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E4 - 9461

V.A.Zagrebnov

ON STATISTICAL MECHANICS OF SYSTEMS WITH HIGHLY SINGULAR TWO-BODY POTENTIALS

(Convergence Theorems)

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ON STATISTICAL MECHANICS OF SYSTEMS WITH HIGHLY SINGULAR TWO-BODY POTENTIALS

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Загребнов В.А.

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О статистической механике систем с существенно сингулярными парными потенциалами (теоремы сходимости)

Рассматривается статистическая механика для систем с существенно сингулярными парными потенциалами. Обсуждается случай частиц с "точечными" парными сердцевинами (потенциалы типа Леннарда-Джонса). Дано строгое математическое обоснование для использования этой физической идеализации с помощью теорем о сходимости при снятии обрезания.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований

Дубна 1976

Zagrebnov V.A.

E4 - 9461

On Statistical Mechanics of Systems with Highly Singular Two-Body Potentials

A natural cut-off procedure for two-body highly singular potentials, discussed in the previous paper (part I), is proposed. The main result is the proof of a convergence theorem for partition sum (or the free energies) when the cut-off parameter is removed to infinity. The question of stability of the cut-off interactions is also discussed. These results are illustrated by a consideration of the Lennard-Jones potential (12-6).

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research

Dubna 1976

1. *INTRODUCTION. CONVERGENCE OF CUT-OFF HAMILTONIANS*

As was pointed out in ref./1/ (part 1), the highly singular two-body potentials are an idealization. So, a cut-off procedure is very natural when we start to consider the physical problems connected with highly singular interactions. Therefore, the Hamiltonian $H_L(\Lambda^N)$ generated by the cut-off interaction $U_N^L(x_1, \dots, x_N) = \frac{1}{2}\sum_{i \neq j}^{N} \Phi_L(x_i - x_j)$ in some sense is close to the original Hamiltonian $H(\Lambda^N)$ defined in the previous work/1/. Before formulating the corresponding results we need some preliminaries.

From the definition of the cut-off interactions:

$$\Phi_L(x) = \begin{cases} \Phi(x) & \{x : \Phi(x) \leq L\} \\ L & \{x : \Phi(x) > L\} \end{cases} \qquad (1.1.)$$

it is clear that $\{U_N^L(x_1, \dots, x_N)\}$ is a monotone sequence of functions $U_N^L(x_1, \dots, x_N) \in L^{\infty}(\Lambda^N)$ such that at each point of $\Lambda^N \setminus S_N$ it converges to $U_N(x_1, \dots, x_N)$

$$\lim_{L \to \infty} U_N^L(x_1, \dots, x_N) = U_N(x_1, \dots, x_N) \quad \text{for} \quad (x_1, \dots, x_N) \in \Lambda^N \setminus S_N .$$

According to the construction of $\{U_N^L(x_1, \dots, x_N)\}$ it is evident that for $\mathrm{Supp}[U_N(x_1, \dots, x_N) - U_N^L(x_1, \dots, x_N)] = S_N + \Sigma_L$

$$\lim_{L\to\infty} \text{mes}\,(S_N + \Sigma_L) = 0 . \qquad (1.2)$$

Now let us consider the sequence $\{U_N^L\}$ as operators in the Hilbert space of states $\mathcal{H}(\Lambda^N) = L^2(\Lambda^N)$.

L e m m a 1.1. Let the cut-off parameters $\{L\}$ form a nondecreasing family, then the functions $\{U_N^L(x_1, \dots, x_N)\}$ form in the Hilbert space $\mathcal{H}(\Lambda^N)$ a monotonic nondecreasing sequence of bounded self-adjoint operators, i.e., for $\forall L < \infty$ $U_N^L \in \mathcal{B}(\mathcal{H})$ and for $L \le L'$ $U_N^L \le U_N^{L'}$ in the sense of quadratic forms.

P r o o f. The Lemma is a straightforward consequence of definition (1.1).

L e m m a 1.2. Let the operators $H_L(\Lambda^N)$ be defined for each cut-off parameter L as the algebraic sum $H_L(\Lambda^N) = H_0(\Lambda^N) + U_N^L$ then these operators are self-adjoint and $D(H_L) = D(H_0)$.

P r o o f. The Lemma is an immediate consequence of the well-known Kato-Rellich Theorem (see Kato /2/ V,§ 4). From Lemma 1.1 the operators $U_N^L \in \mathcal{B}(\mathcal{H})$ and are self-adjoint, hence, $D(U_N^L) \supset D(H_0)$, so operators U_N^L are Kato-small perturbations to the self-adjoint kinetic-energy operator $H_0(\Lambda^N)$.

Corollary 1.1. For nondecreasing family of cut-off parameters $\{L\}$ the self-adjoint operators $\{H_L(\Lambda^N)\}$ form, in the sense of quadratic form, a monotonic nondecreasing sequence, bounded from above by the Hamiltonian $H(\Lambda^N) = (H_0(\Lambda^N) + U_N)_F$ /1/

$$H_{L_1} \le H_{L_2} \le \dots \le H, \quad (L_1 \le L_2 \le \dots). \qquad (1.3.)$$

R e m a r k 1.1. The densely defined, closed symmetric quadratic forms $\tilde{u}_L[\psi]$ associated with bounded self-adjoint operators U_N^L are obviously bounded for $\forall L$. Hence they are also $\tilde{h}_0$ -bounded, so for $\forall L$:

$$\tilde{h}_L = (h_0 + u_L)^{\sim} = \tilde{h}_0 + \tilde{u}_L . \qquad (1.4)$$

Proposition 1.1. (Kato /2/ VIII, §3). Let $\{h_n\}$ be a nondecreasing sequence of densely defined, closed symmetric quadratic forms bounded from below by a constant γ and dominated from above by a similar form $\tilde{h}$:

$$\gamma \le \tilde{h}_1 \le \tilde{h}_2 \le \dots \le \tilde{h} ,$$

and let H_n be the self-adjoint operators associated with $\tilde{h}_n$. Then: (i) the sequence of semibounded from below self-adjoint operators $\{H_n\}$ converges strongly in the generalized sense to a self-adjoint operator H' which is also bounded from below:

$$\text{g.s.s.} - \lim_{n\to\infty} H_n = H',$$

(ii) if $\tilde{h}'[\psi] = (\psi, H'\psi)^{\sim}$ is the associated symmetric form, we have

$$\tilde{h}_n \le \tilde{h}' \le \tilde{h} \qquad \text{for} \quad \forall n = 1, 2, \dots,$$

(iii) for $\forall \psi \in Q(\tilde{h}')$ the form $\tilde{h}'[\psi]$ is the limit of $\{\tilde{h}_n\}$, i.e.,

$$\lim_{n\to\infty} \tilde{h}_n[\psi] = \tilde{h}'[\psi] \qquad \text{for} \quad \psi \in Q(\tilde{h}').$$

This completes the preliminaries. Now we can prove the main results of this section. We start with

R e m a r k 1.2. From Proposition 1.1 and Corollary 1.1

it follows that the cut-off Hamiltonians $H_L(\Lambda^N)$ for $L\to\infty$ converge in the generalized strong sense to self-adjoint operator H' with the properties (i)-(iii), where $\tilde h[\psi] = (\psi, (H_0 + U_N)\psi)^{\sim}$.

Now we can prove that under the conditions of Theorem 2.1 /1/ the Hamiltonians $H'(\Lambda^N) = \text{g.s.s.}-\lim_{L\to\infty} H_L(\Lambda^N)$ and $H(\Lambda^N)$ are equal one to another.

Remark 1.3. (Kato /2/, VIII § 4). From the monotonicity of the sequence $\{\tilde h_L[\psi]\}$ (1.4) (or $H_L(\Lambda^N)$ (1.3)) and $\tilde h_L[\psi] \le \tilde h[\psi]$ it follows that $\lim_{L\to\infty} \tilde h_L[\psi]$ exists at least for $\forall\, \psi \in Q(\tilde h_0)$. Let us define a form

$$h''[\psi] = \lim_{L\to\infty} \tilde h_L[\psi], \quad \psi \in Q(h'') \tag{1.5}$$

with $Q(h'')$ consisting of all $\psi \in \bigcap_L Q(\tilde h_L)$ such that limit (1.5) exists. Point (iii) of Proposition 1.1. shows that $\tilde h'[\psi]$ is a particular case of the general limiting definition (1.5), so $h''[\psi] \supset \tilde h'[\psi]$. If we take into account Remark 1.1, then the limiting form $h''[\psi]$ (1.5) can be represented also (see (1.4)) as

$$h''[\psi] = \tilde h_0[\psi] + \lim_{L\to\infty} (\psi, U_N^L \psi)^{\sim} \tag{1.6}$$

for each $\psi \in Q(\tilde h_0)$ such that the limit in the right-hand side of (1.6) exists.

Corollary 1.2. As follows from definition (1.1) and Lemma 1.1, the operators $\{U_N^L\}$ and the associated sequence of quadratic forms $\tilde u_L[\psi] = (\psi, U_N^L \psi)^{\sim}$ satisfy the conditions of Propositions 1.1. So, g.s.s. $-\lim_{L\to\infty} U_N^L = U'$ and $\lim_{L\to\infty} \tilde u[\psi] = \tilde u'[\psi]$ for $\psi \in Q(\tilde u')$. But in this case it is easy to show that $U' = U(\Lambda^N)$.

Lemma 1.3. Let the cut-off parameter L tends to infinity, then the nondeacresing sequence of bounded self-adjoint operators $\{U_N^L\}$ (1.1) converges in generalized strong sense to the closure of the singular interaction operator $\tilde U_N = U(\Lambda^N)$.

Proof. As was pointed out, the operator of the N-particle singular interaction $U_N(x_1, \dots, x_N)$, $D(U_N) = C_0(\Lambda^N \setminus S_N)$ (see /1/) is essentially self-adjoint, i.e., it has only one self-adjoint extension which coincides with its closure so

$$D(U_N) = \text{Core}\, U(\Lambda^N) \qquad \text{i.e.,}\ (U(\Lambda^N) \restriction D(U_N))^{\sim} = U(\Lambda^N). \tag{1.7}$$

Hence $U(\Lambda^N) \restriction D(U_N) = U_N$ and for $\forall\, \psi \in D(U_N)$

$$\begin{aligned} &\int_{\Lambda^N} dx_1 \dots dx_N [U(\Lambda^N) - U_N^L]^2 |\psi|^2 = \\ &= \int_{\Lambda^N} dx_1 \dots dx_N (U_N - U_N^L)^2 |\psi|^2 \le \\ &\le 2 \int_{S_N + \Sigma_L} dx_1 \dots dx_N [U_N^2 + (U_N^L)^2] |\psi|^2, \end{aligned} \tag{1.8}$$

where $S_N + \Sigma_L = \text{Supp}\,(U_N - U_N^L)$, so the right-hand side of (1.8) for $L\to\infty$ tends to zero, because $\lim_{L\to\infty} \text{mes}\,(S_N + \Sigma_L) = 0$ (1.2). Therefore for $\forall\, \psi \in D(U_N) = \text{Core}\, U(\Lambda^N)$

$$\lim_{L\to\infty} U_N^L \psi = U\psi. \tag{1.9}$$

But if the sequence of self-adjoint operators $\{U_N^L\}$ converges for $L\to\infty$ on the dense in the space $\mathcal{H}(\Lambda^N)$ set $D(U_N)$ to the self-adjoint operator $U(\Lambda^N)$ and if $D(U_N)$ is a core of $U(\Lambda^N)$, then, as is well-known, $\{U_N^L\}$ converges to the operator $U(\Lambda^N)$ strongly in the generalized sense (see, e.g., Kato [2], VIII, § 1):

$$\text{g.s.s.} - \lim_{L\to\infty} U_N^L = U(\Lambda^N) . \tag{1.10}$$

Corollary 1.3. The sequence $\tilde{u}_L[\psi] = (\psi, U_N^L \psi)^\sim$ for $L \to \infty$ and $\psi \in Q(\tilde{u})$ converges to the form $\tilde{u}[\psi] = (\psi, U\psi)^\sim$, so the form $\tilde{u}'[\psi] = \tilde{u}[\psi]$ (see Corollary 1.2). Therefore for $\forall \psi \in Q(\tilde{h}_0) \cap Q(\tilde{u})$ (see (1.6)):

$$\tilde{h}''[\psi] = \tilde{h}_0[\psi] + \lim_{L\to\infty} (\psi, U_N^L \psi)^\sim = \tilde{h}_0[\psi] + \tilde{u}[\psi] . \tag{1.11}$$

From (1.11), Remarks 1.2, 1.3 and point (ii) of Proposition 1.1., it follows that

$$\tilde{h}_0[\psi] + \tilde{u}[\psi] \supset \tilde{h}'[\psi] \leq \tilde{h}[\psi] = (h_0 + u)^\sim [\psi] . \tag{1.12}$$

But the quadratic forms in the left and right-hand sides of (1.12) coincide (see Theorem 2.1 [1]), so

$$\tilde{h}'[\psi] = \tilde{h}[\psi] . \tag{1.13}$$

From the uniqueness of the self-adjoint operators associated with the forms $\tilde{h}'[\psi]$, $\tilde{h}[\psi]$ (1.13) (see proposition 1.1) it follows that $H' = H(\Lambda^N)$, hence (see Remark 1.2):

$$\text{g.s.s.} - \lim_{L\to\infty} H_L(\Lambda^N) = H(\Lambda^N) . \tag{1.14}$$

Therefore, in the present section we have proved the following

Theorem 1.1. Let $H_L(\Lambda^N) = H_0(\Lambda^N) + U_N^L$ be a self-adjoint cut-off Hamiltonian corresponding to the nonsingular N-particle interaction $U_N^L(x_1, \dots, x_N)$ then, for the cut-off parameter L going to infinity, the sequence $\{H_L(\Lambda^N)\}$ converges to the Hamiltonian $H(\Lambda^N)$ strongly in the generalized sense.

Now we are interested in statistical mechanics of systems defined by $H_L(\Lambda^N)$ and $H(\Lambda^N)$. As a first step we mention that from (1.14) the convergence of $\exp(-\beta H_L)$ follows immediately

Corollary 1.4. For $\beta > 0$:

$$s - \lim_{L\to\infty} \exp(-\beta H_L) = \exp(-\beta H) \tag{1.15}$$

uniformly for β in any finite interval of the positive axis R_+^1.

It is clear that (1.15) is insufficient for the proof of the convergence of partition functions $Z_\beta[H_L(\Lambda^N)]$ to $Z_\beta[H(\Lambda^N)]$. But in the next section we will show that (1.15) and some properties of the sequence $\{H_L(\Lambda^N)\}$ allow us to prove the convergence of $\{\exp(-\beta H_L)\}$ in the trace-class topology.

2. *CONVERGENCE THEOREM FOR PARTITION FUNCTIONS* $Z_\beta[H_L(\Lambda^N)]$

To treat the quantum statistical mechanics in a bounded region $\Lambda \subset R^\nu$ of an arbitrary shape it will be very useful

Proposition 2.1. (Weyl's min-max principle, see, e.g., Ruelle [3]). Let A be a self-adjoint operator bounded from below. Let

$$\mu_n(A) = \inf_{\substack{M \\ \dim M = n}} \{ \sup_{\substack{\psi \in M \subset Q(A) \\ \|\psi\| = 1}} (\psi, A\psi) \} . \tag{2.1}$$

Then either (a) μ_n is the n-th eigenvalue from the bottom of the spectrum $\sigma(A)$ (counting multiplicity) or (b) $\mu_n = \inf \sigma_{ess}(A)$, where $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_{disc}(A)$, here $\sigma_{disc}(A)$ is the discrete part of the spectrum $\sigma(A)$. In particular, $\sigma_{ess}(A) = \phi$ if and only if $\lim_{n\to\infty} \mu_n(A) = \infty$.

Now we recall the definition of trace-class operators $\mathfrak{C}_1$.

Definition 2.1. (see, e.g., Reed and Simon /4/). Let $\mathcal{B}(\mathcal{H})$ be the space of all bounded operators on a separable Hilbert space $\mathcal{H}$. The Banach space $\mathfrak{C}_1 \subset \mathcal{B}(\mathcal{H})$ of compact operators with finite $\|\cdot\|_1$-norm:

$$\|A\|_1 = \sum_{k=1}^{\infty} \lambda_k < \infty, \quad A \in \mathfrak{C}_1, \tag{2.2}$$

where the λ_k denote the non-zero repeated singular values of A (i.e., the non-zero eigenvalues of $|A| = \sqrt{A^*A}$), is called the trace-class and $\|\cdot\|_1$ is the trace-norm.

In particular for any positive self-adjoint operator $A \in \mathfrak{C}_1$

$$\|A\|_1 = \mathrm{Tr}\, A = \sum_{k=1}^{\infty} (\psi_k, A\psi_k) = \sum_{n=1}^{\infty} \mu_n(A), \tag{2.3}$$

where $\{\psi_k\}$ is any orthonormal system in $\mathcal{H}$ and $\{\mu_n(A)\}$ are eigenvalues of A (counting multiplicity). These preliminaries allow us to prove the following statement which defines statistical mechanics of the system under consideration (see section 1 and /1/).

Lemma 2.1. Let $\Lambda \subset \boldsymbol{R}^\nu$ be a bounded region of an arbitrary shape and U_N be a highly singular N-particle interaction corresponding to "point" hard core particles (see section 1 /1/). Hamiltonian $H(\Lambda^N)$ of the system is defined as Friedrichs extension of the algebraic sum $H_0 + U_N$ (see /1/), then

(i) the spectrum $\sigma(H)$ is purely discrete,

(ii) for $\beta > 0$ $\exp(-\beta H) \in \mathfrak{C}_1$,

(iii) the partition function $Z_\beta[H(\Lambda^N)] = \mathrm{Tr}\exp[-\beta H(\Lambda^N)]$ is nondecreasing for Λ, i.e.,

$$Z_\beta[H(\Lambda^N)] \le Z_\beta[H(\Lambda'^N)] \quad \text{if} \quad \Lambda \subset \Lambda'. \tag{2.4}$$

Proof. (i) The N-particle interaction $U_N(x_1,\ldots,x_N)$ for highly singular two-body potentials with "point" hard core, acceptable in statistical mechanics, is known to be at least semibounded from below (see /1/ and section 3):

$$U_N(x_1,\ldots,x_N) > -a \quad \text{for} \quad \forall (x_1,\ldots,x_N) \in \Lambda^N. \tag{2.5}$$

Therefore for $\forall \psi \in D(H_0) \cap D(U_N)$

$$h[\psi] = (\psi, H_0\psi) + (\psi, U_N\psi) \ge h_0[\psi] - a(\psi,\psi),$$

or for $\forall \psi \in Q(\tilde{h})$

$$\tilde{h}[\psi] \ge \tilde{h}_0[\psi] - a(\psi,\psi). \tag{2.6}$$

So, from the Weyl's min-max principle (Proposition 2.1)

$$\mu_n(H(\Lambda^N)) \ge \mu_n(H_0(\Lambda^N)) - a. \tag{2.7}$$

Let us now consider a cube $\Lambda_+ \subset \boldsymbol{R}^\nu$ and $\Lambda \subset \Lambda_+$. It is easy to check that in this case the spectrum $\sigma(H_0(\Lambda_+^N))$ is purely discrete and $\lim_{n\to\infty} \mu_n(H_0(\Lambda_+^N)) = \infty$. Thus the same is true for the Hamiltonian $H(\Lambda_+^N)$ (see (2.7)). Moreover, it is clear that for $\Lambda \subset \Lambda_+$ the Hilbert space $\mathcal{H}(\Lambda^N)$ is in a natural way imbedded into $\mathcal{H}(\Lambda_+^N)$, so if $\psi \in D(H(\Lambda^N))$ it is also in $D(H(\Lambda_+^N))$. From here and Weyl's min-max principle (Proposition 2.1), we have

$$\mu_n(H(\Lambda^N)) \geq \mu_n(H(\Lambda_+^N)), \tag{2.8}$$

hence $\lim_{n\to\infty} \mu_n(H(\Lambda^N)) = \infty$, i.e., the spectrum $\sigma(H(\Lambda^N))$ is purely discrete.

(ii) Straightforward calculations show that for the cube $\Lambda_+ \subset \boldsymbol{R}^\nu$ $\exp[-\beta H_0(\Lambda_+^N)] \in \mathfrak{C}_1$, hence $\exp[-\beta H(\Lambda_+^N)] \in \mathfrak{C}_1$ (see (2.7)). From inequality (2.8) it follows that the same is true for $\exp[-\beta H(\Lambda^N)]$ i.e., for $\beta > 0$ $\exp(-\beta H) \in \mathfrak{C}_1$. Therefore (see Definition 2.1)

$$Z_\beta[H(\Lambda^N)] = \mathrm{Tr}\exp[-\beta H(\Lambda^N)] = \sum_{n=1}^{\infty} \exp[-\beta \mu_n(H(\Lambda^N))]. \tag{2.9}$$

(iii) Let us consider $\Lambda \subset \Lambda'$ then from the discussion of point (i) it follows

$$\mu_n(H(\Lambda^N)) \geq \mu_n(H(\Lambda'^N)),$$

thus inequality (2.4) is an immediate consequence of (2.9). This completes the proof.

Corollary 2.1. The cut-off in the singular interaction U_N (see (1.1)) does not change its semiboundedness property (2.5): hence

$$U_N^L(x_1, \ldots, x_N) \geq -a, \ \forall (x_1, \ldots, x_N) \in \Lambda^N.$$

Therefore the self-adjoint cut-off Hamiltonians $H_L(\Lambda^N) = H_0(\Lambda^N) + U_N^L$ (see Section 1):

(i) have a purely discrete spectrum,

(ii) for $\beta > 0$ $\exp[-\beta H_L(\Lambda^N)] \in \mathfrak{C}_1$,

(iii) $Z_\beta[H_L(\Lambda^N)] = \mathrm{Tr}\exp[-\beta H_L(\Lambda^N)]$ is a nondecreasing function of Λ.

L e m m a 2.2. If $L \leq L'$ then for the corresponding trace-class norms:

$$\|\exp(-\beta H_{L'})\|_1 \leq \|\exp(-\beta H_L)\|_1. \tag{2.10}$$

P r o o f. From corollary 2.1 for $L \leq L'$ we get

$$H_L(\Lambda^N) \leq H_{L'}(\Lambda^N), \quad D(H_L) = D(H_{L'}),$$

then from Weyl's min-max principle (Proposition 4.1)

$$\mu_n(H_L) \leq \mu_n(H_{L'}). \tag{2.11}$$

This, together with (2.9), proves inequality (2.10).

Now we prove an important auxiliary statement, required for the proof of the main result of this section, i.e., convergence of partition functions $Z_\beta[H_L(\Lambda^N)]$ to $Z_\beta[H(\Lambda^N)]$.

L e m m a 2.3. Let $\{A_n\}$ and A be trace-class operators with $w-\lim_{n\to\infty} A_n = A$. If the sequence of norms $\{\|A_n\|_1\}$ decreases monotonously together with $\{\|A_n - A_n^{(d)}\|_1\}$ for an arbitrary $d \geq 1$ (where $A_n^{(d)} = P_d A_n P_d$ and P_d is a finite-dimensional projector: $\mathcal{H}^{(d)} = P_d \mathcal{H}$, , $\dim \mathcal{H}^{(d)} = d$), then

$$\|\cdot\|_1 - \lim_{n\to\infty} A_n = A. \tag{2.12}$$

P r o o f. Every operator from $\mathfrak{C}_1$ can be approximated in the trace-class topology by finite-rank operators. Hence for $\forall \epsilon > 0$, we can find such $d(\epsilon)$, that for $d > d(\epsilon)$

$$\|A - A^{(d)}\|_1 < \epsilon \quad \text{and} \quad \|A_1 - A_1^{(d)}\|_1 < \epsilon. \tag{2.13}$$

Hence estimation (2.13) is valid for $\forall n \geq 1$

$$\| A_n - A_n^{(d)} \|_1 < \epsilon . \tag{2.14}$$

Consider now $\| A - A_n \|_1$, then

$$\| A - A_n \|_1 \leq \| P_d (A - A_n) P_d \|_1 + \| A - A^{(d)} \|_1 + \| A_n - A_n^{(d)} \|_1 . \tag{2.15}$$

But on the finite-dimensional space $\mathcal{H}^{(d)} = P_d \mathcal{H}$ all operator topologies are known to be equivalent. Therefore, for n large enough:

$$\| P_d (A - A_n) P_d \|_1 < \epsilon .$$

This estimate together with (2.13)-(2.15) proves the lemma.

Theorem 2.1. Let $\{ H_L (\Lambda^N) \}$ be a sequence of cut-off Hamiltonians (see section 1), then for each $\beta > 0$

$$\| \cdot \|_1 - \lim_{L \to \infty} \exp(-\beta H_L) = \exp(-\beta H). \tag{2.16}$$

Proof. Let us verify the conditions of Lemma 2.3:

(a) from Corollary 1.4. (1.15) $w - \lim_{L \to \infty} \exp(-\beta H_L) = \exp(-\beta H)$ for $\beta > 0$,

(b) for $\forall L$ and $\beta > 0$ $\exp(-\beta H_L) \in \mathfrak{C}_1$ (see Corollary 2.1) and also $\exp(-\beta H) \in \mathfrak{C}_1$ (see Lemma 2.1.);

(c) the sequence of the tarce-norms $\{ \| \exp(-\beta H_L) \|_1 \}$ monotonously decreases when the cutoff parameter L increases to infinity (see Lemma 2.2);

(d) moreover, inequality (2.11) for single eigenvalues of Hamiltonians $H_L (\Lambda^N)$ and $H_{L'} (\Lambda^N)$ (for $L \leq L'$) shows that

$$\sum_{n=d+1}^{\infty} \exp[-\beta \mu_n (H_{L'})] \leq \sum_{n=d+1}^{\infty} \exp[-\beta \mu_n (H_L)],$$

or (see (2.9) and Definition 2.1):

$$\| \exp(-\beta H_{L'}) - P_d \exp(-\beta H_{L'}) P_d \|_1 \leq \| \exp(-\beta H_L) - P_d \exp(-\beta H_L) P_d \|_1 .$$

Therefore the sequence $\{ \exp(-\beta H_L) \}$ satisfies all conditions of Lemma 2.3. Hence (2.16) is valid in the trace-norm topology.

Corollary 2.2. The $\mathrm{Tr}(\cdot)$ is known to be continuous in the trace-norm topology, thus for partition functions

$$Z_\beta [H_L (\Lambda^N)] = \mathrm{Tr} \exp[-\beta H_L (\Lambda^N)]$$

and each $\beta > 0$.

$$\lim_{L \to \infty} Z_\beta [H_L (\Lambda^N)] = Z_\beta [H (\Lambda^N)]. \tag{2.17}$$

The same is obviously true for the free energies $F_L = -\beta^{-1} \ln Z_\beta [H_L]$.

3. *CUT-OFF PROCEDURE AND STABILITY CONDITION, LENNARD-JONES POTENTIAL*

In this section we discuss a purely thermodynamic problem which one immediately faces with if a cut-off procedure is introduced. As was pointed out in /1/ to ensure the correct thermodynamic behaviour (absence of collapse) the Hamiltonian $H(\Lambda^N)$ must be stable (Ruelle /3/):

$$H(\Lambda^N) > -BN \quad \text{for } B > 0 \text{ and } \forall N \geq 1 . \tag{3.1}$$

For highly singular two-body potentials $\Phi(x)$ this means that the N-particle interaction $U_N(x_1, \ldots, x_N)$ is not only semibounded from below (see sections 1) but satisfies the stability condition in the sense of Ruelle [3]:

$$U_N(x_1,\dots,x_N) > -BN \quad \text{for} \quad \forall N \geq 1,\ \forall (x_1,\dots,x_N) \in \Lambda^N \qquad (3.2)$$

and fixed $B > 0$.

The cut-off procedure (see (1.1) leads to the following representation of the stable interaction $U_N(x_1,\dots,x_N)$

$$U_N(x_1,\dots,x_N) = U_N^L(x_1,\dots,x_N) + U_N^+(x_1,\dots,x_N), \qquad (3.3)$$

here the interaction $U_N^+(x_1,\dots,x_N)$ corresponds to a positive two-body potential $\Phi_+(x) = \Phi(x) - \Phi_L(x)$. But now it is an open question whether $U_N^L(x_1,\dots,x_N)$ is stable, at least for cut-off parameters large enough (compare Ruelle [3]), If so, then we can add to the statement of Theorem 2.1 that the sequence of cut-off Hamiltonians $H_L(\Lambda^N)$ in (2.17), (2.18) corresponds to the stable interactions $U_N^L(x_1,\dots,x_N)$ for L large enough.

We can verify this for the case of the widely-used Lennard-Jones potentials (12-6) in three-dimensional space

$$\Phi(x) = 4E\left[\left(\frac{a}{|x|}\right)^{12} - \left(\frac{a}{|x|}\right)^6\right],\ E > 0,\ a > 0. \qquad (3.4)$$

This potential is highly singular and repulsive at the origin and regular out of it. Thus it obviously satisfies all conditions of Theorem 2.1 [1] and Theorems 1.1, 2.1, therefore for this potential the convergence (2.17), (2.18) takes place. At last, potential (3.4) is stable in Ruelle sense (3.2) (see [3] and Theorem 3.1). It can be proved that the cut-off Lennard-Jones potentials $\Phi_L(x)$ (see (1.1) and (3.4)) for $\nu = 3$ and L large enough are stable too.

Proposition 3.1. (Ruelle [3]). Let two-body potential $\Phi(x) = \Phi(|x|)$ be a continuous and positive-type functions, i.e., $\Phi(x) \in L^1(R^\nu)$ and its Fourier transform $\tilde{\Phi}(q) \geq 0$, then such a potential is stable if $\tilde{\Phi}(0) > 0$.

Corollary 3.1. Let two-body potential $\Phi(x) = \Phi_1(x) + \Phi_2(x)$, where $\Phi_1(x) > 0$ and $\Phi_2(x)$ be the same as in Proposition 3.1 then $\Phi(x)$ is stable.

Theorem 3.1. If $\Phi(x)$ is a Lennard-Jones potential (5.4) in R^3, then the cut-off potential $\Phi_L(x)$ defined as in section 1 (1.1) is stable for L large enough.

P r o o f. Let us construct an auxiliary function:

$$\Phi_-(x) = 4E\left[\left(\frac{a^2}{|x|^2 + \xi^2 a^2}\right)^6 - \left(\frac{a^2}{|x|^2 + \xi^2 a^2}\right)^6\right], \qquad (3.5)$$

then a straight forward calculation shows that for $\nu = 3$ and $0 < \xi^2 < \sqrt[3]{2} - 1$

$$\Phi_+(x) = \Phi(x) - \Phi_-(x) \geq 0. \qquad (3.6)$$

The function $\Phi_-(x)$ (3.5) is continuous and bounded from above, so we can chose the cut-off parameter L in such a way that $L \geq \Phi_-(0)$, then

$$\Phi_L(x) \geq \Phi_-(x). \qquad (3.7)$$

If one represents $\Phi_-(x)$ as (see Ruelle [5])

$$\Phi_-(x) = 4E\left[\left(\frac{a^2}{|x|^2+\xi^2 a^2}\right)^3 - \sqrt[3]{2}\left(\frac{a^2}{|x|^2+\xi^2 a^2}\right)^2\right] \times$$
$$\times \left[\left(\frac{a^2}{|x|^2+\xi^2 a^2}\right)^3 + \sqrt[3]{2}\left(\frac{a^2}{|x|^2+\xi^2 a^2}\right)^2 + \sqrt[3]{4}\left(\frac{a^2}{|x|^2+\xi^2 a^2}\right)\right],$$

then one can show, that $\Phi_{-}(x)$ is a positive-type function for $\nu = 3$ and $0 < \xi^{2} < \sqrt[3]{2} - 1$. Therefore the two-body potential $\Phi_{-}(x)$ is stable (Proposition 5.1). The same is obviously true for $\Phi_{L}(x)$ (see (3.7)) if $L \geq \Phi_{-}(0)$. This completes the proof.

Theorem 3.1 completes the discussion of the main result of this paper (see Theorem 2.1 and Corollary 2.2).

ACKNOWLEDGEMENTS

The author is indebted to Dr. E.Christov, Prof. A.Uhlmann and Dr. I.Volovich for numerous useful comments and criticism. I would like to thank Prof. Ja.G.Sinai for a careful reading of the manuscript, helpful suggestions and encouragement. The support and valuable remarks of Prof. D.V.Anosov, Dr. V.K.Fedyanin and Dr. V.K.Melnikov are also gratefully acknowledged.

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Received by Publishing Department on January 16, 1976.