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

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

by

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ABSTRACT. — We consider the Hamiltonian H of a quantum mechanical N-particle system ($N \geqslant 3$) in $\mathbb{R}^n$ with potential $V = \sum_{i<j} V_{ij}$, where $V_{ij} \in L^2_{loc}(\mathbb{R}^n \backslash \{0\})$ and $V_{ij} \geqslant \beta \Gamma_{ij}^{-2}$ for suitable values of β. We prove the essential self-adjointness of H on the space $\mathscr{E} = C_0^\infty(\mathbb{R}^{nN} \backslash s)$ 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 $n \geqslant 5$, 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 $C_0^\infty(\mathbb{R}^n)$ with $0 \leqslant V \in L^2_{loc}(\mathbb{R}^n)$ 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 $V \in L^2_{loc}(\mathbb{R}^n \backslash \{0\})$ 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 $C_0^\infty(\mathbb{R}^n \backslash \{0\})$ if

$$-n(n-4)/4\,|x|^2 \leqslant V \in L^2_{loc}(\mathbb{R}^n \backslash \{0\}).$$

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 $C_0^\infty(\mathbb{R}^{nN} \backslash s)$ whenever $n \geqslant 4$ and $0 \leqslant V_{ij} \in L^2_{loc}(\mathbb{R}^{nN} \backslash s)$ where $s = \{x\,;\, x = (x_1, \ldots, x_N) \in \mathbb{R}^{nN}, x_i = x_j \text{ for some pair } (i, j)\}$. 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: $V_{ij} \in L^2_{loc}(\mathbb{R}^n \backslash \{0\})$, $V_{ij} \geqslant \beta_0/|x_i - x_j|^2$, where $\beta_0 = -n(n-4)/4$.

Recently M. Combescure-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 $n \leqslant 6$ 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, $n \geqslant 5$ (all N) the constant obtained is very far from optimal, namely:

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

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:

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

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

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

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

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

$$\| [H_0 + (\beta_0 + \varepsilon_N)V_0]\psi \| \geqslant \| \varepsilon_N V_0 \psi \| , \qquad \forall \psi \in \mathscr{E}$$

where

$$\varepsilon_N \geqslant (1/2\, \gamma)[(1 - 2/N)n^2(n-4)^2/16 - \gamma^2],$$
$$\beta_0 = -n(n-4)/4 + \gamma , \qquad \forall \gamma > 0$$

(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

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

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

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

Here

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

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

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

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 $I_1 + I_2 + I_3 \geqslant 0$. First, let us give an estimate for I_3. We have

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

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

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

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

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

and the following Hardy-type inequality [*6*]:

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

we get:

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

This completes the proof of Lemma 1.

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

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

where

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

Proof. — Clearly, it is sufficient to show that

$$\| H_0\psi \| \geqslant \| \beta_0 V_0 \psi \|, \qquad \forall\psi \in \mathscr{E}.$$

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:

$$I_3' \geqslant \sum_{i<j} \{ [(N/2) - 1]L_{ij} - N^2[(N/2) - 1]\beta_0^2 C_{ij} \}.$$

$$I_1' + I_3' \geqslant \sum_{i<j} \{ (N/2)L_{ij} - (N^2/4)\beta_0^2(2N - 3)C_{ij} \}$$

$$\geqslant (N/2)\sum_{i<j} \{ (n-4)^2 n^2/16 - (N/2)\beta_0^2(2N-3) \} C_{ij}.$$

Hence, if $\beta_0 \geqslant -n(n-4)/2N\sqrt{4 - 6/N}$, then $I_1' + I_3' \geqslant 0$. It is easy to see that $I_2' \geqslant 0$ when β_0 is chosen as above.

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

Then

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

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

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

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:

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

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

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

Hence the propositions 1) and 2) follow immediately.

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

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

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. Combescure-Moulin and J. Ginibre [*11*].

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

3) The method of deriving the inequality $\|(H_0 + V_+)\psi\| \geqslant \|V_0\psi\|$ from the inequality $\|H_0\psi\| \geqslant \|V_0\psi\|$ 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) $V_{ij} \in L^2_{loc}(\mathbb{R}^n\backslash\{0\})$,

2) $V_{ij} \geqslant \beta_0 \Gamma_{ij}^{-2}$.

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

a) $n = 1, 2, 3$; all $N \geqslant 3$; $\beta_0 > -n(n-4)/4$,

b) $n = 4$; all $N \geqslant 3$; $\beta_0 = 0$,

c) $n \geqslant 5$; all $N \geqslant 3$; $\beta_0 \geqslant -n(n-4)/2N\sqrt{4-6/N}$.

Proof. — Let $V_+ = V - \beta_0 V_0$. According to the results of M. Combescure-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) $\| (H + \nu)\varphi \| \geqslant \| (\lambda - \beta_0)V_0\varphi \|$, $\varphi \in \mathcal{D}(H)$, $\nu > 0$.

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

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

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

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

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

1) $V_{ij} \in L^1_{loc}(\mathbb{R}^n \backslash \{ 0 \})$ and

2) $V_{ij} \geqslant \beta_0 r_{ij}^{-2}$.

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

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

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

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