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**Essential self-adjointness
of many-particle Hamiltonian operators
of Schrödinger type
with singular two-particle potentials**

by

V. F. KOVALENKO and Yu. A. SEMENOV

ABSTRACT. — We consider the Hamiltonian H of a quantum mechanical N -particle system ($N \geq 3$) in \mathbb{R}^n with potential $V = \sum_{i < j} V_{ij}$, where $V_{ij} \in L^2_{loc}(\mathbb{R}^n \setminus \{0\})$ and $V_{ij} \geq \beta \Gamma_{ij}^{-2}$ for suitable values of β . We prove the essential self-adjointness of H on the space $\mathcal{E} = C^\infty_0(\mathbb{R}^{nN} \setminus s)$ where $s = \{x \in \mathbb{R}^{nN}; x_i = x_j \text{ for some pair } (i, j)\}$. The value of β , for which our proof holds is optimal for $n=4$ (all N). For $n=1, 2, 3$ (all N) $\beta > -n(n-4)/4$. For $n \geq 5$, we need the assumption:

$$\beta > -n(n-4)/2N\sqrt{4-6/N}.$$

1. INTRODUCTION

Recently, the problem of essential self-adjointness of the Schrödinger operator $-\Delta + V$ in \mathbb{R}^n with singular potentials has been studied. The essential self-adjointness of the Schrödinger operator $-\Delta + V$ on $C^\infty_0(\mathbb{R}^n)$ with $0 \leq V \in L^2_{loc}(\mathbb{R}^n)$ has been proven under certain conditions on the increase of V at infinity by I. Segal and then by B. Simon, by Yu. Semenov and, finally, by W. Faris [1] [2] [3]. Another approach, namely that of T. Kato [4] made it possible to get rid of the restriction on the growth of V . The problem of potentials such that $V \in L^2_{loc}(\mathbb{R}^n \setminus \{0\})$ has been studied

by H. Kalf and J. Walter [5], by U.-W. Schmincke [6] and finally by B. Simon [7], by D. Robinson [8] and by Yu. Semenov [9], who have shown the essential self-adjointness of $-\Delta + V$ on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ if

$$-n(n-4)/4 |x|^2 \leq V \in L_{loc}^2(\mathbb{R}^n \setminus \{0\}).$$

An attempt to extend this result to include N-particle Hamiltonian was later made by D. Robinson and others [10]. The authors proved the essential

self-adjointness of $H_0 + V = (-1/2) \sum_{i=1}^N \Delta_i + \sum_{i<j} V_{ij}$ on $C_0^\infty(\mathbb{R}^{nN} \setminus s)$ whenever

$n \geq 4$ and $0 \leq V_{ij} \in L_{loc}^2(\mathbb{R}^{nN} \setminus s)$ where $s = \{x; x = (x_1, \dots, x_N) \in \mathbb{R}^{nN}, x_i = x_j \text{ for some pair } (i, j)\}$. Here Δ_i is the Laplace operator with respect to the position x_i of the i -th particle; $V_{ij} = V_{ij}(|x_i - x_j|)$ is a two-particle potential. An interesting conjecture was formulated, in the paper just mentioned, namely that the optimal condition for the problem of N-particles should be the following: $V_{ij} \in L_{loc}^2(\mathbb{R}^n \setminus \{0\})$, $V_{ij} \geq \beta_0 / |x_i - x_j|^2$, where $\beta_0 = -n(n-4)/4$.

Recently M. Combes-Moulin and J. Ginibre [11] gave a partial proof of the conjecture. Modifying Simon's method [7] they obtained the optimal constant $\beta (= \beta_0)$ in the cases $n = 1$ and $n = 4$ (all N) and also for $n \leq 6$ with $N = 3$. For the other values of n and N the values obtained for β were greater than the expected optimal value.

The aim of the present paper is to prove essential self-adjointness of the N-particle Hamiltonian using the method developed by one of the authors for the two-particle case [9]. We obtain an almost optimal constant $\beta = \beta_0 + \varepsilon$, $\forall \varepsilon > 0$ for $n = 1, 2, 3$ (all N). For higher dimensions, $n \geq 5$ (all N) the constant obtained is very far from optimal, namely:

$$\beta \geq -n(n-4)/2N\sqrt{4-6/N}.$$

We also get an additional information on the functions belonging to the domain of the closure $(H_0 + V)^\sim$ for the constants mentioned above.

We show that $\mathcal{D}(H^\sim) \subset \mathcal{D}(V_0)$ where $V_0 = \sum_{i<j} |x_i - x_j|^{-2}$.

2. MAIN INEQUALITIES

From now on we shall consider an N-particle system (with fixed center of mass) in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{n(N-1)})$. The « free » Hamiltonian of the reduced problem is:

$$H_0 = (-1/2) \sum_{i=1}^N \Delta_{x_i} + (1/2N) \left(\sum_{i=1}^N \nabla_{x_i} \right)^2.$$

Denoting $p_i = -i\nabla_{x_i}$ and introducing the relative momentum of the pair of particles (i, j) as $p_{ij} = (1/2)(p_i - p_j)$, we have

$$H_0 = (2/N) \sum_{i < j} p_{ij}^2.$$

Let us introduce the reference potential

$$V_0 = \sum_{i < j} \Gamma_{ij}^{-2}, \quad \text{where } \Gamma_{ij} = |x_i - x_j|.$$

Let us define the symmetric operator $H = H_0 + \lambda V_0$, $\lambda \in \mathbb{R}^1$ on the space $\mathcal{E} = C_0^\infty(\mathbb{R}^{n(N-1)} \setminus s)$ where $s = \{x; x = (x_1, \dots, x_{N-1}) \in \mathbb{R}^{n(N-1)}, x_i = x_j \text{ for some pair } (i, j)\}$.

LEMMA 1. — For each $n = 1, 2, 3, 4$ and for all $N \geq 3$ the following inequality holds

$$\| [H_0 + (\beta_0 + \varepsilon_N)V_0]\psi \| \geq \| \varepsilon_N V_0 \psi \|, \quad \forall \psi \in \mathcal{E}$$

where

$$\varepsilon_N \geq (1/2 \gamma)[(1 - 2/N)n^2(n - 4)^2/16 - \gamma^2],$$

$$\beta_0 = -n(n - 4)/4 + \gamma, \quad \forall \gamma > 0$$

(note that when $n = 4$ then $\beta_0 = \gamma > 0$).

Proof. — Let us denote $\beta_N = \beta_0 + \varepsilon_N$, $\beta = (N/2)\beta_N$; $\varepsilon = (N/2)\varepsilon_N$. Then

$$H_0 + (\beta_0 + \varepsilon_N)V_0 \equiv H_0 + \beta_N V_0 = (2/N) \sum_{i < j} (p_{ij}^2 + \beta \Gamma_{ij}^{-2}),$$

$$(N^2/4)(\| (H_0 + \beta_N V_0)\psi \|^2 - \| \varepsilon_N V_0 \psi \|^2) = I_1 + I_2 + I_3,$$

where

$$I_1 = \sum_{i < j} \{ L_{ij} + 2\beta G_{ij} + (2(n - 4)\beta + \beta^2 - \varepsilon^2)C_{ij} \},$$

$$I_2 = \sum_{i, j, k, l \text{ are different}} \{ \| p_{ki} p_{ij} \psi \|^2 + (\beta^2 - \varepsilon^2) \| \psi \Gamma_{kl}^{-1} \Gamma_{ij}^{-1} \|^2 + 2\beta \| \Gamma_{kl}^{-1} p_{ij} \psi \|^2 \},$$

$$I_3 = \sum_{i, j, k \text{ are different}} \{ \| p_{ki} p_{ij} \psi \|^2 + (\beta^2 - \varepsilon^2) \| \Gamma_{ki}^{-1} \Gamma_{ij}^{-1} \psi \|^2 + (1/2)(n - 4)\beta C_{ki} + 2\beta \| \Gamma_{ki}^{-1} p_{ij} \psi \|^2 \}$$

Here

$$L_{ij} \equiv \| p_{ij}^2 \psi \|^2, \quad G_{ij} \equiv \| \Gamma_{ij}^{-1} p_{ij} \psi \|^2, \quad C_{ij} \equiv \| \Gamma_{ij}^{-2} \psi \|^2.$$

The expression I_1 has been obtained by applying Green's formula and using the following equalities:

$$p_{ij}^2(\Gamma_{ij}^{-2}) = 2(n-4)\Gamma_{ij}^{-4}, \quad \psi p_{ij}^2 \bar{\psi} + \bar{\psi} p_{ij}^2 \psi = p_{ij}^2 |\psi|^2 + 2 |p_{ij} \psi|^2.$$

The expression I_3 has been obtained in a similar way by noting that

$$p_{ij}^2(\Gamma_{ki}^{-2}) = (n-4)2^{-1}\Gamma_{ki}^{-4}.$$

The expression I_2 is given in an explicit way.

Now, we should like to demonstrate that $I_1 + I_2 + I_3 \geq 0$. First, let us give an estimate for I_3 . We have

$$\begin{aligned} I_3 &\geq \sum_{i,j,k \text{ all different}} \{ (n-4)2^{-1}\beta C_{ki} + 2\beta [|\Gamma_{ij}^{-1} p_{ki} \psi|^2 + |p_{ij} p_{ki} \psi|^2] \} \\ &= \sum_{i,j,k \text{ all different}} \{ (n-4)2^{-1}\beta C_{ki} + \beta [|\Gamma_{ki}^{-1} p_{ij} \psi|^2 + |\Gamma_{ij}^{-1} p_{ki} \psi|^2] \\ &\quad + 2^{-1} [|p_{ki} p_{ij} \psi|^2 + |p_{ki} p_{kj} \psi|^2] \} \\ &\geq \sum_{i,j,k \text{ all different}} \{ (n-4)2^{-1}\beta C_{ki} + 2^{-1}\beta G_{ki} + 4^{-1}L_{ki} \} \\ &= \sum_{i < j} 2^{-1}(N-2)[2(n-4)\beta C_{ij} + 2\beta G_{ji} + L_{ij}]. \end{aligned}$$

Here, the inequality $2(a^2 + b^2) \geq (a \pm b)^2$ and the equality $p_{kj} \psi - p_{ij} \psi = p_{ki} \psi$ have been used. By virtue of the inequality $I_2 \geq 0$ we have

$$\begin{aligned} I_1 + I_2 + I_3 &\geq I_1 + I_3 \geq \sum_{i < j} \{ L_{ij} + 2\beta G_{ij} + [\beta^2 - \varepsilon^2 + 2(n-4)\beta] C_{ij} \\ &\quad + 2^{-1}(N-2)[L_{ij} + 2\beta G_{ij} + 2(n-4)\beta C_{ij}] \} \\ &= (N/2) \sum_{i < j} \{ L_{ij} + 2\beta G_{ij} + [2(n-4)\beta + 2N^{-1}(\beta^2 - \varepsilon^2)] C_{ij} \} \equiv (N^2/4) \sum_{i < j} I_{ij}. \end{aligned}$$

Omitting the indices i, j of L, G, C and applying the well-known Rellich inequality [6]:

$$L + sG - 4^{-2}(n-4)^2(n^2 + 4s)C \geq 0, \quad \forall s \in [-n(n-4)2^{-1}, \infty)$$

and the following Hardy-type inequality [6]:

$$4G \geq (n-4)^2 C,$$

we get:

$$\begin{aligned} I &\geq [\beta_N^2 - \varepsilon_N^2 + 2^{-1}(n-4)n\beta_N + n^2(n-4)^2(8N)^{-1}]C \\ &= [n^2(n-4)^2 4^{-2}(2N^{-1} - 1) + \gamma^2 + 2\varepsilon_N \gamma]C \geq 0. \end{aligned}$$

This completes the proof of Lemma 1.

LEMMA 2. — Let $N \geq 3, n \geq 5$. The following inequality holds true:

$$\| [H_0 + (\beta_0 + \varepsilon)V_0]\psi \| \geq \varepsilon \| V_0\psi \|, \quad \forall \psi \in \mathcal{E}, \quad \forall \varepsilon > 0, \quad \varepsilon + \beta_0 \leq 0,$$

where

$$\beta_0 \geq -n(n-4)/2N\sqrt{4-6/N}.$$

Proof. — Clearly, it is sufficient to show that

$$\| H_0\psi \| \geq \| \beta_0 V_0\psi \|, \quad \forall \psi \in \mathcal{E}.$$

We have

$$\| H_0\psi \|^2 - \| \beta_0 V_0\psi \|^2 = 4N^{-2}(I'_1 + I'_2 + I'_3),$$

where

$$I'_1 = \sum_{i < j} \{ L_{ij} - (N^2/4)\beta_0^2 C_{ij} \},$$

$$I'_2 = \sum_{i,j,k,l \text{ are different}} \{ \| p_{ij} p_{kl}\psi \|^2 - (N^2/4)\beta_0^2 \| \Gamma_{ij}^{-1} \Gamma_{kl}^{-1} \psi \|^2 \},$$

$$I'_3 = \sum_{i,j,k \text{ are different}} \{ \| p_{ij} p_{ki}\psi \|^2 - (N^2/4)\beta_0^2 \| \Gamma_{ij}^{-1} \Gamma_{ki}^{-1} \psi \|^2 \}.$$

The terms I'_1, I'_3 can be estimated in a similar way as has been done in the case of Lemma 1:

$$\begin{aligned} I'_3 &\geq \sum_{i < j} \{ [(N/2) - 1]L_{ij} - N^2[(N/2) - 1]\beta_0^2 C_{ij} \}. \\ I'_1 + I'_3 &\geq \sum_{i < j} \{ (N/2)L_{ij} - (N^2/4)\beta_0^2(2N - 3)C_{ij} \} \\ &\geq (N/2) \sum_{i < j} \{ (n - 4)^2 n^2 / 16 - (N/2)\beta_0^2(2N - 3) \} C_{ij}. \end{aligned}$$

Hence, if $\beta_0 \geq -n(n-4)/2N\sqrt{4-6/N}$, then $I'_1 + I'_3 \geq 0$. It is easy to see that $I'_2 \geq 0$ when β_0 is chosen as above.

LEMMA 3. — Let the conditions of Lemma 1 be satisfied. Let us assume that $\lambda \geq \beta_0$ is chosen large enough for $H_0 + \lambda V_0$ to be essentially self-adjoint on \mathcal{E} . Let us denote the closure of $H_0 + \lambda V_0$ by $H_{0\lambda}$. Assume that $0 \leq V_+ \in L^1_{loc}(\mathbb{R}^{m(N-1)} \setminus s)$. Let us define the form-sum $H = H_{0\lambda} \dot{+} V_+$.

Then

1) $\mathcal{D}(H) \subset \mathcal{D}(V_0)$,

2) for any $\varphi \in \mathcal{D}(H)$ and for arbitrary $\nu > 0$ the following inequality holds true:

$$\| (H + \nu)\varphi \| \geq \| (\lambda - \beta_0)V_0\varphi \|.$$

Proof. — Since $\exp(-H_0)$ and $\exp(-\lambda V_0)$ transform positive vectors into positive ones, then, by the Trotter formula, it is easy to see that $\exp(-H_{0\lambda})$ preserves this property. The same remark is valid also for $\exp(-H)$. By representing the operator resolvent by means of the corresponding semigroup, and applying the Trotter formula again, we obtain:

$$\pm (H + \nu)^{-1} \varphi \leq (H_{0\lambda} + \nu)^{-1} |\varphi|$$

for any real-valued $\varphi \in \mathcal{H}$. Multiplying this inequality by $(\lambda - \beta_0)V_0 \geq 0$ and applying Lemma 1 we have

$$\|(\lambda - \beta_0)V_0(H + \nu)^{-1} \varphi\| \leq \|(\lambda - \beta_0)V_0(H_{0\lambda} + \nu)^{-1} |\varphi|\| \leq \|\varphi\|.$$

Hence the propositions 1) and 2) follow immediately.

LEMMA 4. — Let all the assumptions of Lemma 2 be satisfied. Let $0 \leq V_+ \in L^1_{\text{loc}}(\mathbb{R}^{n(N-1)} \setminus S)$. Let us define the form-sum $H = H_0 + V_+$.

Then

- 1) $\mathcal{D}(H) \subset \mathcal{D}(V_0)$,
- 2) for any $\varphi \in \mathcal{D}(H)$ and for arbitrary $\nu > 0$ the following inequality holds:

$$\|(H + \nu)\varphi\| \geq \|\beta_0 V_0 \varphi\|$$

The proof of Lemma 4 is the same as that of Lemma 3.

Remarks Lemma 3 and Lemma 4.

1) The possibility of choosing a suitable $\lambda > 0$ in the formulation of Lemma 3 is ensured for instance, by the work of M. Combes-Moulin and J. Ginibre [11].

2) The proof of the Trotter formula for $V_+ \in L^1_{\text{loc}}(\mathbb{R}^n \setminus \{0\})$ is given in [12].

3) The method of deriving the inequality $\|(H_0 + V_+)\psi\| \geq \|V_0\psi\|$ from the inequality $\|H_0\psi\| \geq \|V_0\psi\|$ is due to E. Davies [13] (see also W. Faris [3] and Yu. Semenov [9]).

3. ESSENTIAL SELF-ADJOINTNESS

Now, we shall formulate and prove our main result. All the notation is the same as above.

THEOREM 1. — Let $V = \sum_{i < j} V_{ij}$. Let us assume that:

- 1) $V_{ij} \in L^2_{\text{loc}}(\mathbb{R}^n \setminus \{0\})$,
- 2) $V_{ij} \geq \beta_0 \Gamma_{ij}^{-2}$.

Then the operator $H = H_0 + V$ is essentially self-adjoint on \mathcal{E} in the following cases

- a) $n = 1, 2, 3$; all $N \geq 3$; $\beta_0 > -n(n-4)/4$,
 b) $n = 4$; all $N \geq 3$; $\beta_0 = 0$,
 c) $n \geq 5$; all $N \geq 3$; $\beta_0 \geq -n(n-4)/2N\sqrt{4-6/N}$.

Proof. — Let $V_+ = V - \beta_0 V_0$. According to the results of M. Combes-Moulin and J. Ginibre [11] the operator $H_0 + \lambda V_0 + V_+$ is essentially self-adjoint on \mathcal{E} for sufficiently big $\lambda > \beta_0$. Let us denote its closure as H . Then, by virtue of Lemma 3, we get:

- 1) $\mathcal{D}(H) \subset \mathcal{D}(V_0)$,
 2) $\|(H + v)\varphi\| \geq \|(\lambda - \beta_0)V_0\varphi\|$, $\varphi \in \mathcal{D}(H)$, $v > 0$.

Then, by the Rellich-Kato-Wust theorem [14], the operator

$$(H - (\lambda - \beta_0)V_0) \upharpoonright \mathcal{E} \equiv (H_0 + V) \upharpoonright \mathcal{E}$$

is essentially self-adjoint.

REMARK 1. — Applying the method based on Kato's inequality and Lemmas 1-2, it is easy to prove the essential self-adjointness of $H_0 + V$ on \mathcal{E} , assuming that the operator $H_0 + \lambda V_0$ is essentially self-adjoint for λ large enough.

REMARK 2. — Let the form $\mathcal{S}_{H_0+V}[u, v] = \langle (H_0 + V)u, v \rangle$ be defined on $\mathcal{E} \times \mathcal{E}$. The problem of closability of \mathcal{S}_{H_0+V} has been considered by D. Robinson [8].

In the work of Yu. Semenov [12] the closability of the form \mathcal{S}_{H_0+V} is discussed for non-negative potentials $V \in L^1_{loc}(\mathbb{R}^n \setminus \{a_1, \dots, a_n\})$ in the two-body problem. The method used in [9] can be immediately extended to the case when $N \geq 3$.

THEOREM 3. — Let $n \geq 3$ and $N \geq 3$. Let $V = \sum_{i < j} V_{ij}$. We assume that

- 1) $V_{ij} \in L^1_{loc}(\mathbb{R}^n \setminus \{0\})$ and
 2) $V_{ij} \geq \beta_0 \Gamma_{ij}^{-2}$.

Then the form $\mathcal{S}_H[u, v] = \langle H_0 u, v \rangle + \langle V u, v \rangle$ with domain $\mathcal{D}(\mathcal{S}_H) = \mathcal{E} \times \mathcal{E}$ is closable (in \mathcal{H}) whenever $\beta_0 > -(n-2)^2/2N$. If, in addition

- 1') $V_{ij} \in L^2_{loc}(\mathbb{R}^n \setminus \{0\})$,

then the Friedrich extension $(H_0 + V)_F$ and the form-sum $H_0 \dot{+} V$ coincide.

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