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# HIGHLY SINGULAR POTENTIALS IN STATISTICAL MECHANICS

## (Definition of Hamiltonian)

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## 1. INTRODUCTION

The class of translation invariant two-body potentials widely used in statistical mechanics includes highly singular potentials of the Lennard-Jones type

$$\Phi(x) = 4E\left(\frac{A}{|x|^{12}} - \frac{B}{|x|^{6}}\right), \; E>0, \; A>0, \; x \in \boldsymbol{R}^{\nu}, \qquad (1.1)$$

or potentials containing a hard core $\Phi_a(x)$, i.e., $\Phi(x) = \Phi_a(x) + \Phi'(x)$, where $\Phi'(x) \in L^{\infty}(\boldsymbol{R}^{\nu})$ or, e.g., $\Phi'(x) = \Phi(x-a)$ (see (1.1)) and

$$\Phi_a(x) = \begin{cases} 0 \text{ for } |x| > a \\ \infty \text{ for } |x| \le a \end{cases} \qquad (1.2)$$

here $\nu = \dim \boldsymbol{R}^{\nu}$. These potentials generate the N-particle interactions $U_N(x_1, \dots, x_N)$:

$$U_N(x_1, \dots, x_N) = \frac{1}{2} \sum_{i \ne j}^{N} \Phi(x_i - x_j), \qquad (1.3)$$

which are far from being small in the usual sense with respect to the kinetic energy operator (see, e.g., Kato/1/ or Simon/2,3/ ). Hence, for the definition of a self-adjoint Hamiltonian corresponding to such an N-particle system the well-known perturbation theory developed by Kato/1/ and Simon/2/ (see also review in/3/ ) for the cases of

$\Phi(x) \in L^2(\boldsymbol{R}^{\nu}) + L^{\infty}(\boldsymbol{R}^{\nu})$ and $\Phi(x) \in R(\boldsymbol{R}^{\nu}) + L^{\infty}(\boldsymbol{R}^{\nu})$

is not directly applicable. In addition, to ensure the existence of thermodynamics, the $N$-particle Hamiltonian must be at least bounded from below (see Ruelle[4,5]).*

Thus, highly singular two-body potentials without hard core which are used in statistical mechanics should be strongly repulsive near the origin ("point" hard core particles). Therefore these potentials are bounded from below and, for example in three-dimensional space $\boldsymbol{R}^3$, behave as (see, e.g., Simon[2,3]):

$$\Phi(x)\Big|_{|x|\to 0} \geq \frac{\lambda}{|x|^a}, \quad a > 2, \ \lambda > 0. \qquad (1.4)$$

Highly singular potentials, attractive near the origin $\lambda < 0$, are not used in statistical mechanics because the corresponding $N$-particle Hamiltonians are known to be unbounded from below.

From the physical point of view it is clear that a positive singularity in the two-body interaction potential is an idealization. This means that the physical properties of an $N$-particle system enclosed in a bounded region $\Lambda \subset \boldsymbol{R}^\nu$ will change in some sense negligibly if we cut off the singularity of the two-body potentials $\Phi(x)$ from above:

$$\Phi(x) \to \Phi_L(x) = \begin{cases} \Phi(x) & x \in \{x : \Phi(x) \leq L\} \\ L & x \in \{x : \Phi(x) > L\} \end{cases} \qquad (1.5)$$

*Moreover for thermodynamic behaviour it must be stable (see Ruelle[5]).



and then choose the cut-off parameter $L$ large enough, e.g., $L = 10^{10}$ eV! From the mathematical point of view this means that the partition function $Z_\beta[H(\Lambda^N)]$ corresponding to a Hamiltonian $H(\Lambda^N)$ with highly singular interaction (1.3) can be approximated by $Z_\beta[H_L(\Lambda^N)]$ which corresponds to a Hamiltonian with cut-off (1.5). This is a background for highly singular two-body potentials to be a correct model for a real particle interaction. Note that $\Phi_L(x) \in L^2(\boldsymbol{R}^\nu) + L^\infty(\boldsymbol{R}^\nu)$ thus the self-adjoint Hamiltonian $H_L(\Lambda^N)$ and the partition function $Z_\beta[H_L(\Lambda^N)]$ both exist and are well defined.

In the present papers (see also part II) we prove a convergence theorem for the sequence of $Z_\beta[H_L(\Lambda^N)]$ when the cut-off is removed to infinity, $L \to \infty$. Our attention will be limited to the case of "point" hard core particles, i.e., to potentials which are strongly repulsive near the origin and regular out of it but not inevitably spherically symmetric. In the next section we start with definition of a self-adjoint Hamiltonian $H(\Lambda^N)$ for an $N$-particle system enclosed in a bounded region $\Lambda \subset \boldsymbol{R}^\nu$ with a smooth boundary $\partial\Lambda = \bar{\Lambda}\backslash\Lambda$. For the highly singular two-body potentials bounded from below ("point" hard core case) we prove the coincidence of two canonical extensions for the sum of kinetic-energy and potential-energy operators: namely the Friedrichs extension and the form sum extension. This fact is of practical use in the sequel. It allows us to prove the convergence of the cut-off Hamiltonians $H_L(\Lambda^N)$ to $H(\Lambda^N)$ in the generalized strong sense (see part II). This result is a background for the proof of the main result of these papers, i.e., a convergence theorem for partition functions $Z_\beta[H_L(\Lambda^N)]$ or correspondingly free energies $F_L(\beta, \Lambda, N) = -\beta^{-1}\ell n\, Z_\beta[H_L(\Lambda^N)]$. This theorem means that a highly singular two-body potentials $\Phi(x)$ can be substituted by the regular one $\Phi_L(x) \in L^2(\boldsymbol{R}^\nu) + L^\infty(\boldsymbol{R}^\nu)$ with an error which is negligible in the thermodynamical sense when the cut-off parameter L is removed to infinity. In conclusion we discuss a question about stability of the cut-off interactions $U_N^L(x_1, \dots, x_N)$:

$$U_N^L(x_1, \dots, x_N) = \frac{1}{2}\sum_{i \neq j}^{N} \Phi_L(x_i - x_j). \tag{1.6}$$

These results are illustrated in detail for the case of the Lennard-Jones potential (12-6) in $\boldsymbol{R}^3$. For this potential we prove that the regular cut-off interactions $U_N^L$ (1.6) are stable when the parameter L is larger than some fixed value $L_0$.

The repulsive highly singular potentials (see (1.4)) are widely discussed within the framework of quantum mechanics for $\Lambda = \boldsymbol{R}^3$ by Kato /6/, Schmincke /7/ and Simon /8/. These authors were especially interested in the non-perturbative problem of essential self-adjointness of one-particle Schrödinger operator. Recently Robinson /9/, Robinson et al. /10/ and Ginibre /11, 12/ have extended these results in $\boldsymbol{R}^\nu$ to N-particle systems interacting via repulsive translation invariant two-body potentials of an arbitrary singularity at the origin. The scattering theory for such sys-



tems was also developed /9,10/*. But in these papers we are interested in the significance of highly singular two-body potentials (repulsive near the origin) from the point of view of statistical mechanics.

In the following we restrict ourselves to the case of "point" hard core particles, the case of hard core particles with nonzero radius a (1.2) will be considered in a subsequent paper.

## 2. DEFINITION OF HAMILTONIAN

In this section we discuss the definition of a self-adjoint Hamiltonian $H(\Lambda^N)$ for an N-particle system enclosed in a bounded region of an arbitrary shape and with a smooth boundary which in the following will be denoted by $\Lambda \subset \boldsymbol{R}^\nu$. The system is supposed to consist of "point" hard core particles with translation invariant highly singular two-body potential of interaction $\Phi(x)$, repulsive near the origin and regular out of this region. Thus, $\Phi(x)$ is semibounded from below. The Hilbert space $\mathcal{H}(\Lambda^N)$ appropriate for a description of the states of this system is $L^2(\Lambda^N)$. In our discussion the statistics of particles is not important, therefore we will ignore the symmetry restrictions for $\phi(x_1, \dots, x_N) \in \mathcal{H}(\Lambda^N)$ and work on $\mathcal{H}(\Lambda^N) = L^2(\Lambda^N)$.

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*I am grateful to Dr. E.Christov for bringing refs. /9-11/ to my attention. Our method of proving of Theorem 2.1 is a modified version of that of Robinson /9/ and Robinson et al. /10/ inspired by the Kato book /1/.

For the definition of self-adjoint extensions of the operators considered in this paper we need a certain amount of quadratic form technique (see, e.g., Kato /1/ ).

Proposition 2.1. (Kato /1/ VI, §2). Let T be a symmetric operator bounded from below and let us associate with T a quadratic form

$$t[\psi]=(\psi, T\psi) \quad \forall \psi \in D(T), \qquad (2.1)$$

thus, t-domain is equal to the domain of the operator T: $Q(t) = D(T)$. Such a form is closable and let us denote its closure by $\tilde{t}[\psi]$. Then this densely defined, closed, symmetric, and semibounded form determines a unique operator $T_{\tilde{t}}$ which is a self-adjoint extension of T such that

$$\tilde{t}[\psi]=(\psi, T_{\tilde{t}}\psi) \qquad \text{for } \forall\psi \in D(T_{\tilde{t}}) \qquad (2.2)$$

and $D(T_{\tilde{t}})$ is a form-core for $\tilde{t}[\psi]$, i.e., $(\tilde{t} \upharpoonright D(T_{\tilde{t}}))^{\sim} = \tilde{t}$.

According to Proposition 2.1 the self-adjoint operator of kinetic energy $H_0(\Lambda^N)$ for the system under consideration can be defined as a self-adjoint extension of a positive symmetric operator $T_N$ with the dense domain $D(T_N)=C_0^\infty(\Lambda^N)$ (consisting of infinitely differentiable functions $\psi(x_1,\ldots,x_N)$ with compact supports $\operatorname{supp}\psi(x_1,\ldots,x_N) \subset \Lambda^N$)

$$T_N=\sum_{i=1}^{N}\left(-\frac{\Delta_i}{2m}\right), \quad D(T_N)=C_0^\infty(\Lambda^N). \qquad (2.3)$$

This is the well-known Friedrichs extension: $(T_N)_F = H_0(\Lambda^N)$ which corresponds to the "zero boundary condition" extension of $T_N$. This extension is very natural from physical point of view, if one considers N-particle systems enclosed in a bounded region (container) $\Lambda \subset \boldsymbol{R}^\nu$.



Next, we look at the operator of the N-particle interaction. It can be formally defined as real function multiplicator $U_N(x_1,\ldots x_N)$ (1.3) with domain $D(U_N) = C_0(\Lambda^N \setminus S_N)$, i.e.,

$$U_N(x_1,\ldots,x_N)=\frac{1}{2}\sum_{i\neq j}^{N}\Phi(x_i-x_j), \quad D(U_N)=C_0(\Lambda^N\setminus S_N). \qquad (2.4)$$

Here $S_N \subset \Lambda^N$ denotes a singular set for "point" hard core particles:

$$S_N=\{(x_1,\ldots,x_N)\in\Lambda^N : x_i=x_j \text{ for some } i\neq j\} \qquad (2.5)$$

The measure of $S_N$ is obviously equal to zero ($\operatorname{mes}S_N=0$). Hence the domain $D(U_N)=C_0(\Lambda^N\setminus S_N)$ is dense in the space $\mathcal{H}(\Lambda^N)$. Therefore the operator (2.4) is symmetric and due to the semiboundedness of two-body potential $\Phi(x)$ (see section 1) is also semibounded from below: $U_N(x_1,\ldots,x_N)\geq -a$. Moreover, it is clear that the operator $U_N$(2.4) is essentially self-adjoint, hence the self-adjoint extension of $U_N$ given by Proposition 2.1 coincides with its closure $\tilde{U}_N$:

$$(U_N)_F=\tilde{U}_N\equiv U(\Lambda^N). \qquad (2.6)$$

Now for constructing a total self-adjoint Hamiltonian $H(\Lambda^N)$, we discuss the addition of a highly singular particle interaction $U_N$ (or $U(\Lambda^N)$) to the kinetic-energy operator $H_0(\Lambda^N)$. This may be done in general at least in two canonical and distinct ways (Kato /1/, VI, §2). Note at first that $D(H_0)\cap D(U_N)\supset C_0^\infty(\Lambda^N\setminus S_N)$ and $\operatorname{mes}S_N=0$ then $D=D(H_0)\cap D(U_N)$ is dense in the space $\mathcal{H}(\Lambda^N)$. So, the algebraic sum $H_0+U_N$

(or $H_0 + U$ ) is densely defined, symmetric, and semibounded from below. The extension of these sums according to Proposition 2.1 gives us the Friedrichs extensions corresponding to zero boundary condition on $\partial\Lambda$: $(H_0 + U_N)_F$, $(H_0 + U)_F$. These extensions are generated by the densely defined, symmetric, semibounded, and closed quadratic forms

$$
\begin{aligned}
(h_0 + u)^{\sim}[\psi] &= [(\psi, H_0 \psi) + (\psi, U_N \psi)]^{\sim}, \\
(h_0 + u_U)^{\sim}[\psi] &= [\psi, H_0 \psi) + (\psi, U \psi)]^{\sim}.
\end{aligned} \tag{2.7}
$$

Another way is the quadratic form extension

$$H_0 \dotplus U_N \qquad H_0 \dotplus U . \tag{2.8}$$

These extensions are generated by the sums of closed quadratic forms. These sums are well-defined and satisfy all requirements of Proposition 2.1:

$$
\begin{aligned}
(\tilde{h}_0 + \tilde{u})[\psi] &= (\psi, H_0 \psi)^{\sim} + (\psi, U_N \psi)^{\sim}, \\
(\tilde{h}_0 + \tilde{u}_U)[\psi] &= (\psi, H_0 \psi)^{\sim} + (\psi, U \psi)^{\sim}.
\end{aligned} \tag{2.9}
$$

In general, addition and closure are not interchangeable, hence these extensions are distinct* . One can easily check that

$$
\begin{aligned}
(h_0 + u)^{\sim} &\subseteq (\tilde{h}_0 + \tilde{u}), \\
(h_0 + u_U)^{\sim} &\subseteq (\tilde{h}_0 + \tilde{u}_U).
\end{aligned} \tag{2.10}
$$

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*The forms $\tilde{u}[\psi] = (\psi, U_N \psi)^{\sim}$ and $\tilde{u}_U[\psi] = (\psi, U\psi)^{\sim}$ clearly coincide, so the self-adjoint operator $H_0 \dotplus U_N$ coincides with $H_0 \dotplus U$ (2.8).



It will be shown, however, that for systems of N "point" hard core particles enclosed in a bounded region $\Lambda \subset \mathbb{R}^\nu$ these two ways coincide. This can be done in the manner of Kato[1] (see V , § 5.2, VI, § 4.3), similar arguments were used by Simon[8] and recently by Robinson[9].

Theorem 2.1. Let the N-particle interaction $U_N(x_1, \dots, x_N)$ associated with a two-body potential, highly singular at the origin and bounded from below (see (2.4)), is such that $U_N \in L^\infty(K)$ for each compact $K \subset \Lambda^N \setminus S_N$, where $S_N$ is the singularity set (2.5). Then for the N-particle system enclosed in a bounded region $\Lambda \subset \mathbb{R}^\nu$ the Friedrichs extensions and the form sum extensions of the operators $H_0 + U_N$ and $H_0 + U$ are equal one to another if $\nu \geq 3$, i.e.,

$$(h_0 + u)^{\sim} = \tilde{h}_0 + \tilde{u} = (h_0 + u_U)^{\sim}$$

or

$$(H_0 + U_N)_F = H_0 \dotplus U_N = (H_0 + U)_F . \tag{2.11}$$

P r o o f. Let us primarily prove the equality $(h_0 + u)^{\sim} = \tilde{h}_0 + \tilde{u}$ corresponding to $(H_0 + U_N)_F = H_0 \dotplus U_N$. As $(h_0 + u)^{\sim} \subseteq \tilde{h}_0 + \tilde{u}$ (see (2.10)), to establish the equality, it suffices to prove that $D = D(H_0) \cap D(U_N)$ is a core not only for $(h_0 + u)^{\sim}$ but also for $\tilde{h}_0 + \tilde{u}$, i.e., $[(\tilde{h}_0 + \tilde{u}) \restriction D]^{\sim} = \tilde{h}_0 + \tilde{u}$ . Therefore for every $\psi \in Q(h_0 + u)$ one should construct a sequence $\{\psi_n\} \in D$ such that

$$\lim_{n\to\infty} \| \psi - \psi_n \| = 0 \text{ and } \lim_{n\to\infty} (\tilde{h}_0 + \tilde{u})[\psi - \psi_n] = 0 . \tag{2.12}$$

If $\psi \in Q(\tilde{h}_0 + \tilde{u})$ has a compact support $K \subset \Lambda^N \setminus S_N$, it is easy to construct a sequence $\{\psi_n\} \in D$ such that all $\psi_n$ have $\operatorname{supp}\psi_n \subset K'$ with

$K\subset K'\subset \Lambda^N\setminus S_N$ and

$$\lim_{n\to\infty}\|\psi-\psi_n\|=0\,,\quad \lim_{n\to\infty}\tilde{h}_0[\psi-\psi_n]=0\,. \tag{2.13}$$

Then from the estimate

$$\tilde{u}[\psi-\psi_n]<\|U_N(x_1,\dots,x_N)\|_{L^\infty(K')}\cdot\|\psi-\psi_n\|^2$$

it follows that $\lim_{n\to\infty}\tilde{u}[\psi-\psi_n]=0$. Therefore in this case $\psi\in Q(\tilde{h}_0+\tilde{u})$ is approximated in the desired manner.

Next consider the general case when $\psi\in Q(\tilde{h}_0+\tilde{u})$. Let us introduce an auxiliary sequence $\{w_n(x)\}$ with the following properties:

a) $w_n(x)\in C_0^\infty(\Lambda_1)$; $0\le w_n(x)\le 1, \Lambda\subset\Lambda_0\subset\Lambda_1\subset R^\nu$;

b) $w_n(x)=1$ for $\{x\in\Lambda_0:|x|>\frac{1}{n}\}$;

$\quad w_n(x)=0 \qquad \{x\in\Lambda_0:|x|<\frac{1}{2n}\}$;

c) $|\nabla w_n(x)|<\frac{A}{|x|}$ for $\{x\in\Lambda_0:|x|<\frac{1}{n}\}$;

$\quad|\nabla w_n(x)|<C \qquad \{x\in R^\nu: x\in\Lambda_1\setminus\Lambda_0\}$.

Bounded regions $\Lambda_0$ and $\Lambda_1$ both are supposed to be spherically symmetric and the origin $0\in\Lambda$. The region $\Lambda_0$ has radius $r(\Lambda_0)=d(\Lambda)+\delta$, and $\Lambda_1$: $r(\Lambda_1)=d(\Lambda)+2\delta$. Here $d(\Lambda)$ denotes the diameter of the container $\Lambda\subset R^\nu$, i.e., $d(\Lambda)=\mathrm{Sup}_{x,y\in\Lambda}|x-y|$, and $\delta>0$ is a fixed number. Now if $\psi\in Q(\tilde{h}_0+\tilde{u})$ then $\psi_n'=W_n\psi\equiv\prod_{1\le i<j\le N}w_n(x_i-x_j)\psi$ is also in $Q(\tilde{h}_0+\tilde{u})$, moreover it has the compact support $\mathrm{supp}\,\psi_n'\subset\Lambda^N\setminus S_N$. Thus, every $\psi_n'$ can be approximated in the desired manner by a sequence of the functions $\{\psi_k^{(n)}\}\in D$ as it was stated above. But

$$(\tilde{h}_0+\tilde{u})[\psi-\psi_n']=(\tilde{h}_0+\tilde{u})[(\psi-\psi_k^{(n)})+(\psi_k^{(n)}-\psi_n')],$$



therefore we have only to prove that

$$\lim_{n\to\infty}\|\psi-\psi_n'\|=0,\ \lim_{n\to\infty}\tilde{u}[\psi-\psi_n']=0,\ \lim_{n\to\infty}\tilde{h}_0[\psi-\psi_n']=0\,. \tag{2.14}$$

The first and the second limits easily follow from the dominated convergence theorem/13/. To prove the third limit we note first that $\psi\in Q(\tilde{h}_0+\tilde{u})$ implies $\psi\in Q(\tilde{h}_0)$. So, $\partial_{x_i}\psi$ exists in the sense of distributions (see Kato/1/ V, §5 and VI, §4), then the vector $\partial_{x_i}\psi\in L^2(\Lambda^N)$, i.e.,

$$\tilde{h}_0[\psi]=\frac{1}{2m}\sum_{i=1}^{N}(\partial_{x_i}\psi,\partial_{x_i}\psi),\quad \psi\in Q(\tilde{h}_0) \tag{2.15}$$

and $\mathrm{Supp}\,\psi\subset\Lambda^N$. Therefore, substituting $(\psi-\psi_n')\in Q(\tilde{h}_0)$ into (2.15) we obtain:

$$\tilde{h}_0[\psi-\psi_n']\le\frac{1}{m}\sum_{i=1}^{N}\{\|(\partial_{x_i}W_n)\psi\|^2+\|(1-W_n)\partial_{x_i}\psi\|^2\}. \tag{2.16}$$

Now $\lim_{n\to\infty}\|(1-W_n)\partial_{x_i}\psi\|=0$ follows from the dominated convergence theorem. The first term in the right-hand side of (2.16) can be estimated from above:

$$\frac{1}{m}\sum_{i=1}^{N}\|(\partial_{x_i}W_n)\psi\|^2\le\frac{2^{N+1}}{m}\int_{\Lambda^N}dx_1\dots dx_N\sum_{1\le i<j\le N}|\partial_{x_i}w_n(x_i-x_j)|^2|\psi|^2. \tag{2.17}$$

Note, that according to the conditions (2.13)(b) and (c) $|\partial_{x_i}w_n(x_i-x_j)|$ does not equal zero only if $\frac{1}{2n}<|x_i-x_j|<\frac{1}{n}$ or $(x_i-x_j)\subset\Lambda_1\setminus\Lambda_0$. But for the latter case $|x_i-x_j|>d(\Lambda)$, so

$\psi(x_1,\dots,x_N)|_{|x_i-x_j|>d(\Lambda)}=0$ because if $\psi\in Q(h_0)$ then $\operatorname{Supp}\psi\subset\Lambda^N$. Hence from (2.17) we have

$$\sum_{i=1}^{N}\|(\partial_{x_i}W_n)\psi\|^2\le 2^{N+1}\sum_{1\le i<j\le N}\int_{\{\Lambda^N:|x_i-x_j|<\frac{1}{n}\}}dx_1\dots dx_N|\partial_{x_i}w_n(x_i-x_j)|^2|\psi|^2. \tag{2.18}$$

Moreover, from (2.13) (c) it follows that

$$\sum_{1\le j<i\le N}\int_{\{\Lambda^N:|x_i-x_j|<\frac{1}{n}\}}dx_1,\dots dx_N|\partial_x w_n(x_i-x_j)|^2|\psi|^2\le$$
$$\le A^2\sum_{1\le i<j\le N}\int_{\{\Lambda^N:|x_i-x_j|<\frac{1}{n}\}}dx_1\dots dx_N\frac{|\psi|^2}{|x_i-x_j|^2}. \tag{2.19}$$

For the evaluation of the right-hand side of (2.19) we need the following lemmas.

L e m m a 2.1. Let $\Lambda\subset\mathbf{R}^\nu$ be a bounded region and operator T be defined on the set $C_0^\infty(\Lambda)$ as $T=-\Delta$. Then for $\nu\ge3$ the following inequality is valid in the sense of quadratic forms:

$$H_0(\Lambda)=(T)_F\ge\frac{1}{4|x|^2},\ \text{i.e.},(\psi,T\psi)^\sim\ge(\psi,\frac{1}{4|x|^2}\psi)^\sim. \tag{2.20}$$

P r o o f. The proof is a straightforward generalization of arguments given by Courant and Hilbert in /14/. For $\psi\in C_0^\infty(\Lambda)$ $(\psi,T\psi)=(\nabla\psi,\nabla\psi)$ then for $\phi=|x|^{1/2}\psi$

$$\int_\Lambda d^\nu x\sum_{a=1}^{\nu}(\partial_a\psi)^2>\frac{1}{4}\int_\Lambda d^\nu x\frac{\phi^2}{|x|^3}-\frac{1}{2}\int_\Lambda d^\nu x\frac{1}{|x|^2}\frac{\partial}{\partial|x|}\phi^2.$$

If we take into account that $\operatorname{Supp}\phi\subset\Lambda$ and $\psi\in C_0^\infty(\Lambda)$, then for $\nu\ge3$

$$(\psi,T\psi)\ge(\frac{1}{4}+\frac{\nu-3}{2})\int d^\nu x\frac{|\psi|^2}{|x|^2}.$$



The closure gives us desirable inequality (2.20).

R e m a r k 2.1. In the same manner it is easy to prove that (2.20) is valid in the case of many variables: if $\Lambda\subset\mathbf{R}^\nu$ is a bounded region and if operators $T_i$ $(i=1,2,\dots,N)$ are defined on the set of functions $\psi(x_1,\dots,x_N)\in C_0^\infty(\Lambda^N)$ by $T_i=-\Delta_i$, then for $\nu\ge3$

$$H_0^{(i)}(\Lambda^N)=(T_i)_F\ge\frac{1}{4|x_i|^2}=V_i,\ \text{i.e.},(\psi,T_i\psi)^\sim\ge(\psi,V_i\psi)^\sim \tag{2.21}$$

for $\forall\, i=1,2,\dots,N$.

L e m m a 2.2. Let $\Lambda\subset\mathbf{R}^\nu$ be a region as in Lemma 2.1 and operators $T_{kn}$ are defined on the set $C_0^\infty(\Lambda^N)$ by $T_{kn}=(p_k-p_n)^2$, where $p_k=\frac{1}{i}\partial_{x_k}$, $p_n=\frac{1}{i}\partial_{x_n}$. Let operator $V_{kn}=\frac{1}{4|x_k-x_n|^2}$ then for $\nu\ge3$ and $\forall k\ne n\in(1,2,\dots,N)$:

$$(T_{kn})_F\ge4V_{kn}\qquad\text{or}\ (\psi,T_{kn}\psi)^\sim\ge4(\psi,V_{kn}\psi). \tag{2.22}$$

P r o o f. Let us introduce, in the configurational space $\Lambda^N\subset\mathbf{R}^{\nu N}$, new variables $(x_1,\dots,\xi_{(k)},\dots,\eta_{(n)},\dots,x_N)\leftrightarrow(x_1,\dots,x_k,\dots,x_n,\dots,x_N)$, $\xi_{(k)}=x_k-x_n$, $\eta_{(n)}=x_k+x_n$. Then for $\forall\psi\in C_0^\infty(\Lambda^N)$ we have

$$(\psi,(p_k-p_n)^2\psi)=4(\partial_{\xi_{(k)}}\phi,\partial_{\xi_{(k)}}\phi), \tag{2.23}$$

here $\phi(x_1,\dots,x_k-x_n,\dots,x_k+x_n,\dots,x_N)=\psi(x_1,\dots,x_N)$, so, $\phi(x_1,\dots,\xi_{(k)},\dots,\eta_{(n)},\dots,x_N)\in C_0^\infty(\Lambda_*^N)$. Using Remark 2.1 we get

$$(\partial_{\xi_{(k)}}\phi,\partial_{\xi_{(k)}}\phi)>\frac{1}{4}(\phi,\frac{1}{|\xi_{(k)}|^2}\phi). \tag{2.24}$$

Then substituting (2.24) into (2.23) and turning to the old variables $(x_1,\dots,x_N)$ we obtain (2.22).

L e m m a 2.3. Let $\Lambda \subset \boldsymbol{R}^{\nu}$ be a bounded region and let the operator $T_N$ be defined by $T_N = \sum_{k=1}^{N} \frac{1}{2m} p_k^2$ with $D(T_N) = C_0^\infty(\Lambda^N)$, where $p_k = \frac{1}{i}\partial_{x_k}$, then the following inequality is valid in the sense of quadratic forms for $\nu \geq 3$:

$$H(\Lambda^N) = (T_N)_F \geq \sum_{1\leq i<j\leq N} \frac{1}{2m(N-1)|x_i - x_j|^2}. \qquad (2.25)$$

P r o o f. For $\psi \in C_0^\infty(\Lambda^N)$ we rewrite the form $t[\psi] = (\psi, T\psi)$ as

$$t[\psi] = (\psi, \sum_{1\leq k<n\leq N} \frac{(p_k + p_n)^2}{2m(N-1)}\psi) + (\psi, \sum_{1\leq k<n\leq N} \frac{(p_k - p_n)^2}{2m(N-1)}\psi). \qquad (2.26)$$

The arguments given in Lemma 2.2 show that the first quadratic form in the right-hand side of (2.26) is positive. The second form can be estimated from below as was shown in Lemma 2.2:

$$(\psi, \sum_{1\leq k<n\leq N} \frac{(p_k - p_n)^2}{2m(N-1)}\psi) \geq \frac{1}{2m(N-1)}(\psi, \sum_{1\leq k<n\leq N} \frac{1}{|x_k - x_n|^2}\psi). \qquad (2.27)$$

The substitution (2.27) into (2.26) and the closure give us the inequality (2.25).

Corollary 2.1. From Lemma 2.3 it follows that $Q(\tilde{t}) \subset Q(\sum_{1\leq i<j\leq N} \frac{1}{2m(N-1)|x_i - x_j|^2})$ if $\nu \geq 3$. But $Q(\tilde{t}) = Q(\tilde{h}_0)$, so, if $\psi \in Q(\tilde{h}_0)$, then $\psi \in D(\frac{1}{|x_i - x_j|^2})$ for $\forall i \neq j \in (1,2,\ldots,N)$ and $\nu \geq 3$.

Thus, if we take into account that in inequality (2.19) $\psi \in Q(\tilde{h}_0) \cap Q(\tilde{u})$, then Co-



rollary 2.1 gives

$$\sum_{1\leq i<j\leq N} \frac{|\psi|^2}{|x_i - x_j|^2} \in L^1(\Lambda^N). \qquad (2.28)$$

Note that for $\lim_{n\to\infty} \text{mes}\{\Lambda^N : |x_i - x_j| < \frac{1}{n}$ for $i \neq j \in (1,2,\ldots,N)\} = 0$, hence (2.28) shows that the right-hand side of (2.19) tends to zero for $\forall \psi \in Q(\tilde{h}_0) \cap Q(\tilde{u})$ as $n \to \infty$, i.e., $\lim_{n\to\infty} \tilde{h}_0[\psi - \psi_n'] = 0$ so (2.14) is proved. Therefore (see (2.11))

$$(h_0 + u)^\sim = \tilde{h}_0 + \tilde{u},$$

or

$$(H_0 + U_N)_F = H_0 \dot{+} U_N. \qquad (2.29)$$

Now from $U_N \subset U(\Lambda^N)$ (2.6), we obtain

$$(h_0 + u_U)^\sim \supseteq (h_0 + u)^\sim. \qquad (2.30)$$

On the other hand, it is well-known (see (2.10) and Proposition 2.1) that

$$(h_0 + u_U)^\sim \subseteq \tilde{h}_0 + \tilde{u}_U = \tilde{h}_0 + \tilde{u}. \qquad (2.31)$$

So the comparison of (2.29) with (2.31) gives (2.11):

$$(h_0 + u)^\sim = \tilde{h}_0 + \tilde{u} = (h_0 + u_U)^\sim.$$

This completes the proof of Theorem 2.1.

## 3. CONCLUSION REMARKS

The coincidences of two canonical ways for definition of self-adjoint extension for N-particle Hamiltonian in container $\Lambda \subset \boldsymbol{R}^{\nu}$ ($\nu \geq 3$) is of practical use in a subsequent paper (part II). It allows up to prove the convergence theorems for the cut-off Hamiltonians $H_L(\Lambda^N)$ and partition functions $Z_\beta[H_L(\Lambda^N)]$ when the cut-off parameter is removed to infinity.

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