L^2_{\text{loc}}(\mathbf{R}^n), \\ & D_j D_k f \in L^1_{\text{loc}}(\mathbf{R}^n), j,k = 1,\cdots,n\} \end{aligned} \tag{1.7}$$

plays an important role in our theory. For each $f \in W(\mathbf{R}^n)$, we define a real-valued measurable fucntion

$$\Phi_{a,V}(x;f) := \sum_{j,k=1}^{n} [D_j(a_{jk}(x)D_k f(x)) - (D_j f(x))\, a_{jk}(x) D_k f(x)] + V(x). \tag{1.8}$$

We introduce

$$\mathcal{W}_{a,V} := \{f \in W(\mathbf{R}^n) | \text{ess.inf}_{x\in\mathbf{R}^n} \Phi_{a,V}(x;f) > -\infty\}, \tag{1.9}$$

where ess.inf denotes essential infimum. In the case where $\mathcal{W}_{a,V} \neq \emptyset$, we define for $f \in \mathcal{W}_{a,V}$

$$E_{a,V}(f) := \text{ess.inf}_{x\in\mathbf{R}^n} \Phi_{a,V}(x;f). \tag{1.10}$$

The fundamental result of this Letter is the following theorem, which gives a criterion of the boundedness from below of $H_{a,V}$ and an estimate for $E_0(H_{a,V})$ simultaneously.

THEOREM 1.1. *Suppose that $\mathcal{W}_{a,V} \neq \emptyset$. Then $H_{a,V}$ is bounded from below and*

$$E_0(H_{a,V}) \geq \sup_{f\in\mathcal{W}_{a,V}} E_{a,V}(f). \tag{1.11}$$

Remark 1.1. We emphasize that, in Theorem 1.1, V is not necessarily essentially bounded from below.

Remark 1.2. One can consider $H_{a,V}$ as a quadratic form with form domain $C_0^\infty(\mathbf{R}^n)$. In this case, the basic assumption (1.3) for V can be weakened to the condition $V \in L^1_{\text{loc}}(\mathbf{R}^n)$.

Remark 1.3. Under the hypothesis of Theorem 1.1, $H_{a,V}$ is bounded from below. Hence it has a self-adjoint extension $\widetilde{H}_{a,V}$, the Friedrichs extension. It follows that $E_0(\widetilde{H}_{a,V}) \geq \sup_{f\in\mathcal{W}_{a,V}} E_{a,V}(f)$.

Remark 1.4. Consider the case where V is essentially bounded from below. Then $\mathcal{W}_{a,V} \neq \emptyset$, since $0 \in \mathcal{W}_{a,V}$. We have $E_{a,V}(0) = \text{ess.inf}\, V(x)$. Hence Theorem 1.1 implies that

$$E_0(H_{a,V}) \geq \sup_{f\in\mathcal{W}_{a,V}} E_{a,V}(f) \geq \text{ess.inf}\, V(x).$$

Thus Theorem 1.1 may impove the classical lower bound ess.inf $V(x)$. As Theorem 1.3 below shows, under an additional condition, (1.11) indeed gives an improved lower bound.

The following theorem shows that inequality (1.11) is best possible in a sense.

THEOREM 1.2. *Suppose that $\overline{H}_{a,V}$ has a real eigenvalue λ with an eigenvector Ω (i.e., $\Omega \in D(\overline{H}_{a,V})$ and $\overline{H}_{a,V}\Omega = \lambda\Omega$) having the following properties: (i) $\Omega > 0$, a.e. ; (ii) $\Omega \in D(H_0) \cap D(V)$ and $\overline{H}_{a,V}\Omega = (H_0 + V)\Omega$; (iii) $f_0 := -\log \Omega \in W(\mathbf{R}^n)$. Then, $f_0 \in \mathcal{W}_{a,V}$ and $H_{a,V}$ is bounded from below with*

$$\lambda = E_0(H_{a,V}) = \sup_{f\in\mathcal{W}_{a,V}} E_{a,V}(f) = E_{a,V}(f_0). \tag{1.12}$$

Remark 1.5. Theorem 1.2, which is a variant of [1, Theorem 1.2], shows that any positive eigenfunction of $\overline{H}_{a,V}$ with suitable regularities is a ground state of $\bar{H}_{a,V}$. We note that there is a similarity between Theorem 1.2 and the Allegretto-Piepenbrink theorem [2, Theorem 2.12] (cf. also Theorem 2.2 in Section 2 below).

Let

$$v_k(x) := \sum_{j=1}^{n} D_j a_{jk}(x), \quad k = 1, \cdots, n. \tag{1.13}$$

and set

$$v(x) := (v_1(x), \cdots, v_n(x)), \quad x \in \mathbf{R}^n. \tag{1.14}$$

THEOREM 1.3. *Consider the case where V is essentially bounded from below and set*

$$V_0 := \text{ess.inf}_{x \in \mathbf{R}^n} V(x). \tag{1.15}$$

Suppose that $a(x)$ and $v(x)$ are bounded on $\mathbf{R}^n$ and that there exists a point $x_0 \in \mathbf{R}^n$ such that $V_0 = V(x_0)$ and, for some $R > 0$,

$$\text{ess.inf}_{|x-x_0|>R} V(x) > V_0, \tag{1.16}$$

$$\inf_{|x-x_0|\leq R} \operatorname{tr} a(x) > (R^2+1)R \sup_{|x-x_0|\leq R} |v(x)|, \tag{1.17}$$

where tr *denotes trace. Then $E_0(H_{a,V}) > V_0$.*

Remark 1.6. We can compute a constnat γ such that $E_0(H_{a,V}) \geq \gamma > V_0$. See (3.11).

Remark 1.7. Obviously (1.17) holds for $a(x) = (\delta_{ij})_{i,j=1,\cdots,n}$. Hence Theorem 1.3 can be applied to the Schrödinger operator H_V. In the context of quantum mechanics, Theorem 1.3 establishes a mathematically rigorous basis for the folklore that quantization should raise the ground state energy for a wide class of scalar potentials bounded from below (this traditional picture comes from the Heisenberg uncertainty principle).

This Letter is organized as follows. In Section 2 (resp. 3) we prove Theorems 1.1 and 1.2 (resp. Theorem 1.3). In Sectioon 4 we apply Theorem 1.1 to the Hamiltonian of the hydrogen-like atom perturbed by a scalar potential and show that the ground state energy is enhanced under the perturbation.

2 Proof of Theorems 1.1 and 1.2

Theorem 1.1 is proven by applying an extension of [1, Corollary 3.4], which, for the reader's convenience, we prove it frist.

We introduce an operator

$$L_j := \sum_{k=1}^{n} b_{jk}(x) D_k, \quad j = 1, \cdots, n. \tag{2.1}$$

on $L^2(\mathbf{R}^n)$ with $D(L_j) = C_0^\infty(\mathbf{R}^n)$. Then we have

$$H_0 = \sum_{j=1}^{n} L_j^* L_j \quad \text{on } C_0^\infty(\mathbf{R}^n). \tag{2.2}$$

For each $f \in W(\mathbf{R}^n)$, we define

$$\widehat{H}_0 f = -\sum_{j,k=1}^{n} D_j(a_{jk}(x) D_k f), \tag{2.3}$$

$$\widehat{L}_j f = \sum_{k=1}^{n} b_{jk}(x) D_k f. \tag{2.4}$$

We denote by $\langle \cdot \rangle$ the expectation value with respect to the n-dimensional Lebesgue measure:

$$\langle f \rangle := \int_{\mathbf{R}^n} f(x) dx, \quad f \in L^1(\mathbf{R}^n). \tag{2.5}$$

LEMMA 2.1 [1, cf. Lemma 3.3]. *Let Ω be an a.e. strictly positive function Ω on $\mathbf{R}^n$ such that $\Omega \in W(\mathbf{R}^n)$ and $\Omega^{-1} \in L^\infty_{\mathrm{loc}}(\mathbf{R}^n)$. Let*

$$\Omega_j := \Omega^{-1} \widehat{L}_j \Omega. \tag{2.6}$$

Then, for all $u \in C_0^\infty(\mathbf{R}^n)$,

$$\langle |u|^2 \Omega^{-1} \widehat{H}_0 \Omega \rangle = \sum_{j=1}^{n} \left\{ 2\mathrm{Re}\, \langle (L_j u)^* u \Omega_j \rangle - \langle |u|^2 |\Omega_j|^2 \rangle \right\}. \tag{2.7}$$

Proof. Let J_ε ($\varepsilon > 0$) be the Friedrichs mollifier and $\Omega_m := J_{1/m}\Omega$, $m = 1, 2, \cdots$. Then $\Omega_m \in C^\infty(\mathbf{R}^n)$. Moreover, for all compact sets K of $\mathbf{R}^n$, $p \in [1, \infty)$, and $j, k = 1, \cdots, n$,

$$\|\Omega_m - \Omega\|_{L^p(K)} \to 0, \tag{2.8}$$

$$\|D_j \Omega_m - D_j \Omega\|_{L^2(K)} \to 0, \tag{2.9}$$

$$\|D_j D_k \Omega_m - D_j D_k \Omega\|_{L^1(K)} \to 0, \tag{2.10}$$

as $m \to \infty$. We have also for all $r > 0$

$$\inf_{|x|<r} \Omega_m(x) \geq \text{ess.inf}_{|x|<r+m^{-1}} \Omega(x) > 0, \tag{2.11}$$

$$\sup_{|x|<r} \Omega_m(x) \leq \text{ess.sup}_{|x|<r+m^{-1}} \Omega(x) < \infty. \tag{2.12}$$

By integration by parts, one can easily show that (2.7) holds with Ω replaced by Ω_m. Then a simple limiting argument using (2.8)–(2.12) gives (2.7) (we need to take a subsequence $\{\Omega_{m_i}\}_{i=1}^{\infty}$ of $\{\Omega_m\}_m$ such that $\Omega_{m_i} \to \Omega$ a.e. as $i \to \infty$ on the support of u). □

THEOREM 2.2. *Suppose that there exists an a.e. strictly positive function Ω on $\mathbf{R}^n$ such that $\Omega \in W(\mathbf{R}^n)$, $\Omega^{-1} \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^n)$, and*

$$\widehat{H}_0\Omega(x) + V(x)\Omega(x) \geq \lambda\Omega(x), \quad \text{a.e.}x, \tag{2.13}$$

with a real constant λ. Then $E_0(H_{a,V}) \geq \lambda$.

Proof. This follows from Lemma 2.1 and a simple application of [1, Theorem 1.1] (take $\Psi = \Omega^{-1}\widehat{H}_0\Omega$ as the vector Ψ in [1, Theorem 1.1]). □

LEMMA 2.3. *Let $f \in W(\mathbf{R}^n)$ and set*

$$\Omega_f = e^{-f}. \tag{2.14}$$

Then $\Omega_f \in W(\mathbf{R}^n)$, $\Omega_f^{-1} \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^n)$ and

$$D_j\Omega_f = -(D_jf)\Omega_f, \quad D_kD_j\Omega_f = [-D_kD_jf + (D_jf)(D_kf)]\Omega_f. \tag{2.15}$$

Proof. Let $f_m = J_{1/m}f$. Then $f_m \in C^{\infty}(\mathbf{R}^n)$ and, for all $r > 0$,

$$\sup_{|x|<r} |f_m(x)| \leq \sup_{|x|<r+m^{-1}} |f(x)| < \infty.$$

Moreover, (2.8)–(2.10) with Ω_m and Ω replaced by f_m and f respectively hold. Let $u \in C_0^{\infty}(\mathbf{R}^n)$ and $\operatorname{supp} u \subset \{x \in \mathbf{R}^n |\ |x| \leq r\}$. By integration by parts, we have $\langle \Omega_{f_m} D_j u\rangle = \langle (D_jf_m)\Omega_{f_m}u\rangle$. Using the elementary inequality

$$|e^s - e^t| \leq |s-t|e^{\max\{s,t\}}, \quad s, t \in \mathbf{R},$$

we have

$$|\langle(\Omega_{f_m} - \Omega_f)u\rangle| \leq e^{\text{ess.sup}_{|x|\leq r+1}|f(x)|} \sup_{x\in\mathbf{R}^n} |u(x)| \left(\int_{|x|\leq r} |f_m(x) - f(x)|dx\right)$$

Hence $\lim_{m\to\infty}\langle\Omega_{f_m}u\rangle = \langle\Omega_f u\rangle$. Similarly $\lim_{m\to\infty}\langle(D_jf_m)\Omega_{f_m}u\rangle = \langle(D_jf)\Omega_f u\rangle$. Hence $\langle(D_jf)\Omega_f)u\rangle = \langle\Omega_f D_j u\rangle$, which means that $D_j\Omega_f = -(D_jf)\Omega_f$. The condition $f \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^n)$ imlpies that $\Omega_f, \Omega_f^{-1} \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^n)$. It follows that $D_j\Omega_f \in L^2_{\mathrm{loc}}(\mathbf{R}^n)$.

In the same way, we can prove the second equation of (2.15) and $D_k D_j \Omega_f \in L^1_{\mathrm{loc}}(\mathbf{R}^n)$. □

We are now ready to prove Theorems 1.1 and 1.2.

Proof of Theorem 1.1

Let $f \in \mathcal{W}_{a,V}$ and $\Omega_f = e^{-f}$. Then the conclusion of Lemma 2.3 holds. By direct computation using (2.15), we have

$$\begin{aligned} \widehat{H}_0\Omega_f(x) + V(x)\Omega_f(x) &= \Phi_{a,V}(x;f)\Omega_f(x) \\ &\geq E_{a,V}(f)\Omega_f(x), \quad \text{a.e.}x. \end{aligned}$$

By this fact and Lemma 2.3, $\Omega = \Omega_f$ satisfies the assumption of Theorem 2.2 with $\lambda = E_{a,V}(f)$. Hence $E_0(H_{a,V}) \geq E_{a,V}(f)$. Thus the assertion of Theorem 1.1 follows. □

Proof of Theorem 1.2

We can write $\Omega = e^{-f_0}$. Then the conclusion of Lemma 2.3 holds with $f = f_0$ and $\Omega_f = \Omega$. Hence $H_0\Omega = \widehat{H}_0\Omega$ and $\widehat{H}_0\Omega(x) + V(x)\Omega(x) = \lambda\Omega(x)$, a.e.$x$, which implies that $\Phi_{a,V}(x;f_0) = \lambda$, a.e.$x$. Hence $f_0 \in \mathcal{W}_{a,V}$ and $E_{a,V}(f_0) = \lambda$. Thus, by Theorem 1.1, we obtain $E_0(H_{a,V}) \geq \lambda$. On the other hand, by a simple limiting argument, one can easily see that $E_0(H_{a,V}) \leq \lambda$. Hence $E_0(H_{a,V}) = \lambda = E_{a,V}(f_0)$. The last equality of (1.12) follows from this fact, $\sup_{f\in\mathcal{W}_{a,V}} E_{a,V}(f) \geq E_{a,V}(f_0)$ and (1.11). □

3 Proof of Theorem 1.3

The idea of the proof is to find a "trial function" f in $\mathcal{W}_{a,V}$ such that $E_{a,V}(f) > V_0$. Let $t, \varrho > 0$ and

$$f_{t,\varrho}(x) = t\sqrt{(x-x_0)^2 + \varrho^2}.$$

Then $f_{t,\varrho} \in W(\mathbf{R}^n)$. By direct computation, we have for all $x \in \mathbf{R}^n$

$$\begin{aligned} \Phi_{a,V}(x;f_{t,\varrho}) &= \frac{t}{[(x-x_0)^2+\varrho^2]^{3/2}}\{(x-x_0)[\mathrm{tr}\, a(x) - a(x)](x-x_0) + \varrho^2 \mathrm{tr}\, a(x)\} \\ &\quad + \frac{tv(x)(x-x_0)}{\sqrt{(x-x_0)^2+\varrho^2}} - \frac{(x-x_0)a(x)(x-x_0)}{(x-x_0)^2+\varrho^2}t^2 + V(x). \end{aligned}$$

Noting that $\mathrm{tr}\, a(x) - a(x)$ is positive semi-definite, we obtain

$$\begin{aligned} \Phi_{a,V}(x;f_{t,\varrho}) &\geq \frac{\varrho^2 \mathrm{tr}\, a(x)}{[(x-x_0)^2+\varrho^2]^{3/2}}t + \frac{tv(x)(x-x_0)}{\sqrt{(x-x_0)^2+\varrho^2}} \\ &\quad - \frac{(x-x_0)a(x)(x-x_0)}{(x-x_0)^2+\varrho^2}t^2 + V(x). \end{aligned} \tag{3.1}$$

To estimate the right hand side of (3.1) from below, we first consider the case where $|x - x_0| \le R$. We set

$$L_R(a) : = \inf_{|x-x_0|\le R} \operatorname{tr} a(x), \tag{3.2}$$

$$a_{R1} : = \sup_{|x-x_0|\le R} \|a(x)\|, \quad v_{R1} := \sup_{|x-x_0|\le R} |v(x)|, \tag{3.3}$$

where $\|a(x)\|$ is the norm of $a(x)$ as a bounded linear operator on $\mathbf{C}^n$. Since $L_R(a) > 0$ by (1.17), it follows that $a_{R1} > 0$. By the fact that, for $|x - x_0| \le R$,

$$\frac{(x-x_0)^2}{(x-x_0)^2 + \varrho^2} \le \frac{R^2}{R^2 + \varrho^2},$$

we have

$$\Phi_{a,V}(x; f_{t,\varrho}) \ge C(t, \varrho),$$

where

$$C(t,\varrho) := \frac{1}{(R^2+\varrho^2)^{3/2}} \left[L_R(a)\varrho^2 - v_{R1} R(R^2+\varrho^2)\right] t - \frac{a_{R1} R^2}{R^2+\varrho^2} t^2 + V_0. \tag{3.4}$$

Let $\varrho > 1$. Then, by (1.17), we can show that

$$L_R(a)\varrho^2 > v_{R1}(R^2 + \varrho^2)R.$$

Hence, putting

$$t_1 := \frac{1}{a_{R1} R^2 \sqrt{R^2+\varrho^2}} \left[L_R(a)\varrho^2 - v_{R1} R(R^2+\varrho^2)\right] > 0, \tag{3.5}$$

we have for all $t \in (0, t_1)$ and $|x - x_0| \le R$

$$\Phi_{a,V}(x; f_{t,\varrho}) \ge C(t,\varrho) > V_0. \tag{3.6}$$

We next consider the case $|x - x_0| > R$. Let

$$a_{R2} : = \sup_{|x-x_0|>R} \|a(x)\|, \quad v_{R2} := \sup_{|x-x_0|>R} |v(x)|, \tag{3.7}$$

$$V_R : = \operatorname{ess.inf}_{|x-x_0|>R} V(x) > V_0. \tag{3.8}$$

Then we have

$$\Phi_{a,V}(x; f_{t,\varrho}) \ge D(t)$$

where

$$D(t) := -v_{R2} t - a_{R2} t^2 + V_R. \tag{3.9}$$

We define a constant $t_2 > 0$ as follows: in the case $a_{R2} > 0$,

$$t_2 := \frac{-v_{R2} + \sqrt{v_{R2}^2 + 4a_{R2}(V_R - V_0)}}{2a_{R2}} > 0. \tag{3.10}$$

In the case $a_{R2} = 0$,

$$t_2 := \frac{V_R - V_0}{v_{R2}}, \tag{3.11}$$

where $t_2 := \infty$ if $v_{R2} = 0$. Then we have for all $t \in (0, t_2)$ and $|x - x_0| > R$

$$\Phi_{a,V}(x; f_{t,\varrho}) \geq D(t) > V_0. \tag{3.12}$$

By (3.6) and (3.12), we obtain

$$E_{a,V}(f_{t,\varrho}) \geq \gamma(t, \varrho) > V_0, \quad t \in (0, \min\{t_1, t_2\}), \ \varrho > 1,$$

where

$$\gamma(t, \varrho) := \min\{C(t, \varrho), D(t)\}. \tag{3.13}$$

Hence, by Theorem 1.1, we have for all $t \in (0, \min\{t_1, t_2\})$ and $\varrho > 1$

$$E_0(H_{a,V}) \geq \gamma(t, \varrho) > V_0. \tag{3.14}$$

□

4 Application to the Hamiltonian of a perturbed hydrogen-like atom

The Hamiltonian of the hydrogen-like atom is given by

$$H_{\text{hyd}} = -\Delta - \frac{Z}{|x|} \tag{4.1}$$

on $L^2(\mathbf{R}^n)$ with Z a positive constant (the physical case is the case $n = 3$). A simple application of Theorem 1.2 shows that H_{hyd} is bounded from below with

$$E_0(H_{\text{hyd}}) = -\frac{Z^2}{(n-1)^2}, \tag{4.2}$$

see [1, §4.1].

We consider a perturbation of H_{hyd} by a nonnegative potential U on $\mathbf{R}^n$:

$$H := H_{\text{hyd}} + U = -\Delta - \frac{Z}{|x|} + U \tag{4.3}$$

with $D(H) = C_0^\infty(\mathbf{R}^n)$. We want to show that the perturbation U with an additional condition enhances the ground state energy of the hydrogen-like atom even in the case $\text{ess.inf}_{x \in \mathbf{R}^n} U(x) = 0$.

THEOREM 4.1. *Let $n \geq 2$ and $U \geq 0$. Suppose that there exists a constant $R > n(n-1)/2Z$ such that*

$$\text{ess.inf}_{|x| \leq R} U(x) > 0. \tag{4.4}$$

Then

$$E_0(H) > E_0(H_{\mathrm{hyd}}). \tag{4.5}$$

Remark. The conclusion of Theorem 4.1 is nontrivial only if $\text{ess.inf.}_{x\in\mathbf{R}^n}U(x) = 0$. As the proof below shows, we can compute a constant δ such that $E_0(H) \geq \delta > E_0(H_{\mathrm{hyd}})$, see (4.25). This gives an estimate for $E_0(H)$.

Proof. We set $r = |x|$, $x \in \mathbf{R}^n$, and

$$\Phi(x; f) := \Phi_{I,V}(x; f) = \Delta f(x) - \sum_{j=1}^{n} |D_j f(x)|^2 - \frac{Z}{r} + U(x), \tag{4.6}$$

wherer $V(x) = -Zr^{-1} + U(x)$. We take as a trial function

$$g_{s,\alpha}(x) = rs + \alpha \log(1+r), \quad x \in \mathbf{R}^n,$$

where $s > 0$ and $\alpha > 0$ are parameters to be chosen suitably. It is easy to see that $g_{s,\alpha} \in W(\mathbf{R}^n)$ with

$$\begin{aligned} D_j g_{s,\alpha}(x) &= \frac{x_j}{r}\left(s + \frac{\alpha}{1+r}\right), \\ D_k D_j g_{s,\alpha}(x) &= \frac{\delta_{jk}}{r}\left(s + \frac{\alpha}{1+r}\right) - \frac{x_j x_k}{r^3}\left(s + \frac{\alpha}{1+r} + \frac{\alpha r}{(1+r)^2}\right). \end{aligned}$$

Hence

$$\Phi(x; g_{s,\alpha}) = \frac{(n-1)(s+\alpha) - Z}{r} - \frac{(n-1)\alpha}{1+r} - \frac{\alpha}{(1+r)^2} - \left(s + \frac{\alpha}{1+r}\right)^2 + U(x). \tag{4.7}$$

Let

$$U_R := \text{ess.inf}_{r\leq R}\, U(x) > 0. \tag{4.8}$$

Take $s, \alpha > 0$ such that

$$(n-1)(s+\alpha) > Z. \tag{4.9}$$

Then, for $r \leq R$, we have

$$\Phi(x; g_{s,\alpha}) \geq \delta_1(s, \alpha, R), \tag{4.10}$$

where

$$\delta_1(s, \alpha, R) := \frac{(n-1)(s+\alpha) - Z}{R} - \alpha n - (s+\alpha)^2 + U_R. \tag{4.11}$$

Let

$$\alpha_1 = \frac{U_R}{n}, \quad \alpha_2 = \frac{-n + \sqrt{n^2 + 4\left(U_R + \frac{Z^2}{(n-1)^2}\right)}}{2}, \tag{4.12}$$

For all $\alpha \in (0, \min\{\alpha_1, \alpha_2\})$, the interval

$$I_1(\alpha) := \left(0, \sqrt{U_R - \alpha n + \frac{Z^2}{(n-1)^2}} - \alpha\right) \tag{4.13}$$

is not empty. We define a set

$$\mathsf{S}_1 := \{(s,\alpha) | 0 < \alpha < \min\{\alpha_1, \alpha_2\}, s \in I_1(\alpha),\ s \text{ and } \alpha \text{ satisfy (4.9)}\}. \tag{4.14}$$

This is a non-empty set. It follows that, for all $(s,\alpha) \in \mathsf{S}_1$, $\delta_1(s,\alpha,R) > E_0(H_{\mathrm{hyd}})$. Hence

$$\text{ess.inf}_{r \le R}\, \Phi(x; g_{s,\alpha}) \ge \delta_1(s,\alpha,R) > E_0(H_{\mathrm{hyd}}), \quad (s,\alpha) \in \mathsf{S}_1. \tag{4.15}$$

We next consider the case $r \ge R$. We set

$$U_R' := \text{ess.inf}_{r \ge R}\, U(x) \ge 0. \tag{4.16}$$

Then we have

$$\Phi(x; g_{s,\alpha}) \ge \delta_2(s,\alpha,R), \tag{4.17}$$

where

$$\delta_2(s,\alpha,R) := -\frac{\alpha n}{1+R} - \left(s + \frac{\alpha}{1+R}\right)^2 + U_R'. \tag{4.18}$$

Let

$$\begin{aligned} \alpha_3 &= \frac{(1+R)Z^2}{n(n-1)^2}, && (4.19)\\ \alpha_4 &= \frac{\left(-n + \sqrt{n^2 + 4\left(U_R' + \frac{Z^2}{(n-1)^2}\right)}\right)(1+R)}{2}. && (4.20) \end{aligned}$$

Then, for all $\alpha \in (0, \min\{\alpha_3, \alpha_4\})$, the interval

$$I_2(\alpha) := \left(0, \sqrt{U_R' - \frac{\alpha n}{1+R} + \frac{Z^2}{(n-1)^2}} - \frac{\alpha}{1+R}\right) \tag{4.21}$$

is not empty. By virtue of the condition $R > n(n-1)/2Z$, we have

$$\alpha_5 := \frac{2(1+R)Z}{R(n-1)}\left(1 - \frac{n(n-1)}{2ZR}\right) > 0. \tag{4.22}$$

Then the set

$$\mathsf{S}_2 := \{(s,\alpha) | 0 < \alpha < \min\{\alpha_3, \alpha_4, \alpha_5\}, s \in I_2(\alpha),\ s \text{ and } \alpha \text{ satisfy (4.9)}\} \tag{4.23}$$

is not empty and, for all $(s,\alpha) \in \mathsf{S}_2$, we have $\delta_2(s,\alpha,R) > E_0(H_{\mathrm{hyd}})$. Hence

$$\text{ess.inf}_{r \ge R} \Phi(x; g_{s,\alpha}) \ge \delta_2(s,\alpha,R) > E_0(H_{\mathrm{hyd}}), \quad (s,\alpha) \in \mathsf{S}_2. \tag{4.24}$$

It follows from (4.15) and (4.24) that, for all $(s,\alpha) \in \mathsf{S}_1 \cap \mathsf{S}_2$,

$$\text{ess.inf}_{x \in \mathbf{R}^n} \Phi(x; g_{s,\alpha}) \geq \delta(s,\alpha,R) > E_0(H_{\text{hyd}}),$$

where

$$\delta(s,\alpha,R) := \min\{\delta_1(s,\alpha,R), \delta_2(s,\alpha,R)\}. \tag{4.25}$$

(Note that $\mathsf{S}_1 \cap \mathsf{S}_2 \neq \emptyset$.) Thus, by Theorem 1.1, we obtain

$$E_0(H) \geq \delta(s,\alpha,R) > E_0(H_{\text{hyd}}), \quad (s,\alpha) \in \mathsf{S}_1 \cap \mathsf{S}_2. \tag{4.26}$$

□

In the following examples, we take $n \geq 2$.

EXAMPLE 4.1. *The Yukawa potential.* Let $0 < \lambda \leq 1$, $m > 0$ be constants and

$$U(x) = \frac{Z(1 - \lambda e^{-mr})}{r} > 0.$$

Then H becomes the Schrödinger operator with the Yukawa potential $-Z\lambda e^{-mr}/r$:

$$H_{\text{Yukawa}} = -\Delta - \frac{Z\lambda e^{-mr}}{r}.$$

It is obvious that, for all $R > 0$, (4.4) is satisfied. Hence we can apply Theorem 4.1 to conclude that

$$E_0(H_{\text{Yukawa}}) > E_0(H_{\text{hyd}}).$$

EXAMPLE 4.2. The Hamiltonian of a quantum system of a charged particle interacting with two fixed electric charges, one positive and the other negative, is given (up to a constant multiple) by

$$H_g = -\Delta - \frac{Z}{|x|} + \frac{g}{|x - x_0|},$$

where $x_0 \in \mathbf{R}^n$ is a fixed point and $g > 0$ is a constant. It is obvious that $U(x) := g/|x - x_0|$ satisfies (4.4) for all $R > 0$. Hence we can apply Theorem 4.1 to conclude that

$$E_0(H_g) > E_0(H_{\text{hyd}}).$$

References

[1] Arai, A., A criterion for the boundedness from below with a class of symmetric operators and its applications, *J. Math. Anal. Appl.* **145**, 539-554 (1990).

[2] Cycon, H. L., Froese, R. G., Kirsch, W. and Simon, B., *Schrödinger Operators*, Springer, Berlin, Heidelberg, 1987.