N-Body Quantum Systems with Singular Potentials

by

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ABSTRACT. – For N-body quantum systems with singular potentials including hard cores we derive a Mourre estimate and give an elementary proof of asymptotic completeness in the short range case. No regularity is required on the boundary of the hard cores and no conditions on the potentials are imposed at finite interparticle distance, besides those allowing one to define self-adjoint Hamiltonians.

RÉSUMÉ. – Pour des systèmes quantiques à N corps avec des potentiels singuliers incluant des noyaux durs nous démontrons une inégalité de Mourre et nous présentons une preuve élémentaire de la complétude asymptotique pour le cas des interactions à courte distance. Nous ne faisons aucune hypothèse de régularité sur le bord des noyaux durs et nous n'imposons pas de conditions sur le potentiel pour des distances finies entre particules, à l'exception de celles qui permettent de définir des hamiltoniens auto-adjoints.

Contents

1 Introduction

This work is devoted to N-body Schrödinger operators with singular potentials including hard cores. We generalize many known results to this larger class of interactions. The most important is asymptotic completeness in the short-range case, which was first obtained by Sigal and Soffer [20]. Others concern the structure of the continuous spectrum and the decay of wave functions of non-threshold bound

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states. These results are proved by means of the Mourre inequality. Their generalization has been made possible by a new variant of this inequality, which is consistent with the restrictions on configuration space imposed by hard cores.

Consider a system of N particles in $\mathbf{R}^\nu$. For quantum asymptotic completeness the following simple hypotheses will be shown to be sufficient. Each pair of particles interacts through a hard core $K \subset \mathbf{R}^\nu$ (compact) and a two-body potential of the form

$$V \in L^1_{\mathrm{loc}}(\mathbf{R}^\nu \backslash K) ,$$

where $V_-(x) = \max(-V(x), 0)$ is form-bounded with respect to the Dirichlet Laplacian in $L^2(\mathbf{R}^\nu \backslash K)$ with a small enough bound, and the decay of V for $|x| \to \infty$ is subject to the short-range condition

$$V(x) = O(|x|^{-\mu}) \qquad \mu > 1 .$$

That is, if K is regarded as a set where $V = +\infty$, then essentially nothing is required on the positive part V_+ beyond the short-range decay. In particular, asymptotic completeness holds for systems with non-integrable point singularities in the pair potentials, typically at $x = 0$, and for systems of bulk particles. We remark that the Hilbert space for such an N-body system is $L^2(\Omega)$, where $\Omega \subset \mathbf{R}^{N\nu}$ is the subset of those configurations which are not forbidden by the hard cores.

The recent and simpler proofs of AC due to Graf and Yafaev take advantage of carefully constructed vector fields in the configuration space $\mathbf{R}^{N\nu}$ [9, 22]. A common feature of these vector fields is that the generated flow does not change the relative configuration of particles which are close to each other. In particular the reduced configuration space Ω of a hard-core system is left invariant by such a flow after adjusting a parameter of the field if necessary. This partly explains the success of these geometric methods in the present work. A new ingredient in our proof of asymptotic completeness, as compared to those in [22, 15], is a time dependence in the vector field which we introduced following an idea of Hunziker, in order to dispense with the use of local decay. This drastically simplifies the proof and also clarifies the role of the Mourre estimate.

The Mourre estimate is the main tool for the proof of AC. In the generalization to hard-core systems it must be generalized as well. To do this we replace the generator of dilations by the generator of the flow, associated with the vector field constructed by Graf [9]. The Mourre estimate obtained in this way goes back to Skibsted and Graf [21, 11], and has the same immediate consequences for the structure of the continuous spectrum as the original one. Moreover it allows one to rederive in our framework the Froese-Herbst theorem on the exponential decay of wave functions belonging to non-threshold bound states, and the result due to Perry which states that the accumulation of eigenvalues at thresholds can occur only from below.

Previously N-body Schrödinger operators including hard-core interactions were investigated by Hunziker [14], Ferrero, Pazzis, and Robinson [6], Boutet de Monvel, Georgescu, and Soffer [3], and most recently by Iftimovici [16]. Hunziker proved existence of the wave operators for particles in three space dimensions and a similar class of interactions as ours. Ferrero et al. considered particles interacting by spherically symmetric two-body potentials which are repulsive or so weakly attractive that no bound states exist. These potentials may be singular at the origin or include a hard core in the form of a ball. For such systems existence and completeness of the single wave operator is proved. Boutet de Monvel et al. studied the spectral properties of N-body hard-core Hamiltonians. They derived a Mourre estimate, the conjugate operator being the generator of dilations, a limiting absorption principle and then obtained information on the point spectrum and absence of singular continuous spectrum in the standard way. Building on this work Iftimovici then proved existence of Abelian limits of the wave operators and their completeness. Let us compare assumptions and methods of [3, 16] with ours. The conditions in [3, 16] on the tails of the short-range parts of the potentials are weaker than ours. Our conditions, however, concern the tails only. The hard cores in [3, 16] are closures of bounded open sets with boundary of class C^1. Additional assumptions have been summarized (for simplicity) in the condition that each hard core be star-shaped with respect to the origin. We require only compactness (see above). As for the methods, those employed by Boutet de Monvel et al. are completely different from ours. They make use of an algebraic framework, the test of which was the main intention of the authors [3]. For the sole purpose of treating N-body systems with singular potentials our approach is much simpler.

The organization of this work is as follows. In Section 2 we define the class of systems we will to study, we list all assumptions and all our main results. Sections 3 and 4 are devoted to the proofs.

2 N-Body Quantum Systems

2.1 Hard-Core Hamiltonians

The purpose of this section is to define self-adjoint Hamiltonians from given formal expressions for Schrödinger operators with hard-core potentials, and to derive general properties of these Hamiltonians like locality and local compactness.

We begin with some notations. Suppose X is a finite-dimensional Eucledian space. If $x, y \in X$ then xy denotes the inner product of x and y and $|x|$ the corresponding norm. This inner product is extended by linearity to the complexification $\bar{X}$ of X. Further Δ and dx are the Laplace-Beltrami operator and the measure in X induced by the metric $g(x, y) := xy$.

Next let $\Omega \neq \emptyset$ be an open subset of X and let $\langle\varphi|\psi\rangle$ be the usual inner product of the Hilbert space $\mathcal{H} = L^2(\Omega, dx)$. We will use the following abbreviated notation for quadratic forms in $\mathcal{H}$. If $f \in L^1_{\mathrm{loc}}(\Omega)$ then $\langle f\rangle$ denotes the form $\langle\varphi|f|\psi\rangle := \int dx\overline{\varphi(x)}f(x)\psi(x)$ with domain $Q(f) = C_0^\infty(\Omega)$. Quite generally $\langle A\rangle$ will denote a quadratic form $\langle\varphi|A|\varphi\rangle$ and $Q(A) \subset \mathcal{H}$ its domain. $\langle\varphi|A|\varphi\rangle$ will frequently be defined by a symmetric operator $A \geq a$ in $\mathcal{H}$, in which case $\langle A\rangle$ denotes the closure of the form $\langle\varphi|A\psi\rangle$ defined on $D(A) \times D(A)$, $D(A)$ being the domain of A. For instance if $D(-\Delta) := C_0^\infty(\Omega)$ then $\langle\varphi| - \Delta|\psi\rangle = \langle\nabla\varphi|\nabla\psi\rangle$ and $Q(-\Delta) = H_0^1(\Omega)$. The self-adjoint operator associated with this form, i.e., the Friedrichs' extension of $-\Delta$, is called Dirichlet Laplacian for Ω [19]. We denote it by $2T$.

Now suppose $V : \Omega \to \mathbf{R}$ has the properties

$$\begin{array}{ll} (V1) & V \in L^1_{\mathrm{loc}}(\Omega) \\ (V2) & \langle\varphi|V_-|\varphi\rangle \leq \alpha\langle\varphi| -\Delta/2\,\varphi\rangle + \beta\langle\varphi|\varphi\rangle \qquad \forall\varphi \in C_0^\infty(\Omega) \\ & \text{for some } \alpha < 1\ . \end{array}$$

$V_- := \max(-V(x), 0)$. Then we define the Hamiltonian H as the unique self-adjoint operator associated with the closure of the form $\langle T\rangle + \langle V\rangle$. This form is indeed closable since it is the sum of the two forms $(\langle T\rangle - \langle V_-\rangle)$ and $\langle V_+\rangle$, which, by $(V2)$, are bounded from below and closable ([17, Chapter 6]). There is an other possible definition of H which reduces to T if $V \equiv 0$: we could have taken the sum of the closures of the forms $(\langle T\rangle - \langle V_-\rangle)$ and $\langle V_+\rangle$ and had then obtained a form possibly extending $\langle H\rangle$. At least if $\Omega = X$ the two definitions however coincide ([4, Theorem 1.13]).

A further consequence of $(V2)$ is that $Q(H) \subset Q(T)$ and

$$\langle\varphi|T|\varphi\rangle \leq \frac{1}{1-\alpha}\langle\varphi|H+\beta|\varphi\rangle \qquad \forall\varphi \in Q(H)\ . \tag{2.1}$$

This follows from the inequality (2.1) on $C_0^\infty(\Omega)$. As a result H has the so called local compactness property:

Lemma 2.1 *Suppose $f \in L^\infty(\Omega)$ and $f(x) \to 0$ $(|x| \to \infty)$. Then for all $z \in \rho(H)$*

$$f(z-H)^{-1/2} \text{ is compact}$$

as an operator on $\mathcal{H}$.

Proof. For any $z \in \rho(H)$ we have

$$f(z-H)^{-1/2} = f(1+T)^{-1/2}(1+T)^{1/2}(z-H)^{-1/2}\ .$$

$(1+T)^{1/2}(z-H)^{-1/2}$ is bounded by (2.1). To prove compactness of $f(1+T)^{-1/2}$ we must show that $f : H_0^1(\Omega) \to L^2(\Omega)$ is compact. Let $\tilde{f}(x) := f(x)$ for $x \in \Omega$ and $\tilde{f}(x) := 0$ otherwise. Then $\tilde{f} : H^1(X) \to L^2(X)$ is compact (see [15]) and maps the subspace $H_0^1(\Omega)$ of $H^1(X)$ into the subspace $L^2(\Omega)$ of $L^2(X)$. Hence $f : H_0^1(\Omega) \to L^2(\Omega)$ is compact. ∎

Let $(\mathcal{H}_s)_{s\in\{-2\ldots 2\}}$ denote the usual scale of Banach spaces associated with H, i.e., $\mathcal{H}_s$ is the completion of $D(H)$ with respect to the norm $\|\varphi\|_s = \|(|H|+1)^{s/2}\varphi\|$. So $\mathcal{H}_2 = D(H)$ and $\mathcal{H}_1 = Q(H)$ equipped with the graph and the form norm of H respectively. $\mathcal{H}_{-s}$ is norm isomorphic to the space $\mathcal{H}_s^*$ of the bounded anti-linear forms in $\mathcal{H}_s$. The isomorphism of $\mathcal{H}_s^*$ and $\mathcal{H}_s$ induced by the Hilbert space structure of $\mathcal{H}_s$ is suppressed.

Let ∂^α be the spatial derivative $\prod_{i=1}^n \left(\frac{\partial}{\partial x^i}\right)^{\alpha_i}$, $n = \dim(X)$, of order $|\alpha|$.

Lemma 2.2 *Let $f \in C^\infty(\Omega)$ with $\partial^\alpha f \in L^\infty(\Omega)$ if $|\alpha| \leq 2$. Then*

(i) Multiplication by f is a bounded operator on $H_0^1(\Omega)$ and $\mathcal{H}_s$,
(ii) $H(f\varphi) = f(H\varphi) - (\nabla f)\nabla\varphi - \frac{1}{2}(\Delta f)\varphi\ , \qquad \varphi \in D(H)\ .$

Proof. (i) $f \in \mathcal{B}(H_0^1(\Omega))$ follows from $\nabla(f\varphi) = (\nabla f)\varphi + f\nabla\varphi$ for $\varphi \in C_0^\infty(\Omega)$, and $f, \nabla f \in L^\infty$. $f \in \mathcal{B}(\mathcal{H}_{-s})$ follows from $\bar{f} \in \mathcal{B}(\mathcal{H}_s)$ by duality. Below we prove $f: D(H) \to D(H)$ and (ii), $f \in \mathcal{B}(\mathcal{H}_2)$ then follows from (ii). For $f \in \mathcal{B}(\mathcal{H}_1)$ it is sufficient that

$$\langle f\varphi|H|f\varphi\rangle \leq c_1\langle\varphi|H + c_2|\varphi\rangle \ , \qquad \varphi \in C_0^\infty(\Omega), \tag{2.2}$$

for some $c_1, c_2 > 0$, because $C_0^\infty(\Omega)$ is dense in $\mathcal{H}_1$. By dropping V_- we see that

$$\langle f\varphi|H|f\varphi\rangle \leq \langle f\varphi|T|f\varphi\rangle + \|f\|_\infty^2\langle\varphi|V_+|\varphi\rangle \ .$$

From this (2.2) follows if we use $f \in \mathcal{B}(H_0^1(\Omega))$ and (2.1) to estimate the first term, and $\langle\varphi|H + \beta - V_+|\varphi\rangle = \langle\varphi|T - V_- + \beta|\varphi\rangle \geq 0$ for the second term on the right hand side.

(ii) For $\varphi, \psi \in C_0^\infty(\Omega)$ we compute

$$\langle\varphi|H|f\psi\rangle = \langle\bar{f}\varphi|H|\psi\rangle - \langle\varphi|\nabla f\nabla\psi\rangle - \frac{1}{2}\langle\varphi|\Delta f\psi\rangle \ .$$

Because of (i), (2.1), and $\nabla f, \Delta f \in L^\infty(\Omega)$ this extends to all $\psi \in Q(H)$. For $\psi \in D(H)$ we conclude $\langle\varphi|H|f\psi\rangle = \langle\varphi|\eta\rangle$ for all φ in the form core $C_0^\infty(\Omega)$ of H, where $\eta = fH\psi - \nabla f\nabla\psi - \frac{1}{2}\Delta f\psi \in \mathcal{H}$. Hence $f\psi \in D(H)$ and $H(f\psi) = \eta$. ∎

2.2 N-Body Quantum Systems

In this section we introduce N-body quantum theory in the generalized form due to Agmon, Froese and Herbst [1, 7]. We first explain the general structure without any reference to a concrete system and then introduce Schrödinger systems with hard-core interactions as a special model.

The General Structure

An *N-body configuration space* (X, L) is a Eucledian space X together with a finite family L of subspaces, closed under intersection, with $\{0\}, X \in L$. For the order relation in L induced by set-theoretic inclusion we use the notation

$$\begin{aligned} a \geq b \ &\Leftrightarrow \ a \supset b \\ a > b \ &\Leftrightarrow \ a \supset b \neq a \ . \end{aligned}$$

The element $\{0\} \in L$ will be denoted by 0 if there is no danger of confusion. Associated with each $a \in L$ there is an N-body configuration space (X^a, L^a) defined by

$$\begin{aligned} X^a \ &:= \ a^\perp \ , \\ L^a \ &:= \ \{b \cap a^\perp | b \geq a\} \ . \end{aligned}$$

Obviously $(X^0, L^0) = (X, L)$. L and L^a have the structure of a lattice, and L^a is isomorphic to the sublattice $\{b \in L | b \geq a\}$ of L through $b \cap a^\perp \to a \oplus (b \cap a^\perp)$. We can therefore use the elements $b \geq a$ of L to label the elements of L^a as well. For each $a \in L$ we further define Π_a and Π^a as the orthogonal projections mapping X

onto the subspaces a and $a^\perp$ respectively. x_a and x^a are shorthands for $\Pi_a x$ and $\Pi^a x$. So $x \in X$ is decomposed as $x = x_a + x^a$ with respect to the decomposition $X = a \oplus a^\perp$. The (a-)*intercluster distance* is

$$|x|_a := \min_{b \not\geq a} |x^b| \ ,$$

in particular $|x|_0 = +\infty$. The b-intercluster distance in (X^a, L^a) is denoted $|.|^a_b$ and extended to all of X by

$$|x|^a_b = \min_{c \geq a, c \not\geq b} |x^c| = |x^a|^a_b \ .$$

An *N-body quantum system* is an N-body configuration space (X, L) together with an assignment

$$L \ni a \to (\mathcal{H}^a, H^a) \ ,$$

where $\mathcal{H}^a$ is a separable Hilbert space and H^a a self-adjoint operator in $\mathcal{H}^a$. Since each $a \in L$ defines an N-body configuration space (X^a, L^a), there is also an N-body quantum system

$$L^a \ni b \to (\mathcal{H}^b, H^b)$$

for each $a \in L$. In this sense *a is a subsystem of* $\{0\}$. To relate the system $a = 0$ to its subsystems one needs auxiliary Hilbert spaces and operators

$$\begin{aligned} \mathcal{H}_a &:= L^2(a) \otimes \mathcal{H}^a \\ H_a &:= \frac{p_a^2}{2} \otimes 1 + 1 \otimes H^a \\ \mathcal{J}_a &\in \mathcal{B}(\mathcal{H}, \mathcal{H}_a) \end{aligned}$$

where $\mathcal{J}_a$ is a yet unspecified embedding operator. The corresponding objects for the subsystems $b \geq a$ of a subsystem $a > 0$ carry an upper index a. This framework is sufficient to formulate all the following results concerning the spectrum of H as well as the long time behavior of continuum states, i.e., existence and completeness of wave operators.

Proofs for a concrete model are done by "induction in subsystems": to establish a property P on the full system $0 \in L$ one shows first that P is true for the single minimal system $X \in L$ and then proves P for 0 assuming P is true for all $a < 0$ using only arguments available on the level of each subsystem $b < 0$ as well. Since such an induction step could be iterated starting at X, this proves P for all $a \in L$.

N-Body Schrödinger-Systems with Hard-Core Interactions

Suppose for each $a \in L$ there is a pair (Ω^a, V^a) where $\emptyset \neq \Omega^a \subset X^a$, open, is such that

$$\Omega_a := a + \Omega^a \supset \Omega \ , \qquad a \in L \ , \tag{2.3}$$

($\Omega := \Omega^0$), and V^a is a potential in Ω^a with the properties ($V1$) and ($V2$) ($V^X = 0$ in $\mathbf{C}$). The differences

$$I_a(x) := V(x) - V^a(x^a) \ , \qquad x \in \Omega$$

($V := V^0$), are called *intercluster potentials.* We can now define our N-body system by setting

- $\mathcal{H}^a := L^2(\Omega^a)$ if $a < X$ and $\mathcal{H}^X := \mathbf{C}$.
- H^a, if $a < X$, is the unique self-adjoint operator associated with the closure of the form $\langle -\Delta^a/2 + V^a \rangle$ defined in $C_0^\infty(\Omega^a)$, and $H^X := 0$ in $\mathbf{C}$. Δ^a is the Laplacian in X^a.
- $\mathcal{J}_a : L^2(\Omega) \to L^2(\Omega_a)$ is the extension of a function to $\Omega_a \supset \Omega$ by 0.

Note that $\mathcal{J}_a^* : L^2(\Omega_a) \to L^2(\Omega)$ is the restriction : $(\mathcal{J}_a^*\varphi) = \varphi|_\Omega$ and that

$$\mathcal{J}_a^*\mathcal{J}_a = 1_\mathcal{H} \quad ; \quad \mathcal{J}_a\mathcal{J}_a^* = \chi(x \in \Omega) \quad \text{in} \quad L^2(\Omega_a) \ .$$

Finally we introduce momentum operators in our various Hilbert spaces. Let $p : D(p) \subset L^2(\Omega) \to L^2(\Omega, \bar{X})$ be the closure of the operator p in $C_0^\infty(\Omega)$ with

$$(p\varphi)(x) := -i(\nabla\varphi)(x) \ .$$

$D(p) = H_0^1(\Omega) = Q(T)$ and p is related to T by $\|p\varphi\|^2 = 2\langle\varphi|T|\varphi\rangle$. With p_k we denote the components of p with respect to any orthonormal basis (e_k) of X, i.e.,

$$(p_k\varphi)(x) := -ie_k(\nabla\varphi)(x) = -i\frac{\partial\varphi}{\partial x_k}(x) \ , \qquad D(p_k) := D(p) \ .$$

Note that the closure of p_k is not self-adjoint in general. The operators p_a, p^a and $p(a)$ in $L^2(a)$, $L^2(\Omega^a)$ and $L^2(\Omega_a)$ respectively are defined analogously to p. If $H_0^1(\Omega)$ is regarded as a subspace of $H_0^1(\Omega_a)$, then $p(a)$ extends p. That is,

$$p(a)\mathcal{J}_a \supset \mathcal{J}_a p \ . \tag{2.4}$$

We may therefore write p instead of $p(a)$ without danger.

2.3 Assumptions and Results

In this section we collect the main results together with the required assumptions on the domains Ω_a and the intercluster potentials I_a.

In the language of standard N-body systems all following assumptions express a decay of the interaction between different clusters as the minimal intercluster distance goes to infinity. This also means that only the regions $\{|x|_a > R_0\} \subset X$ are involved, where R_0 is an arbitrarily large and henceforth fixed constant. We begin with the condition

$$\Omega_a \cap \{x : |x|_a > R_0\} \subset \Omega \ , \qquad a \in L \tag{2.5}$$

which says that the hard core $\Omega_a \backslash \Omega$, where $I_a(x)$ is supposed to be infinite, is contained in $\{|x|_a \leq R_0\}$. (2.5) combined with (2.3) is automatically also satisfied in all subsystems, i.e., for $\Omega_b^a = a^\perp \cap b + \Omega^b$ and all $b \geq a$, as can be seen using the ideas of the proof of Lemma 3.11. The further assumptions are gathered in the list below and cited upon use. In their formulation we use the following terminology: a quadratic form q in a Banach space E is said to be compact, if q is bounded and the operator in $\mathcal{B}(E, E^*)$ associated with q is compact. For a useful compactness criterion see Lemma A.2.

$(I1)$	$I_a : H_0^1(\Omega_{a,R_0}) \to L^2(\Omega_{a,R_0})$ bounded	
$(I2)$	$\|I_a\| \leq \text{const } R^{-\mu}$ in $\mathcal{B}(H_0^1(\Omega_{a,R}), L^2(\Omega_{a,R}))$ where $\mu > 1$	$\forall R \geq \max(1, R_0)$
$(I3)$	$\langle I_a \rangle$ compact	in $H_0^1(\Omega_{a,\varepsilon,R_0})$ $\forall \varepsilon > 0$
$(I4)$	$\langle \nabla G \nabla I_a \rangle$ bounded	in $H_0^1(\Omega_{a,R_0})$
	$\langle \nabla G \nabla I_a \rangle$ compact	in $H_0^1(\Omega_{a,\varepsilon,R_0})$ $\forall \varepsilon > 0$
	if $G \in C^\infty(\Omega)$, $\sup_x \|\partial^\alpha(G(x) - \frac{x^2}{2})\| < \infty$, $\forall \alpha$	

where

$$\begin{aligned} \Omega_{a,R} &:= \{x \in \Omega : |x|_a > R\} \\ \Omega_{a,\varepsilon,R_0} &:= \{x \in \Omega : |x|_a > \max(\varepsilon|x|, R_0)\} \ . \end{aligned}$$

When (In) is imposed on $(I_a)_{a \in L}$ in the following, we will always assume that (In) equally holds for the intercluster potentials $I_b^a = I_b - I_a$ $(b > a)$ of all subsystems $a > 0$. This becomes important in Sections 3 and 4 where theorems are proved by induction in subsystems, and it is automatically satisfied when $(I1)$ to $(I4)$ are derived from assumptions on the potentials v^b in an expansion $V^a(x^a) = \sum_{b \geq a} v^b(x^b)$ of V^a. This is done in the appendix. We mention that the use of the same parameter R_0 in all our conditions above is justified, since each of them is weakened as R_0 is increased.

We can now state our results.

Theorem 2.3 *Suppose the intercluster potentials obey* $(I3)$ *and let* $\Sigma_a := \inf \sigma(H_a)$. *Then*

$$\sigma_{ess}(H) = [\Sigma, \infty)$$

where $\Sigma := \min_{a>0} \Sigma_a$.

All further results are based on the following new variant of Mourre's inequality, where the generator of dilations is replaced by the operator

$$A := \frac{1}{2}(p\nabla G + \nabla G p)$$

involving any function $G \in C^\infty(\Omega, \mathbf{R})$ with the properties

- (i) $G(x) = G(x_a)$ if $|x^a| \leq R_1$
- (ii) for each $a \in L$ there is a function $G^a : X^a \to \mathbf{R}$ such that $G(x) = \frac{1}{2}x_a^2 + G^a(x^a)$ if $|x|_a \geq cR_1$.

Here $c > 1$ is a constant and R_1 a parameter to be adapted to the system under consideration. The vector field ∇G corresponding to such a function was first constructed by Graf to prove asymptotic completeness [9]. Let the commutator of iH with A be defined as

$$\begin{aligned} i[H, A] &:= pG''p - \frac{1}{4}\Delta^2 G - \nabla G \nabla V \qquad (2.6) \\ pG''p &:= \sum_{k,l} p_k(\partial_k \partial_l G) p_l \ . \end{aligned}$$

Assuming ($I4$) this is a bounded quadratic form in $H_0^1(\Omega)$ if $R_1 > \rho R_0$, where $\rho > 1$ is some constant independent of R_0 (see Lemma 3.13). Further let the *Mourre constant* be defined as

$$\Theta(E) := \begin{cases} \inf\{2(E-\lambda)|\lambda \in \tau(H)\ ,\ \lambda \leq E\} & \text{if } E \geq \Sigma \\ 0 \quad \text{otherwise,} & \end{cases}$$

where $\tau(H) := \{E \in \mathbf{R}|E \text{ is eigenvalue of } H^a \text{ for some } a > 0\}$ is the set of *thresholds*. By an inductive argument using Theorem 2.3, $\Sigma \in \tau(H)$, so that Σ is the smallest threshold.

Theorem 2.4 *Suppose* ($I1$), ($I3$) *and* ($I4$) *on the intercluster potentials and let* $R_1 > \rho R_0$. *Then for each* $E \in \mathbf{R}$ *and* $\varepsilon > 0$ *there is a an open interval* $\Delta \ni E$ *and a compact operator* K *in* $\mathcal{H}$ *such that*

$$E_\Delta(H) i[H, A] E_\Delta(H) \geq [\Theta(E) - \varepsilon] E_\Delta(H) + K\ .$$

If $R_1 = 0$ then $G(x) = x^2/2 + \text{const}$, by ($ii$), so that the original Mourre theorem is recovered. As R_1 is increased Theorem 2.4 becomes stronger because the hypotheses on the potentials are weakened, while it may still replace the original Mourre theorem in many applications. Examples for this are the proof of asymptotic completeness, the next theorem below, and the Corollary 3.17 which says that non-threshold eigenvalues of H have finite multiplicity, they can accumulate only at thresholds (or $+\infty$), and $\tau(H)$ is closed and countable.

Theorem 2.5 *Suppose the intercluster potentials obey the hypotheses of Theorem 2.4.*
(1) If $H\psi = E\psi$ *and*

$$\alpha = \sup\{\beta : e^{\beta|x|}\psi \in L^2(\Omega)\}$$

then $E + \frac{\alpha^2}{2}$ *is either a threshold or infinite.*
(2) Eigenvalues of H *can accumulate at thresholds only from below.*

For the proof of these statements, which we patterned after the proofs in [15], the reader is referred to [12]. In the framework of non-singular N-body systems (1) is due to Froese and Herbst [8] and (2) due to Perry [18]. There one knows in addition that the Hamiltonian has no positive eigenvalues [8, 15]. This is not true for H in general (take e.g. a chain!), and its proof after suitably restricting the class of hard cores is an open problem.

Our main result is existence and completeness of the wave operators $\Omega_a \in \mathcal{B}(\mathcal{H}_a, \mathcal{H})$, $a \in L$, formally given by

$$\Omega_a := s - \lim_{t\to\infty} e^{iHt} \mathcal{J}_a^* e^{-iH_a t}[1_a \otimes P_{\text{pp}}(H^a)]\ . \tag{2.7}$$

1_a is the identity in $L^2(a)$ and $P_{\text{pp}}(H^a)$ is the orthogonal projection onto $\mathcal{H}^a_{\text{pp}}$. In particular $\Omega_0 = P_{\text{pp}}(H)$.

Theorem 2.6 *Assume* ($I2$) *on the intercluster potentials. Then the wave operators* $(\Omega_a)_{a\in L}$ *exist,* Ω_a *is isometric from* $L^2(a) \otimes \mathcal{H}^a_{\text{pp}}$ *into* $\mathcal{H}$, *Ran* $\Omega_a \perp$ *Ran* Ω_b *if* $a \neq b$, *and*

$$\bigoplus_{a>0} \mathit{Ran}\ \Omega_a \subset \mathcal{H}_{ac}\ .$$

Theorem 2.7 *Assume $(I2),(I3)$ and $(I4)$ on the intercluster potentials. Then the N-body quantum system defined in Subsection 2.2 is asymptotically complete:*

$$\bigoplus_{a>0} Ran\ \Omega_a = \mathcal{H}_{cont}\ .$$

We conclude this section with some notations. The scale of Banach spaces associated with the self-adjoint operator H_a is denoted by $(\mathcal{H}_{a,s})_{s\in\{-2,\ldots,2\}}$. $\|\cdot\|_{a,s}$ are the corresponding norms. Suppose S is a mathematical statement. We set $\chi(S)=1$ if S is true and $\chi(S)=0$ otherwise. If S depends on a variable then $\chi(S)$ becomes a function of this variable. For instance if $A\subset X$ then $\chi(x\in A)=\chi_A(x)$ where $\chi_A : X\to \mathbf{R}$ is the characteristic function of the set A. Unless clarity demands it we will not distinguish in notation between a function defined on X and its restriction to Ω or Ω_a, and supp(f) will always denote the closure of $\{x : f(x)\neq 0\}$ in X, even if f is only defined on Ω.

3 Spectral Properties

3.1 Introduction

In this section we prove Theorem 2.3 and Theorem 2.4. Before let us dwell upon the conditions (i) and (ii) on the function G involved in Theorem 2.4. The original Mourre estimate is the statement of Theorem 2.4 for $G(x)=x^2/2$. For its proof the only relevant properties of G are smoothness and (ii) on page 8. First, these two properties are sufficient to reduce the problem to an analogous one in subsystems, and second they are automatically inherited by G^a, which allows us to conclude by induction. The gained freedom in the choice of G may now be used to eliminate conditions on the potentials. This is the purpose of condition (i). By (i), $\nabla G\nabla V(x)=\nabla G\nabla I_a(x)$ if $|x^a|\leq R_1$. Since X is covered by sets of the form $\{x|\,|x^a|<\text{const}\ R_0,\ |x|_a>R_0\}$ it follows that only the tails $I_a\restriction\{|x|_a>R_0\}$ of the intercluster potentials are involved in $i[H,A]$, if R_1 is large enough.

There is good reason for rejecting the use of the generator of dilations in the hard-core problem even if the potentials V^a are perfectly smooth on the sets Ω^a, where they are defined. This has to do with the fact that Ω is not invariant under the group of dilations and is further explained in Section 3.4.

In the next Section Theorem 2.3 is proved. In Section 3.3 we construct a function G with the properties (i) and (ii), so as to establish its existence. This construction follows a general strategy which will be employed again in Section 4.2 to construct Y-functions. Section 3.4 is devoted to the proof of Theorem 2.4.

3.2 The HVZ-Theorem

While H is defined by a quadratic form, the Hamiltonians H_a are defined by operators. In order to compare them with H we will need the following form characterization of H_a.

Theorem 3.1 *$\langle H_a\rangle$ is the closure of the form*

$$\langle\varphi|-\Delta/2\,\varphi\rangle+\langle\varphi|V^a|\varphi\rangle$$

defined for $\varphi \in C_0^\infty(\Omega_a)$.

For the purpose of this and the next section this form characterization could be taken for the definition of H_a. The proof of Theorem 3.1 is therefore deferred to an appendix. The strategy is to derive the theorem first for $C_0^\infty(a) \otimes C_0^\infty(\Omega^a)$ instead of $C_0^\infty(\Omega_a)$. This is done by general arguments. Using this one then shows that $Q(H_a) \supset C_0^\infty(\Omega_a)$. In the special case where $V^a \equiv 0$ we obtain the relation

$$T_a = \frac{p_a^2}{2} \otimes 1 + 1 \otimes T^a ,$$

where T_a in $\mathcal{H}_a$ is defined as T in $\mathcal{H}$. By Lemma A.3 it implies that $C_0^\infty(a) \otimes C_0^\infty(\Omega^a)$ considered as a subspace of $C_0^\infty(\Omega_a)$ is dense in $H_0^1(\Omega_a)$. Therefore

$$p(a) = p_a \otimes 1 + 1 \otimes p^a$$

if p_a and p^a are regarded as operators with ranges in $L^2(a, \bar{X})$ and $L^2(\Omega^a, \bar{X})$ respectively. More importantly this theorem provides us with

$$\langle \mathcal{J}_a\varphi | H_a | \mathcal{J}_a\varphi \rangle = \langle \varphi | H | \varphi \rangle - \langle \varphi | I_a | \varphi \rangle , \qquad \varphi \in C_0^\infty(\Omega) \tag{3.1}$$

as a first weak substitute for the equation $H_a = H - I_a$ one usually has in non-singular N-body theory. We shall need however more:

Lemma 3.2 *Let* $\varphi \in \mathcal{H}$ *and suppose either (i):* I_a *obeys* $(I3)$ *and supp*$(\varphi) \subset \{|x|_a \geq \max(R_0 + \delta, \varepsilon|x|)\}$*, or (ii):* I_a *obeys* $(I1)$ *and supp*$(\varphi) \subset \{|x|_a \geq R_0 + \delta\}$*, where* $\delta, \varepsilon > 0$*. Then* $\varphi \in Q(H)$ *implies* $\mathcal{J}_a\varphi \in Q(H_a)$ *and*

$$c_1\|\varphi\|_1 \leq \|\mathcal{J}_a\varphi\|_{a,1} \leq c_2\|\varphi\|_1 \tag{3.2}$$

with constants $c_1, c_2 > 0$ *independent of* φ*. Moreover in the case (ii)* $\varphi \in D(H)$ *implies* $\mathcal{J}_a\varphi \in D(H_a)$ *and*

$$H_a\mathcal{J}_a\varphi = \mathcal{J}_a(H\varphi - I_a\varphi) . \tag{3.3}$$

Proof. Pick $F \in C^\infty(\Omega)$, bounded, with bounded derivatives, $\mathrm{supp}(F) \subset \{|x|_a \geq \max(R_0 + \frac{\delta}{2}, \frac{\varepsilon}{2}|x|)\}$ and $F(x) = 1$ if $|x|_a \geq \max(R_0 + \delta, \varepsilon|x|)$, where $\varepsilon = 0$ in the case (ii). We will prove that $\psi \in Q(H)$ implies $\mathcal{J}_aF\psi \in Q(H_a)$ and

$$c_1\|F\psi\|_1 \leq \|\mathcal{J}_aF\psi\|_{a,1} \leq c_2\|F\psi\|_1. \tag{3.4}$$

(3.2) then follows from $F\varphi = \varphi$. If (3.4) holds true for all $\psi \in C_0^\infty(\Omega)$, then it extends to $Q(H)$. So let $\psi \in C_0^\infty(\Omega)$. By (3.1)

$$\langle \mathcal{J}_aF\psi | H_a | \mathcal{J}_aF\psi \rangle = \langle F\psi | H | F\psi \rangle - \langle F\psi | I_a | F\psi \rangle . \tag{3.5}$$

Now $|\langle F\psi | I_a | F\psi \rangle| \leq c\langle F\psi | (-\Delta + 1) F\psi \rangle = c\langle \mathcal{J}_aF\psi | (-\Delta + 1) \mathcal{J}_aF\psi \rangle$ by assumption on I_a. Using $(V2)$ for V and V^a respectively, this leads to

$$|\langle F\psi | I_a | F\psi \rangle| \leq \text{const } \|F\psi\|_1^2 \tag{3.6}$$
$$|\langle F\psi | I_a | F\psi \rangle| \leq \text{const } \|\mathcal{J}_aF\psi\|_{a,1}^2 \tag{3.7}$$

which, combined with (3.5), proves (3.4).

To prove (3.3) let F be defined as above in the case (ii), and pick $F_a \in C^\infty(\Omega_a)$, bounded, with bounded derivatives, $\mathrm{supp}(F_a) \subset \{|x|_a \geq R_0 + \frac{\delta}{4}\}$ and $F_a(x) = 1$ if $|x|_a \geq R_0 + \delta/2$, so that $F_a(x) = 1$ in $\mathrm{supp}(F)$. By Theorem 3.1 it suffices to show that

$$\langle \psi | H_a | \mathcal{J}_a \varphi \rangle = \langle \psi | \mathcal{J}_a (H\varphi - I_a \varphi) \rangle \qquad \psi \in C_0^\infty(\Omega_a) \ . \tag{3.8}$$

Since $\mathcal{J}_a H \varphi = F_a \mathcal{J}_a H F \varphi$ and $\mathcal{J}_a^* F_a \psi \in C_0^\infty(\Omega)$ if $\psi \in C_0^\infty(\Omega_a)$, (3.8) is equivalent to

$$\langle \psi | H_a | \mathcal{J}_a F \varphi \rangle = \langle \mathcal{J}_a^* F_a \psi | H | F \varphi \rangle - \langle \mathcal{J}_a^* F_a \psi | I_a F \varphi \rangle \qquad \psi \in C_0^\infty(\Omega_a) \ . \tag{3.9}$$

If this holds true for all $\varphi \in C_0^\infty(\Omega)$, then it extends to $Q(H)$ by (3.2), Lemma 2.2 and $(I1)$. But if $\varphi \in C_0^\infty(\Omega)$, then $\langle \psi | H_a | \mathcal{J}_a F \varphi \rangle = \langle \mathcal{J}_a \mathcal{J}_a^* F_a \psi | H_a | \mathcal{J}_a F \varphi \rangle$ which coincides with the right side of (3.9) by formula (3.1). ∎

Lemma 3.3 *For each $\gamma > 0$ there exists a family of functions $(j_a)_{a \in L} \subset C^\infty(X)$ with the properties*

- (i) $\sum_{a \in L} j_a^2(x) \equiv 1$
- (ii) $j_a(\lambda x) = j_a(x)$ *for* $\lambda \geq 1$ *and* $|x|$ *large.*
- (iii) *supp*(j_0) *is compact, and for* $a > 0$
  supp$(j_a) \subset \{x : |x^a| \leq \gamma |x|,\ |x|_a \geq \max(\kappa |x|, R_0 + 1)\}$ *for some* $\kappa > 0$.

The construction of such a partition of unity is standard and can be found e.g. in [15]. It is therefore omitted here. We shall simply speak of Ruelle-Simon partition of unity if the property $\mathrm{supp}(j_a) \subset \{|x^a| \leq \gamma |x|\}$ is not material, and J_a will always stand for $\mathcal{J}_a j_a$. If $(I3)$ holds then

$$J_a \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{a,1}) \tag{3.10}$$
$$J_a^* \in \mathcal{B}(\mathcal{H}_{a,1}, \mathcal{H}_1) \ . \tag{3.11}$$

(3.10) follows from Lemma 3.2 and Lemma 2.2 while (3.11) requires in addition an approximation argument using Theorem 3.1.

The following proof of Theorem 2.3 was inspired by [15] and the beautiful paper [5] of Enss. In the easy part we will need the criterion:

Lemma 3.4 *Let D be a form core of H. Then $\lambda \in \sigma(H)$ if and only if there exists a sequence $(\varphi_n)_{n \in \mathbf{N}} \subset D$ with $\|\varphi_n\| = 1$ $\forall n$ and*

$$\|(H - \lambda)\varphi_n\|_{-1} \to 0 \quad (n \to \infty) \ .$$

Remark. Of course any self-adjoint operator can replace H in this lemma.

Proof. The only-if part follows from the usual Weyl-criterion and $D \subset \mathcal{H}_1$ dense. To prove the converse assume $\lambda \notin \sigma(H)$. Then $(H - \lambda) : \mathcal{H}_1 \to \mathcal{H}_{-1}$ is a linear homeomorphism. Hence there exists a $c > 0$ such that

$$\|(H - \lambda)\varphi\|_{-1} \geq c \|\varphi\|_{+1} \geq c \|\varphi\|$$

for all $\varphi \in \mathcal{H}_1$. ∎

Proof of Theorem 2.3, easy part. We must show that $\sigma(H) \supset \sigma(H_a)$ for all $a > 0$. Let $\lambda \in \sigma(H_a)$ and $(\varphi_n)_{n\in\mathbf{N}} \subset C_0^\infty(\Omega_a)$, $\|\varphi_n\| = 1\ \forall n$, with

$$\|(H_a - \lambda)\varphi_n\|_{a,-1} \to 0 \qquad (n \to \infty) \tag{3.12}$$

as given by the Lemma 3.4. Fix $y \in a$ with $|y|_a > 0$ and set $T_s\varphi(x) := \varphi(x - sy)$ for $s \in \mathbf{R}$. If $\operatorname{supp}(\varphi_n) \subset \{x : |x| \le M_n\}$ then $\operatorname{supp}(T_s\varphi_n) \subset \{x : |x|_a \ge s|y|_a - M_n,\ |x| \le s|y| + M_n\}$ for all $s > 0$. So by choosing $s = s_n$ large enough we can achieve

$$\operatorname{supp}(T_{s_n}\varphi_n) \subset \{x : |x|_a > \max(\varepsilon|x|, R_0 + 2 + n)\}\ , \qquad \text{all } n\ , \tag{3.13}$$

with some $\varepsilon > 0$ independent of n. $\psi_n := \mathcal{J}_a^* T_{s_n}\varphi_n \in \mathcal{H}$ defines our sequence which will serve to prove $\lambda \in \sigma(H)$ by means of Lemma 3.4. By (3.13) and (2.5) we have

$$\psi_n \in C_0^\infty(\Omega)\ ,\ \operatorname{supp}(\psi_n) \subset \Omega_{a,\varepsilon,R_0+2}\ ,\ \|\psi_n\| = 1\ , \qquad \text{all } n\ , \tag{3.14}$$

and we need $\|(H - \lambda)\psi_n\|_{-1} \to 0$ as $n \to \infty$, or equivalently

$$\sup_{v \in C_0^\infty(\Omega),\ \|v\|_1 = 1} |\langle v|H - \lambda|\psi_n\rangle| \to 0 \qquad (n \to \infty)\ . \tag{3.15}$$

To prove (3.15) pick $F \in C^\infty(\Omega)$, bounded, with bounded derivatives, $\operatorname{supp}(F) \subset \Omega_{a,\varepsilon/2,R_0+1}$ and $F = 1$ in $\Omega_{a,\varepsilon,R_0+2}$. Then $F\psi_n = \psi_n$ by (3.14) and therefore

$$\langle v|H - \lambda|\psi_n\rangle = \langle \mathcal{J}_a F v|H_a - \lambda|\mathcal{J}_a\psi_n\rangle + \langle v|I_a F^2|\psi_n\rangle \qquad v \in C_0^\infty(\Omega).$$

Now use $\mathcal{J}_a\psi_n = T_{s_n}\varphi_n$, $T_s H_a = H_a T_s$, Lemma 3.2 and $F \in \mathcal{B}(\mathcal{H}_1)$ to conclude that

$$|\langle v|H - \lambda|\psi_n\rangle| \le \text{const}\ \|v\|_1 \|(H_a - \lambda)\varphi_n\|_{a,-1} + \|v\|_1 \|I_a F^2 \psi_n\|_{-1}\ .$$

By (3.12), (3.15) follows if $\|I_a F^2\psi_n\|_{-1} \to 0$ as $n \to \infty$. $I_a F^2 : \mathcal{H}_1 \to \mathcal{H}_{-1}$ is compact because $F : \mathcal{H}_1 \to H_0^1(\Omega_{a,\varepsilon/2,R_0+1})$ is bounded, and $\psi_n \rightharpoonup 0$ in $\mathcal{H}_1$ because $\psi_n \rightharpoonup 0$ in $\mathcal{H}$ and $\sup_n \|\psi_n\|_1 < \infty$. In fact

$$\|\psi_n\|_1 \le c\|\mathcal{J}_a\psi_n\|_{a,1} = c\|\varphi_n\|_{a,1}$$

$$\|\varphi_n\|_{a,1}^2 \le \|\varphi_n\|_{a,1}\|(H_a - \lambda)\varphi_n\|_{a,-1} + \text{const}$$

by Lemma 3.2. So $\|\psi_n\|_1$ cannot be unbounded. ∎

Proof of Theorem 2.3, hard part. Pick $\lambda \in \sigma_{ess}(H)$ and $(\psi_n)_{n\in\mathbf{N}} \subset D(H)$ with $\|\psi_n\| = 1$, $\psi_n \rightharpoonup 0$ and $\|(H - \lambda)\psi_n\| \to 0$ $(n \to \infty)$. We show that

$$\lambda = \lim_{n\to\infty} \langle \psi_n|H\psi_n\rangle \ge \Sigma\ . \tag{3.16}$$

Let $(j_a)_{a\in L}$ be the Ruelle-Simon partition given by Lemma 3.3. As sums of forms with domain $Q(H)$

$$\begin{aligned} H &= \sum_{a\in L} j_a H j_a - \frac{1}{2}|\nabla j_a|^2 \\ j_a H j_a &= J_a^* H_a J_a + j_a I_a j_a\ . \end{aligned}$$

These two equations combined lead to the first equation of

$$\begin{aligned}\langle\psi_n|H\psi_n\rangle &= \sum_{a>0}\langle J_a\psi_n|H_a|J_a\psi_n\rangle + \langle j_0\psi_n|Hj_0\psi_n\rangle \\ &\quad + \sum_{a\in L}\Big(\langle\psi_n|j_aI_aj_a|\psi_n\rangle - \frac{1}{2}\langle\psi_n||\nabla j_a|^2\psi_n\rangle\Big) \\ &= \sum_{a>0}\langle J_a\psi_n|H_a|J_a\psi_n\rangle + o(1) \qquad (n\to\infty)\ . \end{aligned} \tag{3.17}$$

In the second one we used the assumption on I_a and local compactness in combination with $|\nabla j_a|^2$, $j_0 \to 0$ $(|x|\to\infty)$ and $(H+i)\psi_n \rightharpoonup 0$. Since $H_a \geq \Sigma$ for all $a>0$ and $\sum_{a>0} J_a^* J_a = 1 - j_0^2$, (3.17) implies that

$$\langle\psi_n|H\psi_n\rangle \geq \Sigma(1-\|j_0\psi_n\|^2) + o(1) \qquad (n\to\infty)\ .$$

By the arguments above $\|j_0\psi_n\| \to 0$. This proves (3.16). ∎

3.3 The Graf Function

The main purpose of this section is the construction of a function G with the properties (i) and (ii) on page 8. Since a very similar construction is required for the Yafaev functions in Section 4, it pays to develop the common element, which is a way of partitioning X, in more generality than needed here.

Partitions of the Configuration Space

Let $(s_a)_{a\in L}$ be a collection of real-valued functions in X such that for each $a \in L$:

$$\begin{array}{ll} (S1) & s_a(x) = s_a(x_a) \\ (S2) & s_a(x_a) \geq s_b(x_a) \quad \forall b > a\ . \end{array}$$

These functions define for each $a \in L$ two subsets of X

$$S_a := \{x\in X | s_a(x) \geq s_b(x) \ \ \forall b>a\} \tag{3.18}$$

$$S_a^* := S_a \backslash \bigcup_{b<a} S_b \tag{3.19}$$

By $(S2)$, $a \subset S_a$ for all $a \in L$. The prototype of $s_a(x)$ is $|x_a|$. Then $S_a = a$ and $S_a^* = a^*$ where

$$a^* = a\backslash \bigcup_{b<a} b\ .$$

Other examples are found below and in Subsection 4.2.

Lemma 3.5 *Suppose* $S_a \cap S_b \subset S_{a\cap b}$ $\forall a,b \in L$. *Then*

$$\begin{array}{rl} (i) & X = \bigcup_{a\in L} S_a^* \ \textit{and}\ S_a^*\cap S_b^* = \emptyset \ \textit{if}\ a\neq b\ . \\ (ii) & S_a^* = \{x|s_a(x)\geq s_b(x)\ \forall b\in L \ \textit{and}\ > \ \textit{if}\ a>b\} \\ (iii) & \Pi_b : S_a^* \to S_a^* \ \ \forall b \geq a\ . \end{array}$$

Remark. (iii) combined with (i) implies for $b \geq a$:

$$(x \in S_a^* \Leftrightarrow x_b \in S_a^*) \qquad \text{if } x \in S_b \ . \tag{3.20}$$

Proof. Let $s(x) := \max_{a\in L} s_a(x)$ in this proof. (i) $S_X = X$ and $S_a \subset \bigcup_{b\leq a} S_b^*$ proves the covering property. If $a > b$ then clearly $S_a^* \cap S_b^* = \emptyset$. If $a \not\geq b$ then $a \cap b < b$ and hence $(S_a^* \cap S_b^*) \subset (S_{a\cap b} \cap S_b^*) = \emptyset$.

(ii) Denote by Z_a the set which is claimed to coincide with S_a^*. For any $x \in X$ there is certainly a $c \in L$ such that $s_c(x) \geq s_b(x)\ \forall b$ and c being minimal with this property. Thus $x \in Z_c$ and $X = \bigcup_{c\in L} Z_c$. By (i) it is now enough to show that $Z_a \subset S_a^*$. Obviously $Z_a \subset S_a \subset \bigcup_{b\leq a} S_b^*$. If $b < a$ then $Z_a \cap S_b = \emptyset$. Therefore $Z_a \subset S_a^*$.

(iii) Since $\Pi_b x \in b \subset S_b$, $x_b \in S_c^*$ for some $c \leq b$. Using this, $x \in S_a^*$, $b \geq a$ and $(S1)$ we find $s_c(x) = s_c(x_b) \geq s_a(x_b) = s_a(x) \geq s_c(x)$. Hence by (ii) $s_c(x) = s_a(x) = s(x)$ and $s_a(x_b) = s_c(x_b) = s(x_b)$ which implies $x \in S_c$ and $c \not> a$. For $c \neq a$ we conclude $x \in S_{a\cap c} \cap S_a^* = \emptyset$. Therefore $a = c$ and $x_b \in S_a^*$. ▮

Smoothing of functions on X of the form $f(x)\chi(x \in S_a^*)$ will be done by averaging with respect to parameters defining $s_a(x)$ and thus S_a^*. This amounts to introducing a whole family of functions $s_a(x,\sigma)$. To ensure that the corresponding sets $S_a(\sigma)$ always satisfy the hypothesis of Lemma 3.5 we now construct sub- and supersets $S_a^\pm$ of S_a and impose conditions on them. Let $s_a^\pm(x)$ be real-valued functions on X obeying

$$\begin{array}{lll} (S2)_\pm & s_a^-(x_a) \geq s_b^+(x_a) & \forall b > a \\ (S3) & s_a^-(x) \leq s_a(x) \leq s_a^+(x) & \forall a \in L \ . \end{array}$$

Define $S_a^\pm := \{x \in X | s_a^\pm(x) \geq s_b^\mp(x) \ \ \forall b > a\}$ and suppose

$$(S4) \quad S_a^+ \cap S_b^+ \subset S_{a\cap b}^- \quad \text{if } a \cap b < a, b \ .$$

Then $S_a^- \subset S_a \subset S_a^+$ by $(S3)$ and therefore by $(S4)$ $S_a \cap S_b \subset S_{a\cap b}$, even if $a \cap b < a, b$. Furthermore $(S2)$ has become a consequence of $(S2)_\pm$ and $(S3)$. So all we need to do before applying Lemma 3.5 is to check $(S1)$, $(S2)_\pm$, $(S3)$, and $(S4)$.

The Graf Function

$G(x)$ is a smooth version of the function $G(x,\sigma) = \frac{1}{2}\max_{a\in L}(x_a^2 + \sigma_a)$. The requirements on G impose conditions on the parameters σ_a. The remaining freedom in their choice is used to regularize $G(x,\sigma)$ by averaging with respect to σ.

Pick $\alpha > 0$ and $\varepsilon \in (0, 1/2)$. For each $a \in L$ define

$$\begin{aligned} \sigma_a^- &:= \alpha\varepsilon^{|a|} \\ \sigma_a^+ &:= 2\sigma_a^- \\ s_a(x,\sigma) &:= \tfrac{1}{2}(x_a^2 + \sigma_a) \\ s_a^\pm(x) &:= s_a(x, \sigma^\pm) \end{aligned}$$

where $|a| := \dim(a)$, $\sigma := (\sigma_a)_{a\in L}$ and similar for $\sigma^\pm$. The sets $S_a^\pm$, $S_a(\sigma)$ and $S_a^*(\sigma)$ are defined by $s_a^\pm(x)$ and $s_a(x,\sigma)$ as above. Since $\varepsilon < 1/2$, $\sigma_a^- \geq \sigma_b^+$ for all $b > a$, which implies $(S2)_\pm$. $s_a(x,\sigma)$ obeys $(S3)$ if $\sigma \in \Sigma := \{\sigma | \sigma_a^- \leq \sigma_a \leq \sigma_a^+\}$, $(S1)$ is obvious and the following lemma provides $(S4)$.

Lemma 3.6 *If ε is smaller than some constant independent of α, then*

$$S_a^+ \cap S_b^+ \subset S_{a\cap b}^- \quad \textit{if } a\cap b < a, b\ .$$

Proof. It easily follows from the definitions that

$$\begin{aligned} S_a^-(\varepsilon) &\supset \{x : |x^a|^2 \le (1-2\varepsilon)\varepsilon^{|a|}\alpha\} && (3.21)\\ S_a^+(\varepsilon) &\subset \{x : |x^a|^2 \le 2\varepsilon^{|a|}\alpha\}\ . && (3.22)\end{aligned}$$

Since $\max(|x^a|, |x^b|)$ is a norm in $(a\cap b)^\perp$, there exists a constant M such that

$$|x^{a\cap b}| \le M \max(|x^a|, |x^b|) \qquad \forall a, b \in L\ . \tag{3.23}$$

Choose $\varepsilon : 0 < 2\varepsilon \le (1+M^2)^{-1}$. If $x \in S_a^+ \cap S_b^+$ and $c := a\cap b < a, b$, then (3.23) and (3.22) imply that

$$|x^c|^2 \le M^2 2 \max(\varepsilon^{|a|}, \varepsilon^{|b|})\alpha \le M^2 2\varepsilon\varepsilon^{|c|}\alpha \le (1-2\varepsilon)\varepsilon^{|c|}\alpha\ .$$

Hence $x \in S_c^-(\varepsilon)$ by (3.21). ∎

Henceforth ε is always assumed to be small enough in the sense of Lemma 3.6.

Lemma 3.7

$$|x|_a > \kappa \qquad \textit{if } x \in S_a^+ \setminus \bigcup_{b<a} S_b^-\ ,$$

where $\kappa^2 := \alpha(1-2\varepsilon)\varepsilon^{|X|} > 0$.

Proof. Trivial for $a = 0$. So let $a > 0$ and $x \in S_a^+ \setminus \bigcup_{b<a} S_b^-$. There is a $b \not\geq a$ such that $|x|_a^2 = |x^b|^2$. For this b, $x \notin S_b^-$, because otherwise $b \not< a$ so that $a \cap b < a, b$ and thus $x \in S_a^+ \cap S_b^- \subset S_{a\cap b}^-$ by Lemma 3.6. By choice of x this is impossible. Consequently there is a $c > b$ such that $x_b^2 + \sigma_b^- = 2s_b^-(x) < 2s_c^+(x) \le x^2 + \sigma_c^+$. Therefore $|x|_a^2 = x^2 - x_b^2 > \sigma_b^- - \sigma_c^+ \ge \alpha(1-2\varepsilon)\varepsilon^{|X|}$. ∎

We now define

$$\begin{aligned} G(x,\sigma) &:= \max_{a\in L} s_a(x,\sigma)\\ G_a(x,\sigma) &:= \max_{b\ge a} s_b(x,\sigma) = \frac{x_a^2}{2} + G_a(x^a,\sigma)\end{aligned}$$

Using Lemma 3.5, the properties of the sets $S_a^\pm$, $S_a(\sigma)$ are easily translated into properties of $G(x,\sigma)$.

Lemma 3.8 *For any $\sigma \in \Sigma$*

$$\begin{array}{rll} (i) & G(x,\sigma) = G(x_a,\sigma) & x \in S_a(\sigma)\\ (ii) & G(x,\sigma) = s_a(x,\sigma) & x \in S_a^*(\sigma)\\ (iii) & G(x,\sigma) = G_a(x,\sigma) & \textit{if } |x|_a^2 \ge \sigma_0^+\ .\end{array}$$

Proof. The remarks preceding Lemma 3.6 establish the hypotheses of Lemma 3.5 for $\sigma \in \Sigma$. (ii) follows from the characterization of $S_a^*(\sigma)$ given in Lemma 3.5. (i) If $x \in S_a(\sigma)$ then $x \in S_b^*(\sigma)$ for some $b \leq a$. By (iii) of Lemma 3.5 also $x_a \in S_b^*(\sigma)$. Now (ii) implies $G(x,\sigma) = s_b(x,\sigma) = s_b(x_a,\sigma) = G(x_a,\sigma)$. (iii) We may assume $a > 0$. $|x^b|^2 \geq \sigma_0^+ \geq \sigma_b^+ \ \forall b \not\geq a$ by assumption on x. Hence $|x_b|^2 + \sigma_b^+ \leq x^2 + \sigma_x^- \ \forall b \not\geq a$, which proves (iii) for $\sigma \in \Sigma$. ∎

For each $a \in L$ pick $m_a \in C_0^\infty(\mathbf{R})$ such that $\mathrm{supp}(m_a) \subset [\sigma_a^-, \sigma_a^+]$, $m_a \geq 0$ and $\int d\lambda m_a(\lambda) = 1$. Let $m(\sigma) := \prod_{a\in L} m_a(\sigma_a)$ and

$$G(x) := \int d\sigma m(\sigma) G(x,\sigma) \ . \tag{3.24}$$

$G(x)$ inherits the properties of $G(x,\sigma)$ and is in addition differentiable:

Theorem 3.9 *For any $R_1 \geq 0$ there exists a function $G \in C^\infty(X)$ with the properties:*

(i) $G(x) = G(x_a)$ *if* $|x^a| \leq R_1$.

(ii) *For each $a \in L$ there is a function $G^a : X^a \to \mathbf{R}$ such that* $G(x) = \frac{1}{2}x_a^2 + G^a(x^a)$ *if* $|x|_a \geq cR_1$.

The constant $c > 1$ is independent of R_1.

Proof. If $R_1 = 0$ then $G(x) = \frac{1}{2}x^2$ is such a function. If $R_1 > 0$ let $G(x)$ be given by (3.24) with α defined by $(1-2\varepsilon)\varepsilon^{|X|}\alpha = R_1^2$. Smoothness of G is proved as in [10]. (i) By (i) of Lemma 3.8 and by (3.21), $G(x) = G(x_a)$ in $S_a^- \supset \{x : |x^a| \leq R_1\}$. (ii) follows from (iii) of Lemma 3.8 and $\sigma_0^+ = 2\alpha = R_1^2 2(1-2\varepsilon)^{-1}\varepsilon^{-|X|}$. ∎

Definition 3.10 *A function with the properties described in the theorem will be called a* G-function *in (X, L) with parameter R_1.*

Lemma 3.11 *If $G(x)$ is a G-function in (X, L) with parameter R_1, then for each $a > 0$ G^a is a G-function in (X^a, L^a) with the same parameter.*

Proof. Let $a \in L\backslash\{0\}$ and fix $y \in a^*$. Then $|y|_a > 0$ and thus $|x^a + sy|_a \geq s|y|_a - |x^a| \to \infty$ as $s \to \infty$. So by definition of G^a

$$G^a(x^a) = G(x^a + sy) - \frac{(sy)^2}{2} \qquad |x^a| \leq \text{const} \tag{3.25}$$

if s is large enough. In particular $G \in C^\infty(X)$ implies $G^a \in C^\infty(X^a)$. Now let $b \geq a$ and assume $|(x^a)^b| \leq R_1$. Then $|(x^a + sy)^b| = |(x^a)^b| \leq R_1$ for all s. Choosing s large we find from (3.25) and (i)

$$G^a(x^a) = G(x^a + sy) - \frac{(sy)^2}{2} = G(x_b^a + sy) - \frac{(sy)^2}{2} = G^a(x_b^a)$$

which proves (i) for G^a. To prove (ii) for G^a pick $x^a \in X^a$ and assume $|x^a|_b^a \geq cR_1$ for some $b \geq a$. Then

$$\begin{aligned} |x^a + sy|_b &= \min\left(|x^a + sy|_b^a, |x^a + sy|_a\right) \\ &= \min\left(|x^a|_b^a, |x^a + sy|_a\right) = |x^a|_b^a \geq cR_1 \end{aligned}$$

for large s, because $|x^a + sy|_a \to \infty$ as $s \to \infty$. Hence for s chosen large enough (ii) tells us that

$$
\begin{aligned}
G^a(x^a) = G(x^a + sy) - \frac{(sy)^2}{2} &= \frac{(x^a + sy)_b^2}{2} + G^b((x^a + sy)^b) - \frac{(sy)^2}{2} \\
&= \frac{(x_b^a)^2}{2} + G^b(x^b)
\end{aligned}
$$

which completes the proof. ∎

As a technical tool we will need partitions of unity adapted to G-functions.

Lemma 3.12 *For any $R_1 \geq 0$ there is a collection of functions $(\eta_a)_{a\in L} \subset C^\infty(X)$ with the properties*

$$
\begin{array}{rl}
(i) & \partial^\alpha \eta_a \in L^\infty(X) \qquad \forall \alpha,\ a \in L\ . \\
(ii) & \sum_{a\in L} \eta_a(x)^2 \equiv 1 \\
(iii) & supp(\eta_a) \subset \{x : |x^a| \leq R_1,\ |x|_a \geq \rho^{-1} R_1\}
\end{array}
$$

where $\rho > 1$ is independent of R_1.

In applications of this partition of unity, the parameter R_1 will be assumed to coincide with the parameter of the G-function currently considered. This is done to achieve $\eta_a G(x) = \eta_a G(x_a)$.

Proof. If $R_1 = 0, \eta_X(x) \equiv 1$ and $\eta_a = 0$ for all $a < X$. Now let $R_1 > 0$. We use the machinery developed to construct $G(x)$, but now define α by $2\alpha = (\frac{1}{2}R_1)^2$. From $S_a^+ \subset \{x : |x^a|^2 \leq 2\alpha\}$ and Lemma 3.7 it follows that

$$
S_a^*(\sigma) \subset \{x : |x^a| \leq \frac{1}{2} R_1,\ |x|_a \geq \delta R_1\}\ , \qquad \sigma \in \Sigma,
$$

where $\delta < 1$ is independent of R_1. Consequently the functions $\chi(x \in S_a^*(\sigma)),\ a \in L$ satisfy (ii) and (iii). Differentiability and (i) are easiest established if we mollify them as follows. Let $\varphi \in C_0^\infty(\Omega)$ with $\mathrm{supp}(\varphi) \subset \{x : |x| \leq \frac{1}{2}\delta R_1\}$, $\varphi \geq 0$, and $\int dx \varphi(x) = 1$. For arbitrary but fixed $\sigma \in \Sigma$ define $\tilde{\eta}_a := \varphi * \chi(S_a^*(\sigma))$. $\tilde{\eta}_a$ has all the required properties except that $\sum \tilde{\eta}_a \equiv 1$ instead of (ii). Therefore the functions

$$
\eta_a(x) := \frac{\tilde{\eta}_a(x)}{\left(\sum_{b\in L} \tilde{\eta}_b(x)^2\right)^{1/2}}
$$

are in $C^\infty(X)$ and satisfy (i) to (iii). ∎

Lemma 3.13 *Assume $(I4)$ on the intercluster potentials and let G be a G-function in (X, L) with parameter R_1. Then*

$$
\begin{array}{rll}
(i) & \sup_{x\in X} \left|\partial^\alpha \left(G(x) - \frac{1}{2}x^2\right)\right| < \infty & \textit{all } \alpha \\
(ii) & (1+T)^{-1/2} \nabla G \nabla V (1+T)^{-1/2} \in \mathcal{B}(\mathcal{H}) & \textit{if } R_1 > \rho R_0
\end{array}
$$

with ρ as defined in Lemma 3.12.

Proof. (i) is proved by induction.

$$\sup_{x^a\in X^a}\left|\partial^\alpha\left(G^a(x^a)-\frac{1}{2}(x^a)^2\right)\right|<\infty \qquad \forall\alpha \tag{3.26}$$

is trivial for $a=X$. Now suppose (3.26) holds for all $a>0$. If $|x|_a\geq cR_1$, then $G(x)-\frac{1}{2}x^2=G^a(x^a)-\frac{1}{2}(x^a)^2$ by (ii) of Theorem 3.9 and therefore

$$\sup_{|x|_a\geq cR_1}\left|\partial^\alpha\left(G(x)-\frac{1}{2}x^2\right)\right|<\infty \qquad \forall\alpha, a>0$$

by the induction hypothesis. Because $\bigcup_{a>0}\{|x|_a\geq cR_1\}=X\backslash$ compact , this proves (i). (ii) Let $(\eta_a)_{a\in L}$ be the partition of unity given by Lemma 3.12. Then

$$\nabla G\nabla V(x)=\sum_{a>0}\nabla G\nabla I_a\eta_a^2(x)$$

by construction of $(\eta_a)_{a\in L}$. Since $\mathrm{supp}(\eta_a)\subset\{x:|x|_a\geq\rho^{-1}R_1\}$ (ii) follows from $(I4)$ if $R_1>\rho R_0$. ∎

3.4 A Mourre Estimate

In this subsection we prove Theorem 2.4 following the strategy employed for the proof of the original Mourre theorem in [15]. The use of A instead of the generator of dilations requires only a minor modification thereof.

One ingredient in the proof in [15] is the virial theorem. Somewhat surprising our proof of this theorem for A depends on the fact that G has property (i) in Theorem 3.9. This, however, has a good reason which is explained in the remark after Lemma 3.15. We regard it as an indication that A is the proper substitute for the generator of dilations in the hard-core problem.

Theorem 3.14 *Assume $(I1)$ and $(I4)$ on the intercluster potentials and let $R_1>\rho R_0$. If $\varphi,\psi\in D(H)$, $H\varphi=E\varphi$, and $H\psi=E\psi$, then*

$$\langle\varphi|i[H,A]|\psi\rangle=0\ .$$

In the next theorem we use the notations

$$\begin{aligned}
G_\varepsilon(x) &:= \frac{1}{\varepsilon}\left(1-e^{-\varepsilon G}\right)\\
A_\varepsilon &:= \frac{1}{2}(p\nabla G_\varepsilon+\nabla G_\varepsilon p)\\
i[H,A_\varepsilon] &:= pG_\varepsilon''p-\frac{1}{4}\Delta^2G_\varepsilon-\nabla G_\varepsilon\nabla V\ .
\end{aligned}$$

G_ε'', Δ^2G_ε are bounded, and if $R_1>\rho R_0$, $\nabla G_\varepsilon\nabla V$ is relatively form-bounded with respect to T. Hence $\langle i[H,A_\varepsilon]\rangle$ is bounded in $H_0^1(\Omega)$.

Lemma 3.15 *Assume $(I1)$ and $(I4)$ on the intercluster potentials and let $R_1>\rho R_0$. If $\varphi\in D(H)$ then*

$$i\langle H\varphi|A_\varepsilon\varphi\rangle-i\langle A_\varepsilon\varphi|H\varphi\rangle=\langle\varphi|i[H,A_\varepsilon]|\varphi\rangle\ .$$

Remark. Since A_ε is H-bounded and $i[H,A_\varepsilon]$ is form-bounded with respect to H, this theorem implies that $A_\varepsilon \upharpoonright D(H)$ is essentially self-adjoint (cf. Nelson's commutator theorem, see [19, Theorem X.37]), a property which we would not expect if the flow corresponding to ∇G left Ω. This explains why the structure of ∇G is important for the proof.

Proof of Theorem 3.14. It is enough to do the proof in the case $\psi = \varphi$. Since $A_\varepsilon \subset A_\varepsilon^*$, Lemma 3.15 implies that $\langle\varphi|i[H,A_\varepsilon]|\varphi\rangle = 0$. So it remains to show that $\langle\varphi|i[H,A_\varepsilon]|\varphi\rangle \to \langle\varphi|i[H,A]|\varphi\rangle$ as $\varepsilon \to 0$. This is done by applying Lebesgue's dominated convergence theorem to each of the three terms in the definition of $i[H,A_\varepsilon]$ separately. ∎

Proof of Lemma 3.15. The strategy is to localize both quadratic forms, the one on the left and the one on the right side, by a suitable partition of unity. In step 1 and step 2 we show that the localization errors, and in step 3 that the localized parts coincide. Let $(\eta_a)_{a\in L}$ be the partition of unity of Lemma 3.12. To localize a bounded form q in $\mathcal{H}_2$ we will use the following technique. Let $K \in \mathcal{L}(\mathcal{H}_2, \mathcal{H}_{-2})$ be the operator corresponding to the form q. By Lemma 2.2 multiplication with η_a is a bounded operator in $\mathcal{H}_2$, $\mathcal{H}$ and $\mathcal{H}_{-2}$. One therefore has the usual localization formula

$$K = \sum_{a\geq 0} \eta_a K \eta_a + \frac{1}{2}[[K,\eta_a],\eta_a] \ .$$

If $K = AB$ with $B \in \mathcal{B}(\mathcal{H}_2,\mathcal{H})$ and $A \in \mathcal{B}(\mathcal{H},\mathcal{H}_{-2})$ the double commutator on the right side is evaluated by the "Leibnitz rule"

$$[[AB,\eta_a],\eta_a] = A[[B,\eta_a],\eta_a] + 2[A,\eta_a][B,\eta_a] + [[A,\eta_a],\eta_a]B \ .$$

Henceforth $\varphi_a = \eta_a\varphi$.

Step 1.

$$i\langle\varphi|[H,A_\varepsilon]|\varphi\rangle = \sum_{a>0} i\langle\varphi_a|[H,A_\varepsilon]|\varphi_a\rangle - \langle\varphi|\nabla\eta_a G_\varepsilon'' \nabla\eta_a|\varphi\rangle \ .$$

Split $p_k G_{\varepsilon,kl} p_l$ into $G_{\varepsilon,kl}p_l \in \mathcal{B}(\mathcal{H}_2,\mathcal{H})$ and $p_k \in \mathcal{B}(\mathcal{H},\mathcal{H}_{-2})$ and apply the Leibnitz rule to the double commutator. The terms with $a=0$ vanish because $G(x) = G(0)$ on $\mathrm{supp}(\eta_{a=0})$.

Step 2.

$$i\langle H\varphi|A_\varepsilon\varphi\rangle - i\langle A_\varepsilon\varphi|H\varphi\rangle = \sum_{a>0} i\langle H\varphi_a|A_\varepsilon\varphi_a\rangle - i\langle A_\varepsilon\varphi_a|H\varphi_a\rangle - \langle\varphi|\nabla\eta_a G_\varepsilon''\nabla\eta_a|\varphi\rangle \ .$$

H and A_ε are bounded operators from $\mathcal{H}_2$ to $\mathcal{H}$ and from $\mathcal{H}$ to $\mathcal{H}_{-2}$. Applying the Leibnitz rule to HA_ε and $A_\varepsilon H$ and subtracting the results gives a sum of three threefold commutators. One vanishes because $[[A_\varepsilon,\eta_a],\eta_a] = 0$, the other two yield the localization error.

Step 3.

$$i\langle H\varphi_a|A_\varepsilon\varphi_a\rangle - i\langle A_\varepsilon\varphi_a|H\varphi_a\rangle = \langle\varphi_a|pG_\varepsilon''p - \tfrac{1}{4}\Delta^2 G_\varepsilon - \nabla G_\varepsilon \nabla V|\varphi_a\rangle \ .$$

In the proof of this step, (*iii*) refers to (*iii*) in Lemma 3.12. By this property and Lemma 3.2

$$H_a\mathcal{J}_a\varphi_a = \mathcal{J}_a(H\varphi_a - I_a\varphi_a) \; .$$

Let $\tilde{A}_\varepsilon := \frac{1}{2}(p(a)\nabla G_\varepsilon + \nabla G_\varepsilon p(a))$. Then by (2.4) $\mathcal{J}_a A_\varepsilon = \tilde{A}_\varepsilon \mathcal{J}_a$ in $D(H)$. Therefore

$$\begin{aligned} & i[\langle H\varphi_a|A_\varepsilon\varphi_a\rangle - \langle A_\varepsilon\varphi_a|H\varphi_a\rangle] \\ &= i[\langle H_a\mathcal{J}_a\varphi_a|\tilde{A}_\varepsilon\mathcal{J}_a\varphi_a\rangle - \langle \tilde{A}_\varepsilon\mathcal{J}_a\varphi_a|H_a\mathcal{J}_a\varphi_a\rangle] \qquad (3.27) \\ & \quad + i[\langle I_a\varphi_a|A_\varepsilon\varphi_a\rangle - \langle A_\varepsilon\varphi_a|I_a\varphi_a\rangle] \qquad (3.28) \end{aligned}$$

Consider (3.28). If $\varphi \in C_0^\infty(\Omega)$ then

$$i[\langle I_a\varphi_a|A_\varepsilon\varphi_a\rangle - \langle A_\varepsilon\varphi_a|I_a\varphi_a\rangle] = -\langle\varphi_a|\nabla G_\varepsilon\nabla I_a|\varphi_a\rangle = -\langle\varphi_a|\nabla G_\varepsilon\nabla V|\varphi_a\rangle$$

where we used (*iii*) again. This extends to $Q(H)$ since the forms on both sides are bounded in $\mathcal{H}_1$ and $C_0^\infty(\Omega)$ is dense in $\mathcal{H}_1$.

To evaluate (3.27) note that, by (*iii*), $\tilde{A}_\varepsilon\mathcal{J}_a\varphi_a = (B_a \otimes 1)\mathcal{J}_a\varphi_a$ where $B_a = \frac{1}{2}(p_a\nabla G_\varepsilon(x_a) + \nabla G_\varepsilon(x_a)p_a)$. Furthermore $H_a = (\frac{1}{2}p_a^2 \otimes 1) + (1 \otimes H^a)$ and $D(H_a) = D(\frac{1}{2}p_a^2 \otimes 1) \cap D(1 \otimes H^a)$. $1 \otimes H^a$ can be interchanged with $B_a \otimes 1$ and gives thus no contribution. For all $\alpha, \beta \in C_0^\infty(a)$ we have

$$i\langle\tfrac{1}{2}p_a^2\alpha|B_a\beta\rangle - i\langle B_a\beta|\tfrac{1}{2}p_a^2\alpha\rangle = \langle\alpha|p_aG_\varepsilon''(x_a)p_a - \tfrac{1}{4}\Delta^2G_\varepsilon(x_a)|\beta\rangle \; .$$

This extends to $D(p_a^2)$ because $C_0^\infty(a)$ is a core of p_a^2. The corresponding equation for $\frac{1}{2}p_a^2 \otimes 1$ and $B_a \otimes 1$ in $\mathcal{H}_a$ extends from $D(\frac{1}{2}p_a^2) \otimes L^2(\Omega^a)$ to $D(\frac{1}{2}p_a^2 \otimes 1) \supset D(H_a)$. This proves the first equation of

$$\begin{aligned} & i\left[\langle(\tfrac{1}{2}p_a^2 \otimes 1)\mathcal{J}_a\varphi_a|\tilde{A}_\varepsilon\mathcal{J}_a\varphi_a\rangle - \langle\tilde{A}_\varepsilon\mathcal{J}_a\varphi_a|(\tfrac{1}{2}p_a^2 \otimes 1)\mathcal{J}_a\varphi_a\rangle\right] \\ &\quad = \langle\mathcal{J}_a\varphi_a|p_aG_\varepsilon''(x_a)p_a - \tfrac{1}{4}\Delta^2G_\varepsilon(x_a)|\mathcal{J}_a\varphi_a\rangle = \langle\varphi_a|pG_\varepsilon''(x)p - \tfrac{1}{4}\Delta^2G_\varepsilon(x)|\varphi_a\rangle \; . \end{aligned}$$

The second follows from (*iii*). The proof of step 3 is thus complete. Step 1, 2 and 3 combined prove the theorem. ▮

Henceforth (*I*1), (*I*3), (*I*4) and $R_1 > \rho R_0$ are tacitly assumed, and $\Delta \ni E$ denotes an open interval Δ containing E. Theorem 2.4 has the following two important corollaries.

Corollary 3.16 *If $E \in \mathbf{R}$ in not an eigenvalue of H, then for each $\varepsilon > 0$ there is a $\Delta \ni E$ such that*

$$E_\Delta(H)i[H, A]E_\Delta(H) \geq [\Theta(E) - \varepsilon]E_\Delta(H) \; .$$

Corollary 3.17 *Non-threshold eigenvalues of H have finite multiplicities and can accumulate only at thresholds or $+\infty$. $\tau(H)$ is closed and countable.*

The proof of Theorem 2.4 goes by induction and makes use of these corollaries for subsystems. For their proofs the reader is referred to [15] or [4].

Proof of Theorem 2.4. Let $B_\Delta(H) := E_\Delta(H) i[H,A] E_\Delta(H)$ for short. Since $B_\Delta(H^X) = 0$ and $\Theta^X(E) \equiv 0$ the theorem for $a = X$ is obviously true. Let $G_a := \frac{1}{2}x_a^2 + G^a$. For $a > 0$ define

$$i[H_a, A_a] := pG_a''p - \frac{1}{4}\Delta^2 G_a - \nabla G_a \nabla V^a$$

as a form in $\mathcal{H}_a$ with domain $H_0^1(\Omega_a)$, and let

$$B_\Delta(H_a) := E_\Delta(H_a) i[H_a, A_a] E_\Delta(H_a) \ .$$

We claim that for each $E \in \mathbf{R}$ and $\varepsilon > 0$ there is a $\Delta \ni E$ such that

$$B_\Delta(H_a) \geq [\Theta(E+\varepsilon) - 3\varepsilon] E_\Delta(H_a) \ . \tag{3.29}$$

In [15] this is proved in three steps for $x^2/2$ instead of $G(x)$. Steps 1 and 2 carry over literally including proofs. With our definition of $B_\Delta(H_a)$ this is also true for the third step, which is the statement above. One only needs to note that

$$i[H_a, A_a] = p_a^2 \otimes 1 + 1 \otimes i[H^a, A^a]$$

in the sense of a form sum. It is the step 1 where the virial theorem is used. We now derive the theorem from (3.29).

Let $(j_a)_{a \in L} \subset C^\infty(X)$ be a Ruelle-Simon partition of unity (cf. Lemma 3.3). By the properties of G and j_a we may achieve that $j_a G = j_a G_a$ by scaling the functions j_a. For given $E \in R$, $\varepsilon > 0$ pick Δ that satisfies (3.29) and $f \in C_0^\infty(\Delta)$ with $f \equiv 1$ in some $\Delta_1 \ni E$. Because p_k is in $\mathcal{B}(\mathcal{H}_1, \mathcal{H})$ and $\mathcal{B}(\mathcal{H}, \mathcal{H}_{-1})$, and multiplication by j_a is a bounded operator in $\mathcal{H}_1$, $\mathcal{H}$ and $\mathcal{H}_{-1}$, the operator $i[H,A] \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{-1})$ can be localized using the technique employed in the proof of the virial theorem. This gives

$$i[H,A] = \sum_{a \geq 0} j_a i[H,A] j_a - \frac{1}{2} \nabla j_a G'' \nabla j_a \ .$$

By construction of j_a and assumption on ∇I_a we have for $a > 0$

$$j_a i[H,A] j_a = J_a^* i[H_a, A_a] J_a - j_a^2 \nabla G_a \nabla I_a$$

as a sum of bounded forms in $H_0^1(\Omega)$. Since $H_0^1(\Omega) \supset \mathcal{H}_1$ this can also be read as a sum of operators in $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_{-1})$. Combining these two equations we find

$$f(H) i[H,A] f(H) = \sum_{a>0} f(H) J_a^* i[H_a, A_a] J_a f(H) + \text{compact} \ .$$

The next step is to replace $J_a f(H)$ by $f(H_a) J_a$. To this end we need that

$$(H_a + i)^{1/2} [J_a f(H) - f(H_a) J_a] \in \mathcal{B}(\mathcal{H}, \mathcal{H}_a) \text{ and is compact} \ . \tag{3.30}$$

Boundedness follows from $J_a \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{a,1})$ and compactness is shown after this proof. Using (3.30), the construction of f, inequality (3.29), $\mathcal{J}_a^* \mathcal{J}_a = 1_\mathcal{H}$ and finally local compactness to restore the $a = 0$ term we arrive at

$$f(H) i[H,A] f(H) \geq [\Theta(E+\varepsilon) - 3\varepsilon] f(H)^2 + \text{compact} \ .$$

After multiplying from both sides with $E_{\Delta_1}(H)$ we get an estimate that is apparently weaker but in fact equivalent to the Mourre estimate. To see this, note that $\tau(H)$ is closed as a consequence of Corollary 3.17 for subsystems. Hence for $E \notin \tau(H)$ and ε small enough $\Theta(E+\varepsilon) - 2\varepsilon = \Theta(E)$. ▮

Proof of (3.30). By the functional calculus of Helffer and Sjöstrand [13] it is enough to prove that

$$(H_a + i)^{1/2}[J_a(z-H)^{-1} - (z-H_a)^{-1}J_a] \in \mathcal{B}(\mathcal{H}, \mathcal{H}_a)$$

is compact for $\mathrm{Im}(z) \neq 0$. Taking the resolvents out of the square brackets and using Lemma 3.2 and Lemma 2.2 to evaluate $J_a H - H_a J_a$ we arrive at

$$(H_a + i)^{1/2}(z-H_a)^{-1}\left[\mathcal{J}_a(i\nabla j_a p + \frac{1}{2}\Delta j_a) + J_a I_a\right](z-H)^{-1} .$$

The first two terms in this sum are compact by local compactness. To see compactness of the third term pick a bounded function $f \in C^\infty(\Omega)$ with bounded derivatives, $\mathrm{supp}(f) \subset \{x : |x|_a \geq R_0 + 1/2\}$ and $j_a = j_a f$. Then

$$(z-H_a)^{-1/2} J_a I_a (z-H)^{-1} = (z-H_a)^{-1/2} J_a (z-H)^{1/2} (z-H)^{-1/2} f I_a f (z-H)^{-1}$$

which is compact by $(I3)$ and $J_a^* \in \mathcal{B}(\mathcal{H}_{a,1}, \mathcal{H}_1)$ ▮

4 Asymptotic Completeness

4.1 Introduction

In this section we prove existence and completeness of the wave operators (2.7) as well as the remaining statements in Theorem 2.6. Up to technical difficulties due to the hard cores, the proof of completeness is a simplified version of the one given in [15], which in turn is a variant of Yafaev's proof [22].

Our proof of completeness of the wave operators is divided into two independent parts. The first part consists of the construction of (unbounded) operators W and $(W_a)_{a\in L}$ with domain $D(H)$ such that

$$\|W\varphi - \sum_{a>0} e^{iHt}\mathcal{J}_a^* e^{-iH_a t} W_a \varphi\| \to 0 \qquad (t \to \infty) \tag{4.1}$$

for all $\varphi \in D(H)$, while in the second part we show that Ran W is dense in $\mathcal{H}_{\mathrm{cont}}$. Completeness then follows by an inductive argument and from the fact that the range of a wave operator is closed.

The construction of the asymptotic observable W and the so called Deift-Simon wave operators W_a is based on a suitable partition of the configuration space X and a time dependent function $g_t(x)$ on X related to this partition. These geometric objects differ from those introduced in the last section, although there are common features. Most important with regard to the hard cores is that $\nabla g_t(x)$, like $\nabla G(x)$, is "parallel to $\partial\Omega$" near $\partial\Omega$ at least for large t. Unlike the Graf function, however, g_t is homogeneous for large $|x|$ and this is important in the proof of existence of

W_a. The change of $g_t(x)$ with time t can be understood as coming from a rescaling of the underlying partition of X with a factor t^δ for some suitable $\delta < 1$. Thanks to this rescaling the operators W, W_a exist globally (with respect to the energy) and independent of the spectral properties of H.

Density of Ran W in $\mathcal{H}_{\text{cont}}$ is derived from the following stronger result: the closure $\overline{W}$ of W is self-adjoint, commutes with H, and

$$\overline{W}^2 \geq \theta(H) > 0 \qquad \text{in } \mathcal{H}_{\text{cont}} , \tag{4.2}$$

where $\theta(E)$ is the Mourre constant. The first inequality is precisely what one expects from physical reasoning: for a state of the systems which breaks up into independently moving bound clusters, W^2 measures the asymptotic value (or a quantity slightly larger) of twice the kinetic energy associated with the centers of mass of the clusters. This should be bounded below by $\theta(E)$ if the total energy of the state is centered around E. The inequality (4.2) confirms this. It is the proof of (4.2) (both inequalities) where Theorem 2.4 and its corollaries are used.

This section is organized as follows. In Subsection 4.2 we construct the partition of X mentioned above and the associated functions g and g_a which are used later in the definitions of W and W_a. In 4.3 the propagation estimate is derived which will be the main tool to prove existence of these operators. There we also collect some notations used later on. In 4.4 existence of $W_a, W_a^\dagger$ and W is proved. In 4.5 we first prove existence of the wave operators, then (4.2) and finally asymptotic completeness.

4.2 Yafaev Functions

This section is devoted to the construction of the functions g and g_a which occur in the definitions of asymptotic observable and Deift-Simon wave operators. The construction closely parallels the one of the Graf function and in particular it is also based on the general results at the beginning of Subsection 3.3. We shall call functions sharing the properties of g and g_a Y-functions (Y for Yafaev). The importance of this notion is that the Hessian of any Y-function is dominated by the Hessian of a convex Y-function, and that any convex Y-function obeys our propagation estimate.

Pick $\alpha \geq 0,\ \varepsilon \in (0, 1/2)$ and define

$$\begin{array}{rcll} \sigma_a^- &:=& (1-\varepsilon^{|a|})^{-1/2} & a > 0 \\ \sigma_a^+ &:=& (1-2\varepsilon^{|a|})^{-1/2} & a > 0 \\ \sigma_0^\pm &:=& \alpha & \\ s_a(x,\sigma) &:=& \sigma_a |x_a| & a > 0 \\ s_0(x,\sigma) &:=& \alpha & \\ s_a^\pm(x) &:=& s_a(x,\sigma^\pm) & a \in L \ . \end{array}$$

$|a|, \sigma,\ \sigma^\pm,\ \Sigma,\ S_a^\pm,\ S_a(\sigma)$ and $S_a^*(\sigma)$ are defined as in Subsection 3.3. We write $S_a^\pm(\alpha, \varepsilon)$ for $S_a^\pm$ when we want to exhibit the dependence on α and ε. $(S1),\ (S2)_\pm$ and $(S3)$ are again satisfied and $(S4)$ is provided by:

Lemma 4.1 *If ε is smaller than some constant independent of α, then*

$$S_a^+ \cap S_b^+ \subset S_{a\cap b}^- \quad \textit{if } a \cap b < a, b \ .$$

Proof. We only show that

$$
\begin{aligned}
S_a^-(\varepsilon) &\supset \{x : |x^a|^2 \leq (1-2\varepsilon)\varepsilon^{|a|}|x|^2\} && (4.3)\\
S_a^+(\varepsilon) &\subset \{x : |x^a|^2 \leq 2\varepsilon^{|a|}|x|^2\} && (4.4)
\end{aligned}
$$

for all $a \in L$. Due to the similarity of (4.3) and (4.4) to (3.21) and (3.22) the rest of the proof is then a copy of the proof of Lemma 3.6 with α replaced by $|x|^2$. The cases $a = 0$ and $a = X$ are almost trivial, let us assume $0 < a < X$. Then $x \in S_a^+$ implies

$$
|x^a|^2 \leq \left(1 - \frac{(\sigma_X^-)^2}{(\sigma_a^+)^2}\right)|x|^2 \leq \left(1 - \frac{1}{(\sigma_a^+)^2}\right)|x|^2 = 2\varepsilon^{|a|}|x|^2 ,
$$

which is (4.4). In order that $x \in S_a^-$ it suffices that

$$
|x^a|^2 \leq \left(1 - \frac{(\sigma_b^+)^2}{(\sigma_a^-)^2}\right)|x|^2 \qquad \forall b > a .
$$

But if $b > a$ then

$$
1 - \frac{(\sigma_b^+)^2}{(\sigma_a^-)^2} = \frac{\varepsilon^{|a|} - 2\varepsilon^{|b|}}{1 - 2\varepsilon^{|b|}} > (1-2\varepsilon)\varepsilon^{|a|} .
$$

∎

Henceforth ε is always assumed to be small enough in the sense of this lemma.

Lemma 4.2

$$
|x|_a \geq \kappa|x| \qquad \textit{if } x \in S_a^+ \setminus \bigcup_{b<a} S_b^- ,
$$

where $\kappa^2 = (1-2\varepsilon)\varepsilon^{|X|} > 0$.

Proof. If $|x|_a = |x|$ this is trivial, and otherwise it follows from the proof of Lemma 3.7 with the new definition for $s_a^{\pm}(x)$ given above. ∎

We now define

$$
\begin{aligned}
g(x,\sigma) &:= \max_{a\in L} s_a(x,\sigma)\\
g_a(x,\sigma) &:= g(x,\sigma)\chi(x \in S_a^*(\sigma)) .
\end{aligned}
$$

Lemma 4.3 *For any* $\sigma \in \Sigma$

$$
\begin{array}{rll}
(i) & g(x,\sigma) = \sum_{a\in L} g_a(x,\sigma) & \\
(ii) & g(x,\sigma) = s_a(x,\sigma) & x \in S_a^*(\sigma)\\
(iii) & g_a(x,\sigma) = g_a(x_b,\sigma) & x \in S_b(\sigma) .
\end{array}
$$

Proof. (i) and (ii) follow from (i) and (ii) of Lemma 3.5. (iii) Let $x \in S_b(\sigma)$. $g(x,\sigma) = g(x_b,\sigma)$ is seen in the same way as (i) of Lemma 3.8. If $b \not\geq a$ then $\chi(x \in S_a^*(\sigma)) = 0 = \chi(x_b \in S_a^*(\sigma))$ because $a \cap b < a$ and hence $S_b \cap S_a^* \subset (S_{b\cap a} \cap S_a^*) = \emptyset$. If $b \geq a$ then $\chi(x \in S_a^*(\sigma)) = \chi(x_b \in S_a^*(\sigma))$ because $x \in S_a^* \Leftrightarrow x_b \in S_a^*$ by the remark after Lemma 3.5. ∎

To regularize the functions $g(x,\sigma)$ and $g_a(x,\sigma)$ choose $m_a \in C_0^\infty(\mathbf{R})$ as in Subsection 3.3 and set $m(\sigma) := \prod_{a>0} m_a(\sigma_a)$ and

$$g(x) \;:=\; \int d\sigma m(\sigma) g(x,\sigma) \tag{4.5}$$

$$g_a(x) \;:=\; \int d\sigma m(\sigma) g_a(x,\sigma)\ , \qquad a \in L\ . \tag{4.6}$$

Definition 4.4 *A function $f : X \to \mathbf{R}$ is a* Y-function *if $f \in C^\infty(X)$ and there are constants $\alpha, \beta, \varepsilon \in \mathbf{R}_+,\ \alpha < \beta$, such that*

$$\begin{array}{ll} (i) & f(x) = f(x_a) \qquad x \in S_a^-(\alpha,\varepsilon),\ a \in L \\ (ii) & f(\lambda x) = \lambda f(x) \quad \text{if } \lambda \geq 1,\ |x| \geq \beta\ , \end{array}$$

and ε is small enough in the sense of Lemma 4.1.

Lemma 4.5 *The functions g and $(g_a)_{a\in L}$ constructed above are Y-functions, g is convex, $\sum_{a\in L} g_a(x) = g(x) \geq \max(\alpha, |x|)$ and moreover*

$$\begin{array}{ll} (i) & supp(g_0) \subset \{x : |x| \leq \alpha\} \\ (ii) & supp(g_a) \subset \{x : |x|_a \geq \kappa |x|,\ |x| \geq \alpha(1-2\varepsilon)^{1/2}\} \quad \text{if } a > 0\ , \end{array}$$

where $\kappa > 0$.

Proof. The support properties follow from $\text{supp}(g_a) \subset S_a^+ \setminus \bigcup_{b<a} S_b^-$, Lemma 4.2, and from

$$S_0^-(\alpha,\varepsilon) \;\supset\; \{x : |x| \leq (1-2\varepsilon)^{1/2}\alpha\} \tag{4.7}$$

$$S_0^+(\alpha,\varepsilon) \;\subset\; \{x : |x| \leq \alpha\}\ . \tag{4.8}$$

Apart from the differentiability the other statements follow easily from the construction and Lemma 4.3. To prove $g_a \in C^\infty(X;\mathbf{R})$ for $a > 0$, let $\rho = (\rho_b)_{b>0} \in \mathbf{R}^{\#L-1}$ and define

$$f_a(\rho) := \int \prod_{b>0} d\sigma_b m_b(\sigma_b) \sigma_a \rho_a \Theta(\sigma_a\rho_a - \max_{b>0}(\alpha, \sigma_b\rho_b))\ . \tag{4.9}$$

Here $\Theta(.)$ is the characteristic function of $[0,\infty)$. Then $g_a(x) = f_a(\rho)|_{\rho_b = |x_b|}$. Since f_a is independent of ρ_b if ρ_b is small, the last equation remains true when $|x_b|$ is replaced by a suitable function $\rho_b \in C^\infty(X;\mathbf{R}_+)$ which coincides with $|x_b|$ outside a neighborhood of $b^\perp$. Hence $g_a = f_a \circ \rho$ for some $\rho \in C^\infty(X;\mathbf{R}_+^{\#L-1})$. To see that $f_a \in C^\infty(\mathbf{R}_+^{\#L-1};\mathbf{R})$ substitute $\sigma_b \to \frac{\sigma_b}{\rho_b}$ in (4.9) and use that $m_b \in C_0^\infty(\mathbf{R}_+)$. The same arguments with $\sigma_a\rho_a$ replaced by α in (4.9) show that also $g_0 \in C^\infty(X)$. ∎

We will often need a partition of unity $(\rho_a)_{a\in L} \subset C^\infty(X,\mathbf{R})$ adapted to given Y-functions, i.e., with the properties

$$\begin{array}{lll} (i) & \partial^\alpha \rho_a \in L^\infty(X) & \forall \alpha,\ a \in L \\ (ii) & \sum_{a\in L} \rho_a(x)^2 \equiv 1 & \\ (iii) & \text{supp}(\rho_a) \subset S_a^-(\alpha,\varepsilon) \cap \{x : |x|_a \geq c\} & \forall a \in L \end{array}$$

for some $c > 0$. To obtain such a partition pick $(j_a)_{a\in L}$ as given by Lemma 3.3 with $\gamma^2 \leq (1-2\varepsilon)\varepsilon^{|X|}$ and set $\rho(x) = j_a(\lambda x),\ \lambda > 0$. By (4.3) and (4.7) $(\rho_a)_{a\in L}$ then has the desired properties if λ is large enough.

Theorem 4.6 *Suppose f is any Y-function. Then there exists a convex Y-function $\tilde g$ such that*

$$\pm f''(x) \le \tilde g''(x) \qquad x \in X \ .$$

Proof. Let α, β be the parameters of f. For any fixed $y \in X \backslash \{0\}$ we will construct a convex Y-function g_y which is a local bound in the sense that

$$\begin{aligned} \pm f''(x) &\le g_y''(x) \qquad x \in U_y & (4.10)\\ \pm f''(\lambda x) &\le g_y''(\lambda x) \qquad x \in U_y \cap \{|x| \ge \beta\},\ \lambda \ge 1 & (4.11) \end{aligned}$$

where U_y is a neighborhood of y. A finite sum $\tilde g$ of such local bounds satisfies (4.10) and (4.11) with U_y replaced by the compact set $\{\alpha(1-2\varepsilon)^{\frac{1}{2}} \le |x| \le \beta\}$. Since convex Y-functions form a positive cone, and since $f(x) = f(0)$ for $|x| \le \alpha(1-2\varepsilon)^{\frac{1}{2}}$, the theorem then follows. Now let $y \in X \backslash \{0\}$. Since $y \in a^*$ for some $a > 0$, there exists a convex Y-function h (constructed like $g = \sum g_a$) with $h(x) = \sigma |x_a|$ and $h(\lambda x) = \lambda h(x)$ for $\lambda \ge 1$, both in a neighborhood of y. Thus

$$h''(x) = \sigma \frac{\pi_a(x)}{|x_a|}$$

near y, where $\pi_a(x)$ is the projection

$$\pi_a(x) z = z_a - \frac{x_a(x_a z)}{|x_a|^2} \ ,$$

which has rank $\dim(a) - 1$. Near y, $f(x) = f(x_a)$, so that $f''(x) \le \text{const}\ 1_a$. But if $\alpha(1-2\varepsilon)^{\frac{1}{2}} \le |x| \le \beta$, $f''(x)$ may have full rank in a. For this reason we modify h as follows. Let $m \in C_0^\infty(\mathbf{R}_+)$, with $\int m(\lambda) d\lambda = 1$, $m \ge 0$ and $m(h(y)) > 0$, and define

$$g_y(x) := \int d\lambda m(\lambda) \max(\lambda, h(x)) \ .$$

Then a simple computation yields

$$\begin{aligned} (\partial_i \partial_k g_y)(x) &= (\partial_i \partial_k h)(x) \int_0^{h(x)} d\lambda\, m(\lambda) + (\partial_i h)(x)(\partial_k h)(x) m(h(x)) \\ &= \sigma \frac{\pi_a(x)_{ik}}{|x_a|} \int_0^{h(x)} d\lambda\, m(\lambda) + \sigma (1 - \pi_a(x))_{ik} m(h(x)) \end{aligned}$$

where the second equality holds for $x \in \lambda U_y$, $\lambda \ge 1$ and a neighborhood U_y of y. Hence

$$\begin{aligned} g_y''(x) &\ge \text{const}\ 1_a\ , \qquad x \in U_y & (4.12)\\ g_y''(\lambda x) &\ge \text{const}\ \frac{\pi_a(x)}{\lambda}\ , \qquad x \in U_y,\ \lambda \ge 1 & (4.13) \end{aligned}$$

with positive constants, if U_y is small enough. Since

$$f''(\lambda x) \le \text{const}\ \frac{\pi_a(x)}{\lambda}\ , \qquad x \in S_a^- \cap \{|x| \ge \beta\}, \lambda \ge 1\ ,$$

by homogeneity of f, after multiplying g_y with a constant, (4.10) and (4.11) follow from (4.12) and (4.13) for the neighborhood $U_y \cap S_a^-$ of y. ∎

Lemma 4.7 *Assume (I2) on the intercluster potentials. Suppose g is a Y-function and let $g_t(x) = t^\delta g(t^{-\delta}x)$ for some $\delta \in (0,1)$. Then*

$$\begin{array}{lll} (i) & \sup_{x\in X} \left|\partial_t^k \partial^\alpha g_t(x)\right| \leq const\ t^{\delta(1-|\alpha|)-k} & all\ t \geq 1,\ if\ |\alpha| + k > 0\ . \\ (ii) & \|(1+T)^{-1/2}\nabla g_t \nabla V(1+T)^{-1/2}\| \leq const\ t^{-\delta\mu} & for\ t\ large\ enough. \end{array}$$

Proof. (i) For $k = 0$ this follows from $\partial^\alpha g_t = t^{-\delta|\alpha|}(\partial^\alpha g)_t$ and $\|(\partial^\alpha g)_t\|_\infty = O(t^\delta)$ if $\alpha \neq 0$. Now let $k > 0$. $\partial_t^k \partial^\alpha g_t(x) = 0$ if $|x| \geq t^\delta\beta$ because then $g_t(x)$ and hence $\partial^\alpha g_t(x)$ is independent of t. To obtain the bound if $|x| \leq t^\delta\beta$, compute

$$\partial_t^k \partial^\alpha g_t(x) = \partial_t^k \left[t^{-\delta|\alpha|}(\partial^\alpha g)_t(x)\right]$$

by means of the Leibnitz rule and use that $\sup_{|x|\leq t^\delta\beta} |\partial_t^m f_t(x)| \leq \text{const}\ t^{\delta-m}$ whenever $f_t(x) = t^\delta f(t^{-\delta}x)$ and f is smooth.

(ii) Let $(\rho_a)_{a\in L}$ be the partition of unity subordinate to $(S_a^-(\alpha,\varepsilon))_{a\in L}$, as defined on page 26, (α,ε) being the parameters of g. Let $\rho_{a,t}(x) := \rho_a(t^{-\delta}x)$. Then

$$\nabla g_t \nabla V = \sum_{a>0} \rho_{a,t}^2 \nabla g_t \nabla I_a$$

by construction of $(\rho_a)_{a\in L}$ and property (i) of Y-functions. It remains to prove the lemma for each term in the sum. To this end write

$$\rho_{a,t}^2 \nabla g_t \nabla I_a = ip\nabla g_t I_a \rho_{a,t}^2 - I_a \rho_{a,t}^2 \nabla g_t ip - \nabla\left(\rho_{a,t}^2 \nabla g_t\right) I_a$$

and use $\text{supp}(\rho_{a,t}) \subset \{x : |x|_a \geq ct^\delta\}$ and $(I2)$. ∎

4.3 A Propagation Estimate

The purpose of this section is to prove the propagation estimate which will serve us later to prove existence of the Deift-Simon wave operators and the asymptotic observable. The tacit assumption here is $(I2)$. To begin with we fix some notations.

Suppose $(A_t)_{t>0}$ is a family of operators in $\mathcal{H}$ and $D \subset D(A_t)$ is a subspace which is invariant under the time evolution generated by H. Then $A(t) := e^{iHt}A_t e^{-iHt}$ is defined in D for all $t > 0$. φ_t will always denote $e^{-iHt}\varphi$ if $\varphi \in \mathcal{H}$. So

$$\langle\varphi_t|A_t\psi_t\rangle = \langle\varphi|A(t)\psi\rangle \qquad \text{for } \varphi,\psi \in D\ .$$

Further suppose B_t is a form or an operator in $\mathcal{H}$ with domain D and

$$\frac{d}{dt}\langle\varphi_t|A_t\psi_t\rangle = \langle\varphi_t|B_t|\psi_t\rangle \qquad \forall\varphi,\psi \in D\ .$$

Then we say $DA_t = B_t$ in D. Formally the *Heisenberg derivative* DA_t is given by

$$DA_t = i[H, A_t] + \frac{dA_t}{dt}\ .$$

If f is a Y-function, then f_t denotes the scaled function $f_t(x) := t^\delta f(t^{-\delta}x)$, $t \in \mathbf{R}_+$, for some $0 < \delta < 1$ to be specified. g and $(g_a)_{a\in L}$ will always be the Y-functions constructed in Subsection 4.2 for some fixed (α, ε). They are involved in the operators

$$\begin{array}{lll} B_t \equiv i[H, g_t] := \frac{1}{2}(p\nabla g_t + \nabla g_t p) & D(B_t) = H_0^1(\Omega) & \\ B_{a,t} \equiv i[H_a, g_{a,t}] := \frac{1}{2}(p\nabla g_{a,t} + \nabla g_{a,t} p) & D(B_{a,t}) = H_0^1(\Omega_a) & a \in L \\ & & \\ \gamma_t := i[H, g_t] + \partial_t g_t & D(\gamma_t) = D(B_t) & \\ \gamma_{a,t} := i[H_a, g_{a,t}] + \partial_t g_{a,t} & D(\gamma_{a,t}) = D(B_{a,t}) & a \in L \end{array}$$

Note that the subindex a also indicates on which Hilbert space these operators act. By Lemma 4.5 we have the relation

$$\gamma_t = \sum_{a\in L} \mathcal{J}_a^* \gamma_{a,t} \mathcal{J}_a \ . \tag{4.14}$$

Next we define the forms

$$\begin{array}{ll} i[H, B_t] := p g_t'' p - \frac{1}{4}\Delta^2 g_t - \nabla g_t \nabla V & \text{for } t \text{ large} \\ i[H_a, B_{a,t}] := p g_{a,t}'' p - \frac{1}{4}\Delta^2 g_{a,t} - \nabla g_{a,t} \nabla V^a & \text{for } t \text{ large} \end{array}$$

which, by Lemma 4.7, are bounded in the Banach spaces $H_0^1(\Omega)$ and $H_0^1(\Omega_a)$ respectively. Their designation as commutators is justified by

Lemma 4.8 *Suppose $\varphi, \psi \in D(H)$. Then*

$$i\langle H\varphi|B_t\psi\rangle - i\langle B_t\varphi|H\psi\rangle = \langle\varphi|i[H, B_t]|\psi\rangle$$

for all t large enough.

Remark. The proof only requires that g in the definition of B_t is a Y-function.

Proof. This lemma coincides with Lemma 3.15 if we substitute A_ε for B_t in the latter. Also the proof can be taken over literally after the following few substitutions. Replace G_ε by g_t then A_ε becomes B_t. To localize now use the functions $\rho_{a,t}(x) := \rho_a(t^{-\delta}x)$ instead of (η_a), where (ρ_a) is the partition of unity subordinate to S_a^- defined on page 26. Then $\mathrm{supp}(\rho_{a,t}) \subset \{x : |x|_a \geq t^\delta c\}$; hence if $t^\delta c > R_0$ the use of Lemma 3.2 is justified and $I_a \rho_{a,t}(1+T)^{-1/2}$ is bounded. ∎

Lemma 4.9 *$D(\gamma_t - 2\partial_t g_t) = i[H, B_t] - \partial_t^2 g_t$ in $D(H)$ if t is large enough.*

Proof. By definition of γ_t and B_t, $\gamma_t - 2\partial_t g_t = B_t - \partial_t g_t$. Using (i) of Lemma 4.7 we compute for $\varphi \in D(H)$

$$\begin{aligned} \frac{d}{dt}\langle\varphi_t|(B_t - \partial_t g_t)\varphi_t\rangle &= \langle -iH\varphi_t|(B_t - \partial_t g_t)\varphi_t\rangle + \langle (B_t - \partial_t g_t)\varphi_t| - iH\varphi_t\rangle \\ &\quad + \langle\varphi_t|(\partial_t B_t - \partial_t^2 g_t)\varphi_t\rangle \ , \qquad t \geq 1 \end{aligned}$$

where $\partial_t B_t = 1/2(p\nabla\partial_t g_t + \nabla\partial_t g_t p)$. Since $iH\partial_t g_t - \partial_t g_t iH = \partial_t B_t$ in $D(H)$ by (ii) of Lemma 2.2, the result follows from Lemma 4.8 for t large enough. ∎

Theorem 4.10 *If g is a convex Y-function, $\delta \in (1/3, 1)$ and $\delta\mu > 1$, then*

$$\int_1^\infty dt \langle \varphi_t | p g_t'' p | \varphi_t \rangle \le c_1 \langle \varphi | H + c_2 | \varphi \rangle \qquad \forall \varphi \in Q(H) \ ,$$

where $c_1, c_2 > 0$ are constants independent of φ.

Proof. Since $D(H)$ is a form core of H and $0 \le \langle \varphi_t | p g_t'' p | \varphi_t \rangle \le a_1 \langle \varphi | H + a_2 | \varphi \rangle$ for all $\varphi \in Q(H)$, $t \ge 1$, and constants $a_1, a_2 \in \mathbf{R}_+$, it suffices to show that

$$\int_{t_0}^{t_1} dt \langle \varphi_t | p g_t'' p | \varphi_t \rangle \le c_1 \langle \varphi | H + c_2 | \varphi \rangle \qquad \forall \varphi \in D(H),\ \forall t_1 > t_0 \ , \tag{4.15}$$

for constants $t_0, c_1, c_2 \in \mathbf{R}_+$. By Lemma 4.9 there is a t_0 such that

$$\langle \varphi_t | \gamma_t - 2\partial_t g_t | \varphi_t \rangle |_{t_0}^{t_1} = \int_{t_0}^{t_1} dt \langle \varphi_t | p g_t'' p - \tfrac{1}{4}\Delta^2 g_t - \nabla g_t \nabla V - \partial_t^2 g_t | \varphi_t \rangle \ .$$

We now put all terms except $\langle \varphi_t | p g_t'' p | \varphi_t \rangle$ to the left side and then estimate the left side from above using Lemma 4.7. $\gamma_t - 2\partial_t g_t$ is bounded with respect to $\langle H \rangle$ uniformly in $t \ge 1$ because $\nabla g_t,\ \partial_t g_t = O(1)$. $\partial_t g_t^2 = O(t^{\delta - 2})$, $\Delta^2 g_t = O(t^{-3\delta})$ and $\nabla g_t \nabla V$ is $\langle H \rangle$-bounded with bound (const $t^{-\delta\mu}$) for t large enough. After enlarging t_0 if necessary these terms give thus integrable contribution by assumption on δ. This proves (4.15) and hence the theorem. ▮

4.4 Deift-Simon Wave Operators

Formally let

$$W = s - \lim_{t\to\infty} e^{iHt} \gamma_t e^{-iHt} \qquad \text{in } \mathcal{B}(\mathcal{H}_2, \mathcal{H})$$

and for each $a \in L$

$$\begin{aligned} W_a &= s - \lim_{t\to\infty} e^{iH_a t} \gamma_{a,t} \mathcal{J}_a e^{-iHt} && \text{in } \mathcal{B}(\mathcal{H}_2, \mathcal{H}_a) \\ W_a^\dagger &= s - \lim_{t\to\infty} e^{iHt} \mathcal{J}_a^* \gamma_{a,t} e^{-iH_a t} && \text{in } \mathcal{B}(\mathcal{H}_{a,2}, \mathcal{H}) \end{aligned}$$

Theorem 4.11 *Assume (I2) on the intercluster potentials. If $\delta \in (1/3, 1)$ and $\delta\mu > 1$, then W, W_a and $W_a^\dagger$ exist and $W_0 = 0$.*

Remark. While the support property of g_a plays a prominent role in the proof of existence of W_a for $a > 0$, existence of W_0 requires nothing on g_0 but that g_0 is a Y-function. In particular it follows that also W exists. Existence of $W_a^\dagger$ will later serve us to prove existence of the wave operators.

In the proof it pays to work with an another, equivalent definition of the Deift-Simon wave operators. Let

$$\begin{aligned} W_a(t) &:= e^{iH_a t} [\gamma_{a,t} - 2\partial_t g_{a,t}] F_a e^{-iHt} \\ W_a^\dagger(t) &:= e^{iHt} F_a^* [\gamma_{a,t} - 2\partial_t g_{a,t}] e^{-iH_a t} \end{aligned}$$

where $F_a := \mathcal{J}_a f_a$ and $f_a \in C^\infty(\Omega)$ is a bounded function with bounded derivatives, $\operatorname{supp} f_a \subset \{|x|_a \ge R_0 + 1\}$ and $f_a(x) = 1$ if $|x|_a \ge R_0 + 2$. In particular $F_0 = \mathcal{J}_0 = 1_{\mathcal{H}}$. Since $\partial_t g_{a,t} = O(t^{\delta - 1})$ and $\operatorname{supp}(g_{a,t}) \subset \{x : |x|_a \ge t^\delta c\}$ by Lemma 4.5, $W_a = s - \lim_{t\to\infty} W_a(t)$ and $W_a^\dagger = s - \lim_{t\to\infty} W_a^\dagger(t)$ if these strong limits exist. We next anticipate some technical steps of the proof of Theorem 4.11.

Lemma 4.12

$$iH_a(B_{a,t}F_a) - (B_{a,t}F_a)iH = i[H_a, B_{a,t}]F_a - iB_{a,t}(F_aI_a)$$

in $\mathcal{B}(\mathcal{H}_2, \mathcal{H}_{a,-2})$, if t is large enough.

Proof. The second statements of Lemma 2.2 and Lemma 3.2 imply that

$$F_aH = H_aF_a + F_aI_a + \mathcal{J}_a(i\nabla f_a p + \frac{1}{2}\Delta f_a) \qquad \text{in } D(H) .$$

In particular $F_a \in \mathcal{B}(\mathcal{H}_2, \mathcal{H}_{a,2})$. Noting that $\mathrm{supp}(g_{a,t}) \cap \mathrm{supp}(\partial^\alpha f_a) = \emptyset$ for large t, we thus find

$$B_{a,t}F_aH = B_{a,t}H_aF_a + B_{a,t}F_aI_a \qquad \text{in } \mathcal{B}(\mathcal{H}_2, \mathcal{H}_{a,-2})$$

for t large enough. The result now follows from Lemma 4.8, formulated for the case where $I_a \equiv 0$ and $\Omega_a = \Omega$, and the remark succeeding it. ∎

Lemma 4.13

$$\|W_a(t)(H+c)^{-1} - (H_a+c)^{-1}W_a(t)\| \to 0 \qquad (t \to \infty)$$

for $c \in \rho(H) \cap \rho(H_a)$.

Proof. Since $\partial_t g_{a,t} = O(t^{\delta-1})$ in $\mathcal{B}(\mathcal{H})$ for $t \geq 1$, this term in the definition of $W_a(t)$ is irrelevant here. By Lemma 4.12

$$\begin{aligned} &B_{a,t}F_a(H+c)^{-1} - (H_a+c)^{-1}B_{a,t}F_a \\ &\quad = (H_a+c)^{-1}\left(i[H_a, B_{a,t}]F_a - iB_{a,t}(F_aI_a)\right)(H+c)^{-1} \\ &\quad = (H_a+c)^{-1}\left((pg''_{a,t}p - \frac{1}{4}\Delta^2 g_{a,t} - \nabla g_{a,t}\nabla V^a)F_a - iB_{a,t}(F_aI_a)\right)(H+c)^{-1} \end{aligned}$$

which goes to 0 in $\mathcal{B}(\mathcal{H})$ as $t \to \infty$ by Lemma 4.7 (for the case $I_a = 0$, $\Omega_a = \Omega$), the support property of $g_{a,t}$ and $(I2)$. ∎

Proof of theorem 4.11. Pick some real $c \in \rho(H) \cap \rho(H_a)$ and let $R := (H+c)^{-1}$ and $R_a := (H_a+c)^{-1}$. Since $\|W_a(t)R\|$ and $\|W_a^\dagger(t)R_a\|$ are uniformly bounded for $t \geq 1$, it suffices to show that $s - \lim_{t\to\infty} W_a(t)R^2$ and $s - \lim_{t\to\infty} W_a^\dagger(t)R_a^2$ exist. By Lemma 4.13 this is equivalent to existence of $s - \lim_{t\to\infty} R_aW_a(t)R$ and $s - \lim_{t\to\infty} RW_a^\dagger(t)R_a$, which in turn follows if

$$\int_t^\infty ds \left| \frac{d}{ds}\langle\varphi|R_aW_a(s)R\psi\rangle \right| = \left\{ \begin{array}{l} O(1)\|\varphi\| \\ O(1)\|\psi\| \end{array} \right. \qquad (t \to \infty) .$$

We prove this in two steps. Fix $a \in L$, $\varphi \in \mathcal{H}_a$, $\psi \in \mathcal{H}$ and let $\varphi_{a,t} := e^{-iH_at}\varphi$ and $\psi_t := e^{-iHt}\psi$.

Step 1.

$$\left|\frac{d}{dt}\langle\varphi|R_aW_a(t)R\psi\rangle\right| \le |\langle R_a\varphi_{a,t}|pg''_{a,t}p|F_aR\psi_t\rangle| + f(t)\|\varphi\|\|\psi\|$$

where $f(t)$ is integrable near infinity.

Using (i) of Lemma 4.7 one proves differentiability and finds

$$\begin{aligned}\frac{d}{dt}\langle\varphi|R_aW_a(t)R\psi\rangle &= i\langle H_aR_a\varphi_{a,t}|(B_{a,t}-\partial_tg_{a,t})F_aR\psi_t\rangle \\ &\quad -i\langle(B_{a,t}-\partial_tg_{a,t})R_a\varphi_{a,t}|F_aHR\psi_t\rangle \\ &\quad +\langle R_a\varphi_{a,t}|(\partial_tB_{a,t}-\partial_t^2g_{a,t})F_aR\psi_t\rangle\end{aligned}$$

as expected, where $\partial_tB_{a,t}=\frac{1}{2}(p\nabla\partial_tg_{a,t}+\nabla\partial_tg_{a,t}p)$. Simplifying this by means of Lemma 4.12 and using $i[H_a,\partial_tg_{a,t}]=\partial_tB_{a,t}$ we arrive at

$$\frac{d}{dt}\langle\varphi|R_aW_a(t)R\psi\rangle = \langle\varphi_{a,t}|R_a\left(i[H_a,B_{a,t}]F_a-\partial_t^2g_{a,t}F_a-i(B_{a,t}-\partial_tg_{a,t})F_aI_a\right)R\psi_t\rangle$$

for large t. In the center there is a sum of operator in $\mathcal{B}(\mathcal{H}_2,\mathcal{H}_{a,-2})$. The resolvents included it is a sum of operators in $\mathcal{B}(\mathcal{H})$ of which all but $R_apg''_{a,t}pF_aR$ are integrable in norm for large t . This follows from $(I2)$, $\mathrm{supp}(g_{a,t})\subset\{|x|_a\ge ct^\delta\}$ and Lemma 4.7. Step 1 is now obvious.

Step 2.

$$\int_t^\infty ds\left|\langle R_a\varphi_{a,s}|pg''_{a,s}p|F_aR\psi_s\rangle\right| = \left\{\begin{array}{l} O(1)\|\varphi\| \\ O(1)\|\psi\|\end{array}\right. \qquad (t\to\infty)\ .$$

By Theorem 4.6 there exists a convex Y-function $\tilde{g}$ such that $\pm g''_a\le\tilde{g}''$ and thus $\pm g''_{a,t}\le\tilde{g}''_t$ if $\tilde{g}_t(x):=t^\delta\tilde{g}(t^{-\delta}x)$. Hence

$$|\langle\eta|pg''_{a,t}p|\eta\rangle|\le\langle\eta|p\tilde{g}''_tp|\eta\rangle \qquad \forall\eta\in H_0^1(\Omega_a)\ .$$

This and Hölder's inequality account for

$$\begin{aligned}&\int_t^\infty ds|\langle R_a\varphi_{a,s}|pg''_{a,s}p|\mathcal{J}_aR\psi_s\rangle| \\ &\le \left(\int_t^\infty ds\langle R_a\varphi_{a,s}|p\tilde{g}''p|R_a\varphi_{a,s}\rangle\right)^{1/2}\left(\int_t^\infty ds\langle\mathcal{J}_aR\psi_t|p\tilde{g}''p|\mathcal{J}_aR\psi_t\rangle\right)^{1/2}\ .\end{aligned}$$

On the left we can substitute F_a for $\mathcal{J}_a$ if t is large, and on the right we may drop the $\mathcal{J}_a$'s. Step 2 then follows from Theorem 4.10.

Step 1 and step 2 prove existence of the operators W_a, $W_a^\dagger$ and, by the remark after the theorem, existence of W. To prove that $W_0=0$ observe that

$$\frac{d}{dt}\langle\varphi_t|g_{0,t}\psi_t\rangle = \langle\varphi_t|(i[H,g_{0,t}]+\partial_tg_{0,t})\psi_t\rangle = \langle\varphi_t|\gamma_{0,t}\psi_t\rangle \xrightarrow{t\to\infty} \langle\varphi|W_0\psi\rangle$$

for all $\varphi,\psi\in D(H)$, since $g_{0,t}$ and its derivatives are bounded and W_0 exists. This and $g_{0,t}=O(t^\delta)$ where $\delta<1$ imply

$$0=\lim_{t\to\infty}\frac{1}{t}\langle\varphi_t|g_{0,t}\psi_t\rangle = \lim_{t\to\infty}\frac{1}{t}\int_1^t ds\langle\varphi_s|\gamma_{0,s}\psi_s\rangle = \langle\varphi|W_0\psi\rangle \qquad \forall\varphi,\psi\in D(H)\ .$$

Hence $W_0=0$. ∎

4.5 Existence and Completeness of the Wave Operators

To prove existence of the wave operators Ω_a we will use existence of $W_a^\dagger$ and the formula

$$\Omega_a\varphi = W_a^\dagger \frac{1}{\sigma|p_a|}\varphi$$

valid for some set of states $\varphi \in L^2(a)\otimes\mathcal{H}^a_{\mathrm{pp}}$ which depends on the parameters (α,ε) in the construction of $W_a^\dagger$. A dense set is obtained by varying these parameters.

Proof that Ω_a exists. It suffices to show that

$$\lim_{t\to\infty} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}\psi_a\otimes\psi^a$$

exists if $H^a\psi^a = E\psi^a$ and $\psi_a \in D \subset L^2(a)$, where D is dense in $L^2(a)$. We choose $D = \bigcup_{\varepsilon>0} D_\varepsilon$ with $D_\varepsilon := \{\varphi \in D(p_a^2) | \varphi = \chi(p_a \in S_a^-(\alpha,\varepsilon)\setminus \bigcup_{b<a} S_b^+(\alpha,\varepsilon))\varphi\ , \alpha = \varepsilon\}$. So let $\psi^a \in \mathcal{H}^a$ with $H^a\psi^a = E\psi^a$, $\psi_a \in D_\varepsilon$ for some $\varepsilon > 0$ and define $\gamma_{a,t}$ as before, but with g_a constructed using the parameters $(\alpha = \varepsilon, \varepsilon)$, so that

$$g_a(x_a)\chi(x_a \in S_a^-\setminus \bigcup_{b<a} S_b^+) = \sigma|x_a|\chi(x_a \in S_a^-\setminus \bigcup_{b<a} S_b^+)\ , \tag{4.16}$$

for some constant σ. Below we show that

$$\|\gamma_{a,t}e^{-iH_a t}\psi_a\otimes\psi^a - e^{-iH_a t}\sigma|p_a|\psi_a\otimes\psi^a\| \to 0 \qquad (t\to\infty)\ . \tag{4.17}$$

This and the existence of $W_a^\dagger$ imply

$$\begin{aligned}
\lim_{t\to\infty} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}\psi_a\otimes\psi^a &= \lim_{t\to\infty} e^{iHt}\mathcal{J}_a^*\gamma_{a,t}e^{-iH_a t}\frac{1}{\sigma|p_a|}\psi_a\otimes\psi^a \\
&= W_a^\dagger\frac{1}{\sigma|p_a|}\psi_a\otimes\psi^a
\end{aligned}$$

which proves existence of Ω_a. Note that $|p_a|^2 > \alpha^2(1-2\varepsilon)$ in $\mathrm{supp}(\hat{\psi}_a)$.

Since $\Delta g_{a,t} = O(t^{-\delta})$ and $H^a\psi^a = E\psi^a$, (4.17) follows if

$$\nabla g_{a,t} p e^{-itp_a^2/2}\psi_a\otimes\psi^a = e^{-itp_a^2/2}\sigma|p_a|\psi_a\otimes\psi^a + o(1) \qquad (t\to\infty)\ . \tag{4.18}$$

To prove this we split p into $p_a + p^a$ on the left side and treat the two terms thereby arising separately. To begin with we recall that

$$\left\| e^{-itp_a^2/2}f(p_a)\psi_a - f(\frac{x_a}{t})e^{-itp_a^2/2}\psi_a\right\| \to 0 \qquad (t\to\infty) \tag{4.19}$$

if $f \in L^\infty(a)$ (cf. [19, Theorem IX.31]). By assumption on ψ_a this implies

$$\nabla g_{a,t}p_a e^{-itp_a^2/2}\psi_a\otimes\psi^a = \nabla g_a(\frac{x}{t^\delta})\chi(\frac{x_a}{t} \in S_a^-\setminus \bigcup_{b<a} S_b^+)e^{-itp_a^2/2}p_a\psi_a\otimes\psi^a + o(1)\ ,$$

which is still correct after multiplying the right side with $\chi(|x^a| \le t^\delta)$. But if $|x^a| \le t^\delta$, $\frac{x_a}{t} \notin S_0^+$ and t is large, then $x \in S_a^-$ by (4.7) and (4.3), so that $\nabla g_a(t^{-\delta}x) = \nabla g_a(t^{-\delta}x_a)$. From the homogeneity of ∇g_a in $S_a^-\setminus\bigcup_{b<a} S_b^+$ it thus follows that

$$\nabla g_{a,t}p_a e^{-itp_a^2/2}\psi_a\otimes\psi^a = \nabla g_a(\frac{x_a}{t})\chi(\frac{x_a}{t} \in S_a^-\setminus \bigcup_{b<a} S_b^+)e^{-itp_a^2/2}p_a\psi_a\otimes\psi^a + o(1)\ .$$

By (4.19) and (4.16) this proves (4.18) for p_a instead of p. The same arguments show that p^a gives no contributions in the limit $t \to \infty$ since $\nabla g_a(p_a)p^a = 0$. ▮

The other statements of Theorem 2.6 follow essentially from the following basic escape property.

Lemma 4.14 *For any $\varphi \in L^2(a) \otimes \mathcal{H}^a_{\rm pp}$ and $\delta \in (0,1)$*

$$\left\| \chi(|x|_a \le t^\delta) e^{-iH_a t} \varphi \right\| \to 0 \qquad (t \to \infty) \ .$$

Proof. It suffices to consider vectors φ of the form $\varphi = \varphi_a \otimes \varphi^a$ with $H^a \varphi^a = \lambda \varphi^a$ and $\varphi \in D$ dense in $L^2(a)$. For D we choose

$$D = \bigcup_{v>0} \{\varphi \in L^2(a) | \varphi = \chi(p_a \in v S^*_a)\varphi\}$$

with $S^*_a = S^*_a(\sigma)$, $\sigma \in \Sigma$ as in Subsection 3.3 with ε small enough for Lemma 3.6. D is dense in $L^2(a)$ because $\chi(x \in vS^*_a) \to \chi(x \in a^*)$ as $v \downarrow 0$ for all $x \in a$. If $\varphi_a \in D$ then $\varphi_a = \chi(p_a \in vS^*_a)\varphi_a$ for some $v > 0$. Together with Theorem IX.31 in [19] this implies the first equation of

$$\begin{aligned}
e^{-iH_a t}\varphi_a \otimes \varphi^a &= \chi(\frac{x_a}{vt} \in S^*_a) e^{-iH_a t}\varphi_a \otimes \varphi^a + o(1) \\
&= \chi(\frac{x}{vt} \in S_a)\chi(\frac{x_a}{vt} \in S^*_a) e^{-iH_a t}\varphi_a \otimes \varphi^a + o(1) \\
&= \chi(\frac{x}{vt} \in S^*_a) e^{-iH_a t}\varphi_a \otimes \varphi^a + o(1)
\end{aligned}$$

where $\|o(1)\| \to 0$ as $t \to \infty$. In the second equation we used that $x/vt \notin S_a$ implies $|x^a| \ge vtc$ for some $c > 0$ and that φ^a is a bound state. The third equation follows from the remark after Lemma 3.5. To complete the proof we note that $vtS^*_a \subset \{x : |x|_a > t^\delta\}$ for large t , by Lemma 3.7. ▮

Proof of Theorem 2.6. Let $C_a := \{x \in \Omega_a : |x|_a > 1, |x^a| \le 1\}$, $a \in L$. Lemma 4.14 and an argument given in its proof show that

$$\left\| e^{-iH_a t}\varphi - \chi(t^\delta C_a) e^{-iH_a t}\varphi \right\| \to 0 \qquad (t \to \infty) \tag{4.20}$$

for $\varphi \in L^2(a) \otimes \mathcal{H}^a_{\rm pp}$, so that we may substitute $\chi(t^\delta C_a)e^{-iH_a t}\varphi$ for $e^{-iH_a t}\varphi$ in the definition of the wave operators. Then $C_a \cap C_b = \emptyset$ for $a \ne b$ implies Ran $\Omega_a \perp$ Ran Ω_b, and isometry follows from $t^\delta C_a \subset \Omega$ for $t^\delta \ge R_0$ and from (4.20). ▮

Lemma 4.15 and Lemma 4.16 provide technical results needed in the proof of Theorem 4.17.

Lemma 4.15 *Suppose $u \in C^\infty(\Omega; \mathbf{R})$ and $\partial^\alpha u \in L^\infty(\Omega)$ if $0 < |\alpha| \le 2$.*
(i) If $\varphi \in D(H) \cap D(u)$, then $e^{-iHt}\varphi \in D(H) \cap D(u)$ for all t and

$$u e^{-iHt}\varphi = e^{-iHt}u\varphi + \int_0^t ds e^{iH(t-s)} \left(\nabla u p - i\frac{\Delta u}{2} \right) e^{-iHs}\varphi \ . \tag{4.21}$$

(ii) If $f \in C_0^\infty(\mathbf{R})$ then $f(H) : D(H) \cap D(x) \to D(H) \cap D(x)$.

Proof. (i) First suppose u is in addition bounded. (4.21) then follows by differentiating $\langle e^{-iHt}\psi|ue^{-iHt}\varphi\rangle$, $\psi,\varphi \in D(H)$, and then integrating again. For general u, $u_\varepsilon = \frac{1}{\varepsilon}\tanh(\varepsilon u)$ and its derivatives up to second order are bounded, so that

$$u_\varepsilon e^{-iHt}\varphi = e^{-iHt}u_\varepsilon\varphi + \int_0^t dse^{iH(t-s)}(\nabla u_\varepsilon p - i\frac{\Delta u_\varepsilon}{2})e^{-iHs}\varphi \ .$$

In the limit $\varepsilon \to 0$ the right side converges to the right side of (4.21). The left side is of the form $uf(\varepsilon u)e^{-iHt}\varphi$ where $f(\varepsilon u)e^{-iHt}\varphi \to e^{-iHt}\varphi$ as $\varepsilon \to 0$. Since multiplication with u is a closed operator, (i) follows.

(ii) Let $\varphi \in D(H) \cap D(x)$. Using $f(H)\varphi = \int dt\hat{f}(t)e^{-iHt}\varphi$ and (i) we obtain for each component x_k of x:

$$\langle x_k\psi|f(H)\varphi\rangle = \langle\psi|f(H)x_k\varphi\rangle + \langle\psi|\eta\rangle \ , \qquad \text{all } \psi \in D(x)$$

where $\eta := \int dt \int_0^t dse^{iH(t-s)}p_k e^{-iHs}\varphi \in L^2(\Omega)$. Thus $f(H)\varphi \in D(x_k)$ for all k. ∎

Lemma 4.16 *$Dg_t = \gamma_t$ in $D(H) \cap D(x)$.*

Proof. Since e^{-iHt} maps $D(H) \cap D(x)$ onto itself it suffices to show that

$$\frac{d}{d\tau}\langle\varphi_\tau|g_{t+\tau}|\varphi_\tau\rangle\Big|_{\tau=0} = \langle\varphi|\gamma_t|\varphi\rangle \qquad \forall\varphi \in D(H)\cap D(x),\ \forall t > 0 \ .$$

The left side coincides with

$$\langle -iH\varphi|g_t\varphi\rangle + \langle g_t\varphi| - iH\varphi\rangle + \langle\varphi|\partial_t g\varphi\rangle$$

if $g_{t+\tau}e^{-iH\tau}\varphi \to g_t\varphi$ as $\tau \to 0$. To establish this strong continuity note that $e^{-iH\tau}g_{t+\tau}\varphi \to g_t\varphi$ as $\tau \to 0$ because $\partial_t g_t = O(1)$, and that

$$\left(e^{-iH\tau}g_{t+\tau} - g_{t+\tau}e^{-iH\tau}\right)\varphi \to 0 \qquad (\tau \to 0)$$

by Lemma 4.15. It remains to show that

$$\langle -iH\varphi|g_t\varphi\rangle + \langle g_t\varphi| - iH\varphi\rangle = \langle\varphi|B_t|\varphi\rangle \ . \tag{4.22}$$

To see this pick $\chi \in C^\infty(X)$ with $\chi(x) = 1$ if $|x| \le 1$ and $\chi(x) = 0$ if $|x| \ge 2$, and let $\chi_n(x) = \chi(\frac{x}{n})$ restricted to Ω. Then $\varphi_n = \chi_n\varphi \in D(H)\cap D(x)$ and (4.22) for φ_n follows from Lemma 2.2 since g_t is bounded on $\mathrm{supp}(\varphi_n)$. (4.22) is now obtained in the limit $n \to \infty$ since B_t is H-bounded and $H\varphi_n \to H\varphi$ as a consequence of Lemma 2.2. ∎

Theorem 4.17 *Assume the intercluster potentials obey $(I2), (I3)$ and $(I4)$. Then the closure $\overline{W}$ of W is self-adjoint, commutes with H, $D(\overline{W}) \cap \mathcal{H}_{cont} \subset Q(\theta(H))$ and*

$$\overline{W}^2 \ge \theta(H) > 0 \qquad \text{in } D(\overline{W}) \cap \mathcal{H}_{cont} \ , \tag{4.23}$$

where $\theta(E)$ is the Mourre constant.

Proof. If

$$e^{-iHt}W = We^{-iHt} \qquad \text{in } D(H),\ t \in \mathbf{R} \tag{4.24}$$

then $\langle H\varphi|W\varphi\rangle = \langle W\varphi|H\varphi\rangle$ for all $\varphi \in D(H)$, so that W is essentially self-adjoint by Nelson's commutator theorem (i.e. Theorem X.37 in [19]) since W is symmetric and H-bounded. (4.24) implies moreover that $e^{-iHt}\overline{W} \subset \overline{W}e^{-iHt}$ and thus that the self-adjoint operator $\overline{W}$ commutes with H. To prove (4.24) pick $\varphi \in D(H)$. Then

$$W\varphi - e^{iHs}We^{-iHs}\varphi = \lim_{t\to\infty} e^{iH(t+s)}[\gamma_{t+s} - \gamma_t]e^{-iH(t+s)}\varphi\ .$$

Since $\partial_t g_t = O(t^{\delta-1})$ the limit on the right side vanishes if $\|(B_{t+s}-B_t)(H+i)^{-1}\| \to 0$ as $t \to \infty$. Now this follows easily from

$$(B_{t+s} - B_t)\varphi = \int_t^{t+s} d\tau \left(\partial_\tau \nabla g_\tau p - \frac{i}{2}\partial_\tau \Delta g_\tau\right)\varphi$$

for $\varphi \in D(H)$, from $\partial_t \nabla g_t = O(t^{-1})$ and from $\partial_t \Delta g_t = O(t^{-\delta-1})$.

Let $S = \tau(H) \cup \{E \in \mathbf{R} | E \text{ is eigenvalue of } H\}$. $\theta(H) > 0$ in $\mathcal{H}_{\text{cont}}$ follows from $\theta(E) > 0$ in $\mathbf{R}\backslash\tau(H)$ and $E_{\tau(H)}(H)\mathcal{H}_{\text{cont}} = \{0\}$ by Corollary 3.17. To prove the first inequality suppose for each $\varepsilon > 0$ and $E \in \mathbf{R}\backslash S$ there exists an open interval $\Delta \ni E$ such that

$$\|W\varphi\|^2 \geq [\theta(E) - \varepsilon]\|\varphi\|^2 \qquad \forall \varphi \in \mathcal{H}_\Delta\ . \tag{4.25}$$

We may assume $|\Delta| \leq \varepsilon$. Then $\theta(E) \geq \theta(E+\varepsilon) - 2\varepsilon \geq \theta(H) - 2\varepsilon$ in $\mathcal{H}_\Delta$ and thus

$$\|W\varphi\|^2 \geq \langle\varphi|(\theta(H) - 3\varepsilon)\varphi\rangle \qquad \forall \varphi \in \mathcal{H}_\Delta\ . \tag{4.26}$$

By covering a given compact set $I \subset \mathbf{R}\backslash S$ with finitely many disjoint intervals Δ_i with $|\Delta_i| \leq \varepsilon$, we see that (4.26) also holds for $\varphi \in \mathcal{H}_I$. Since $\varepsilon > 0$ was arbitrary this implies (4.23) for $\mathcal{H}_{\text{cont}}$ replaced by $\mathcal{H}_I$, from which the theorem follows by approximation arguments using that S is countable. It remains to prove the assumption we started with. (4.25) follows if it holds in a dense subspace of $\mathcal{H}_\Delta$. $\mathcal{H}_\Delta \cap D(x)$ is such a subspace because $f(H)(1+x^2)^{-1/2}\varphi \in \mathcal{H}_\Delta \cap D(x)$ for all $f \in C_0^\infty(\Delta)$ by Lemma 4.15, and because these states are dense in $\mathcal{H}_\Delta$. Suppose $\varphi \in D(H) \cap D(x)$. Then

$$g(t)\varphi = g(1)\varphi + \int_1^t ds\gamma(s)\varphi \qquad \forall t \geq 1\ . \tag{4.27}$$

The Riemannian integral on the left exists because $s \to \gamma(s)\varphi$ is continuous. This and Lemma 4.16 prove (4.27). So

$$W\varphi = \lim_{t\to\infty} \frac{1}{t} g(t)\varphi\ . \tag{4.28}$$

Now let G be a G-function with parameter $R_1 > \rho R_0$. Using $g_t^2(x) \geq x^2 \geq 2G(x) -$ const $\forall t > 0$ by Lemma 4.5 and Lemma 3.13, we conclude from (4.28)

$$\|W\varphi\|^2 = \lim_{t\to\infty} \frac{1}{t^2}\|g(t)\varphi\|^2 \geq \liminf_{t\to\infty} \frac{2}{t^2}\langle\varphi_t|G|\varphi_t\rangle\ . \tag{4.29}$$

To bound $\langle\varphi_t|G|\varphi_t\rangle$ from below we need that

$$\begin{aligned}\langle\varphi_t|G|\varphi_t\rangle &= \langle\varphi|G|\varphi\rangle + t\mathrm{Re}\langle p\varphi|\nabla G\varphi\rangle \\ &\quad + \int_0^t ds\int_0^s dr\langle\varphi_r|pG''p - \tfrac{1}{4}\Delta^2 G - \nabla G\nabla V|\varphi_r\rangle \end{aligned}\tag{4.30}$$

for $t>0$. For $G_\varepsilon = \frac{1}{\varepsilon}(1-e^{-\varepsilon G})$ instead of G this is proved using Lemma 3.15. (4.30) then follows in the limit $\varepsilon\downarrow 0$. Now let $E\in\mathbf{R}\backslash S, \varepsilon>0$ and $\Delta\ni E$ be the interval provided by Corollary 3.16. Applying this corollary to (4.30) with $\varphi\in\mathcal{H}_\Delta\cap D(x)$ leads to

$$\langle\varphi_t|G|\varphi_t\rangle \geq [\theta(E)-\varepsilon]\|\varphi\|^2\frac{t^2}{2} + O(t) \qquad (t\to\infty)\ .$$

Combined with (4.29) this proves (4.25) and thus the theorem. ▮

In particular $\mathrm{Ker}(\overline{W}|_{\mathcal{H}_{\mathrm{cont}}}) = \{0\}$. Since $\overline{W}$ is self-adjoint and commutes with H this implies:

Corollary 4.18 *Ran W is dense in $\mathcal{H}_{cont}$.*

Remark. $\mathrm{Ker}(\overline{W}) = \mathcal{H}_{\mathrm{pp}}$.

Proof of Theorem 2.7. The proof goes by induction in subsystems. The induction hypothesis is

$$\mathcal{H}^a = \bigoplus_{b\geq a}\mathrm{Ran}\ \Omega_b^a \qquad \forall a>0. \tag{4.31}$$

For $a=X$ this is trivially true. We begin by deriving from (4.31) a statement on $\mathrm{Ran}\ \Omega_b,\ b\geq a$. By definition of the wave operators and $\mathcal{J}_a^*(1_a\otimes(\mathcal{J}_b^a)^*) = \mathcal{J}_b^*$,

$$s-\lim_{t\to\infty} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}(1_a\otimes\Omega_b^a) = \Omega_b\ , \qquad b\geq a\ .$$

Combined with (4.31) this implies that

$$\mathrm{Ran}\left(s-\lim_{t\to\infty} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}\right) \subset \bigoplus_{b\geq a}\mathrm{Ran}\ \Omega_b\ , \qquad \forall a>0\ , \tag{4.32}$$

i.e. the strong limits on the left exist and their ranges have this property. Now let $\varphi\in\mathcal{H}_{\mathrm{cont}}\cap D(H)$. By Corollary 4.18 and the fact that $\mathrm{Ran}\ \Omega_b$ is closed it suffices to show $W\varphi\in\bigoplus_{b>0}\mathrm{Ran}\ \Omega_b$ in order to prove (4.31) for $a=0$. Using (4.14), existence of the Deift-Simon wave operators and $W_0=0$ we find

$$\begin{aligned} W\varphi &\cong e^{iHt}\gamma_t e^{-iHt}\varphi \\ &= \sum_{a\in L} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}e^{iH_a t}\gamma_{a,t}\mathcal{J}_a e^{-iHt}\varphi \\ &\cong \sum_{a>0} e^{iHt}\mathcal{J}_a^* e^{-iH_a t}W_a\varphi\ , \end{aligned}$$

where $u(t)\cong v(t)$ means $\lim_{t\to\infty}\|u(t)-v(t)\| = 0$. By (4.32) this completes the proof of Theorem 2.7. ▮

Appendix

In this section we define the potentials V^a of an N-body system by sums of potentials $(v^b)_{b\geq a}$ and impose conditions on these v^b which imply those on the intercluster potentials in Subsection 2.3. In the standard case v^b is typically defined in terms of a two-body potential (see [1, 15, 12]). After this the proof of theorem 3.1 is given.

For each $a \in L$ let a pair (ω^a, v^a) be given such that

- $\emptyset \neq \omega^a \subset X^a$, open, and $X^a \backslash \omega^a$ is compact
- $v^a : \omega^a \to \mathbf{R}$ obeys $(V1)$ and $(V2)$ with 0 as minimal α in $(V2)$. $v^X = 0$ in $\mathbf{C}$.

Define for each $a \in L$

$$\begin{aligned} \Omega^a &:= \bigcap_{b\geq a} (a^\perp \cap b) + \omega^b && \text{(A.1)} \\ V^a(x^a) &:= \sum_{b\geq a} v^b(x^b) \qquad x^a \in \Omega^a \ . \end{aligned}$$

For the intercluster potentials one then obtains

$$I_a(x) = \sum_{b \not\geq a} v^b(x^b) \qquad x \in \Omega \ .$$

The assumptions on ω^a and v^a now imply our basic requirements on Ω^a and V^a. In fact $\Omega_a \supset \Omega$ is obvious from $\Omega_a = \bigcap_{b\geq a}(b + \omega^b)$ and $\Omega_a \cap \{x : |x|_a > R_0\} \subset \Omega$ for some $R_0 \in \mathbf{R}$ follows from the compactness of $X^a \backslash \omega^a$. $(V1)$ and $(V2)$ for V^a follow easily from the properties of v^b and $V^a_-(x^a) \leq \sum_{b\geq a} v^b_-(x^b)$. The following further assumptions on v^a are suitable to derive $(I1)$ to $(I4)$.

$(v1)$	$v^a : H^1_0(\lvert x^a\rvert > R_0) \to L^2(\lvert x^a\rvert > R_0)$ bounded	
$(v2)$	$\lVert v^a\rVert \leq \text{const } R^{-\mu}$ in $\mathcal{B}(H^1_0(\lvert x^a\rvert > R), L^2(\lvert x^a\rvert > R))$	$\forall R \geq \max(1, R_0)$
$(v3)$	$\langle v^a \rangle$ compact	in $H^1_0(\lvert x^a\rvert > R_0 - 1)$
$(v4)$	$\langle \lvert\nabla v^a\rvert \rangle$, $\langle x^a \nabla v^a \rangle$ compact	in $H^1_0(\lvert x^a\rvert > R_0 - 1)$
$(v5)$	$\lvert v^a(x^a)\rvert \chi(\lvert x^a\rvert \geq R_0 - 1) \leq \text{const } \lvert x^a\rvert^{-\mu}$	*a.e.*

Theorem A.1 *Suppose the potentials $(v^a)_{a\in L}$ obey (vn), for some $n \in \{1 \ldots, 4\}$. Then I_a satisfies (In). $(v5)$ implies $(I1)$ to $(I4)$.*

Proof. Since $I_a = \sum_{b\not\geq a} v^b \circ \Pi^b$ it suffices to prove (In) for $v^b \circ \Pi^b$ with $b \not\geq a$. The proof that (vn) implies the boundedness statement in (In) is similar for all n. We only show $(v2) \Rightarrow (I2)$: Pick $R \geq \max(1, R_0)$. Then by assumption on v^b

$$\langle \varphi | |v^b|^2 | \varphi \rangle \leq cR^{-2\mu} \langle \varphi | (-\Delta^b + 1) \varphi \rangle \qquad \varphi \in C^\infty_0(|x^b| > R) \tag{A.2}$$

where c is independent of φ and R. For $\varphi \in C^\infty_0(b + \{|x^b| > R\})$ apply (A.2) to the partial function $x^b \to \varphi(x_b, x^b)$ and note that $-\Delta^b \leq -\Delta$. This leads to

$$\langle \varphi | |v^b \circ \Pi^b|^2 | \varphi \rangle \leq cR^{-2\mu} \langle \varphi | (-\Delta + 1) \varphi \rangle \qquad \varphi \in C^\infty_0(b + \{|x^b| > R\}) \ . \tag{A.3}$$

Since $b + \{|x^b| > R\} \supset \Omega_{a,R}$, (A.3) holds in particular for all $\varphi \in C^\infty_0(\Omega_{a,R})$, which proves $(I2)$.

$(v3) \Rightarrow (I3)$: If q is a bounded sesquilinear form in a Banach space E, then $\|q\|$ denotes the norm of the operator in $\mathcal{B}(E,E^*)$ associated with q. Let $j \in C^\infty(b^\perp)$ with $0 \le j \le 1$, $j(x^b) = 0$ if $|x^b| \le R_0 - 1/2$, $j(x^b) = 1$ if $|x^b| \ge R_0$. Let $\tilde{v}^b(x) = v^b(x)$ in ω^b and $\tilde{v}^b(x) = 0$ in $b^\perp \backslash \omega^b$. Then $(v3)$ implies that $\langle j\tilde{v}^b j\rangle$ is compact in $H^1(b^\perp)$ because the operator $J : H^1(b^\perp) \to H^1_0(|x^b| > R_0 - 1)$ defined by $(J\varphi)(x) = (j\varphi)(x)|_{\{|x^b|>R_0-1\}}$ is bounded. Therefore there exists a sequence $(v^b_n) \subset C^\infty_0(b^\perp)$ such that

$$\|\langle v^b_n - j\tilde{v}^b j\rangle\| \overset{(n\to\infty)}{\longrightarrow} 0 \qquad \text{in } H^1(b^\perp)$$

(see appendix of [7]), and in particular

$$\|\langle v^b_n - v^b\rangle\| \overset{(n\to\infty)}{\longrightarrow} 0 \qquad \text{in } H^1_0(|x^b| > R_0)\ .$$

Using $b + \{|x^b| > R_0\} \supset \Omega_{a,\varepsilon,R_0}$ and arguing as in the proof of $(I2)$ we obtain

$$\|\langle (v^b_n - v^b)\circ \Pi^b\rangle\| \overset{(n\to\infty)}{\longrightarrow} 0 \qquad \text{in } H^1_0(\Omega_{a,\varepsilon,R_0})\ . \tag{A.4}$$

$\langle v^b_n \circ \Pi^b\rangle$ is compact in $H^1_0(\Omega_{a,\varepsilon,R_0})$ by local compactness. Hence (A.4) proofs $(I3)$.

$(v4) \Rightarrow (I4)$: The proof of $(I3)$ also implies that $\langle |\nabla v^b|\rangle$ and $\langle x^b \nabla v^b\rangle$ are compact in $H^1_0(\Omega_{a,\varepsilon,R_0})$. $(I4)$ now follows from

$$|\langle \varphi|\nabla G \nabla v^b|\varphi\rangle| \le \text{const } \langle\varphi||\nabla v^b||\varphi\rangle + |\langle\varphi|x^b\nabla v^b|\varphi\rangle| \qquad \varphi \in H^1_0(\Omega_{a,\varepsilon,R_0})$$

and the compactness criterion Lemma A.2.

$(v5) \Rightarrow (In)$: For $n \in \{1,2,3\}$ $(v5)$ implies (vn) and therefore (In). $(v5) \Rightarrow (I4)$: We only prove the compactness statement, boundedness is proved by the same method. Let $F = G - \frac{x^2}{2}$. Then

$$\langle \nabla G \nabla v^b\rangle = \langle \nabla F \nabla v^b\rangle + \langle x^b \nabla v^b\rangle \tag{A.5}$$

where both forms on the right side are compact in $H^1_0(\Omega_{a,\varepsilon,R_0})$. To prove this for the first term write

$$\langle \nabla F \nabla v^b\rangle = \langle ip\nabla F v^b\rangle - \langle \nabla F v^b ip\rangle - \langle \Delta F v^b\rangle\ .$$

Each of the three forms on the right side is compact because

$$\begin{aligned} p_k :\ & H^1_0(\Omega_{a,\varepsilon,R_0}) \to L^2(\Omega_{a,\varepsilon,R_0}) \quad \text{bounded} \\ \Delta F v^b, (\partial_{x^k} F)v^b :\ & H^1_0(\Omega_{a,\varepsilon,R_0}) \to L^2(\Omega_{a,\varepsilon,R_0}) \quad \text{compact}\ . \end{aligned} \tag{A.6}$$

(A.6) follows from the assumptions on F and $|v^b(x^b)| \le \text{const } |x|^{-\mu}$ in $\Omega_{a,\varepsilon,R_0}$. Since $\mu > 1$ the same arguments with ∇F replaced by x^b show that $\langle x^b \nabla v^b\rangle$ is compact.
∎

Lemma A.2 *Let $\mathcal{H}$ be a separable Hilbert space and $A \in \mathcal{B}(\mathcal{H})$. Then A is compact if and only if*

$$\varphi_n \rightharpoonup 0 \quad \text{in } \mathcal{H} \quad \Rightarrow \quad \langle \varphi_n|A\varphi_n\rangle \to 0 \tag{A.7}$$

Proof. We use that A is compact if and only if $\varphi_n \rightharpoonup 0$ implies $A\varphi_n \to 0$ as $n \to \infty$. The only-if part is then obvious. To prove the converse first assume $A \geq 0$. (A.7) implies that $\sqrt{A}\varphi_n \to 0$, so that $\sqrt{A}$ and hence A is compact. Now let $A = A^*$, $P_+ = \chi_{[0,\infty)}(A)$, $P_- = \chi_{(-\infty,0)}(A)$ and $A_\pm = \pm P_\pm A P_\pm$. Since $\varphi_n \rightharpoonup 0$ implies $P_\pm\varphi_n \rightharpoonup 0$, (A.7) holds for the non-negative operators $A_\pm$ as well. Therefore $A_\pm$ and $A_+ - A_- = A$ are compact. For general $A \in \mathcal{B}(\mathcal{H})$ there are self-adjoint operators A_1, A_2 such that $A = A_1 + iA_2$. As (A.7) for A implies (A.7) for A_i, A_i and thus A is compact. ∎

Lemma A.3 *Suppose A_i is a self-adjoint operator in the Hilbert space $\mathcal{H}_i$ and let $A = \sum_{i=1}^N 1 \otimes \ldots A_i \ldots \otimes 1$ in $\bigotimes_{i=1}^N \mathcal{H}_i$.*

(i) If A_i is bounded from below, then $\langle A \rangle = \sum_{i=1}^N \langle 1 \otimes \ldots A_i \ldots \otimes 1 \rangle$.

(ii) If D_i is a form core of A_i then $\bigotimes_{i=1}^N D_i$ is a form core of A and $\langle \varphi_1 \otimes \ldots \varphi_N | A | \psi_1 \otimes \ldots \psi_N \rangle = \sum_{i=1}^N \langle \varphi_1 | \psi_1 \rangle \ldots \langle \varphi_i | A_i | \psi_i \rangle \ldots \langle \varphi_N | \psi_N \rangle$ for $\varphi_i, \psi_i \in D_i$, as expected.

Proof. (*i*) Since $\langle 1 \otimes \ldots A_i \ldots \otimes 1 \rangle$ is closed and bounded from below, so is $\sum_{i=1}^N \langle 1 \otimes \ldots A_i \ldots \otimes 1 \rangle$ [17]. Let B denote the unique self-adjoint operator associated with this form. $B = A$ follows if $B \supset A \restriction D$ where $D = D(A_1) \otimes \ldots \otimes D(A_N)$, because A is essentially self-adjoint on D. Let $\varphi \in D$, then $\varphi \in \bigcap_{i=1}^N Q(1 \otimes \ldots A_i \ldots \otimes 1) = Q(B)$ and

$$\langle \psi | B | \varphi \rangle = \sum_{i=1}^N \langle \psi | 1 \otimes \ldots A_i \ldots \otimes 1 | \varphi \rangle = \langle \psi | A \phi \rangle \qquad \forall \psi \in Q(B) \ .$$

This shows that $\varphi \in D(B)$ and $B\varphi = A\varphi$.

(*ii*) We will first prove (*ii*) for $D_i = Q(A_i)$. Let $\varphi_i \in Q(A_i)$, $(\varphi_i^n)_{n \in \mathbf{N}} \subset D(A_i)$ and $\varphi_i^n \to \varphi$ $(n \to \infty)$ w.r.t. the form norm of A_i. Then $|A| \leq \sum_{i=1}^N 1 \otimes \ldots |A_i| \ldots \otimes 1$ implies that $(\varphi^n) = (\varphi_1^n \otimes \ldots \otimes \varphi_N^n)$ is a Cauchy sequence w.r.t. the form norm of A. Since $\varphi^n \to \varphi = \varphi_1 \otimes \ldots \otimes \varphi_N$ and $\langle A \rangle$ is closed, $\varphi \in Q(A)$ and $\varphi^n \to \varphi$ w.r.t. the form norm of A. This shows that $Q(A_1) \otimes \ldots \otimes Q(A_N)$ is a subset of $Q(A)$. It is also a form core because $Q(A_i) \supset D(A_i)$ and $D(A_1) \otimes \ldots \otimes D(A_N)$ is an operator core and thus a form core of A. To prove the formula for $\langle \varphi_1 \otimes \ldots \otimes \varphi_N | A | \psi_1 \otimes \ldots \otimes \psi_N \rangle$ approximate $\varphi_i, \psi_i \in Q(A_i)$ in the same way we approximated φ_i above.

If $D_i \subset Q(A_i)$ is a form core, then the arguments at the beginning show that $D_1 \otimes \ldots \otimes D_N$ is dense in $Q(A_1) \otimes \ldots \otimes Q(A_N)$ w.r.t. the form norm of A. This completes the proof. ∎

Proof of Theorem 3.1. Let h_a, t_a and h^a be the closures of the forms

$$\begin{aligned}
\langle \varphi | h_a | \varphi \rangle &= \langle \varphi | -\Delta/2\varphi \rangle + \langle \varphi | V^a | \varphi \rangle \\
\langle \varphi | t_a | \varphi \rangle &= \langle \varphi | -\Delta_a/2\varphi \rangle \\
\langle \varphi | h^a | \varphi \rangle &= \langle \varphi | -\Delta^a/2\varphi \rangle + \langle \varphi | V^a | \varphi \rangle
\end{aligned}$$

defined in $C_0^\infty(\Omega_a)$. Closability of these forms follows from arguments given in Subsection 2.1. We claim that

$$h_a \overset{(a)}{\supset} \langle H_a \rangle \overset{(b)}{=} \langle T_a \otimes 1 \rangle + \langle 1 \otimes H^a \rangle \overset{(c)}{\supset} t_a + h^a \overset{(d)}{\supset} h_a \ .$$

The theorem then follows. (d) is evident and (b) follows from (i) of Lemma A.3. (ii) of this lemma says that

$$\begin{aligned}
\langle H_a \rangle &= \overline{\langle H_a \rangle \restriction C_0^\infty(a) \otimes C_0^\infty(\Omega^a)} && \text{(A.8)}\\
\langle T_a \otimes 1 \rangle &= \overline{\langle T_a \otimes 1 \rangle \restriction C_0^\infty(a) \otimes C_0^\infty(\Omega^a)} && \text{(A.9)}\\
\langle 1 \otimes H^a \rangle &= \overline{\langle 1 \otimes H^a \rangle \restriction C_0^\infty(a) \otimes C_0^\infty(\Omega^a)}\ . && \text{(A.10)}
\end{aligned}$$

If we identify $C_0^\infty(a) \otimes C_0^\infty(\Omega^a)$ with a subspace of $C_0^\infty(\Omega_a)$ (A.8) proves (a). By (A.9) and (A.10) (c) will follow if we show that

$$\begin{aligned}
\overline{\langle T_a \otimes 1 \rangle \restriction C_0^\infty(a) \otimes C_0^\infty(\Omega^a)} &\supset t_a \restriction C_0^\infty(\Omega_a) && \text{(A.11)}\\
\overline{\langle 1 \otimes H^a \rangle \restriction C_0^\infty(a) \otimes C_0^\infty(\Omega^a)} &\supset h^a \restriction C_0^\infty(\Omega_a)\ . && \text{(A.12)}
\end{aligned}$$

We only prove (A.12). The proof of (A.11) is similar.

Let $\varphi \in C_0^\infty(\Omega_a)$ be fixed and suppose $(\alpha_n)_{n \in \mathbf{N}} \subset C_0^\infty(a)$ is an orthonormal basis of $L^2(a)$. $\varphi(x^a)$ denotes the partial function $x_a \to \varphi(x_a, x^a)$. $\varphi(x^a) \in C_0^\infty(a)$ and can thus be expanded in the basis (α_n) with coefficients

$$\beta_n(x^a) = \langle \alpha_n | \varphi(x^a) \rangle = \int \bar{\alpha}_n(x_a) \varphi(x_a, x^a) dx_a \qquad n \in \mathbf{N}\ .$$

Let $\varphi_N(x_a, x^a) := \sum_{k=0}^N \alpha_k(x_a) \beta_k(x^a)$. Then $(\varphi_N)_{N \in \mathbf{N}} \subset C_0^\infty(a) \otimes C_0^\infty(\Omega^a)$. We will show that $\varphi_N \to \varphi$ in $L^2(\Omega_a)$ and that (φ_N) is a Cauchy-sequence with respect to the form norm of $1 \otimes H^a$. Since $\langle 1 \otimes H^a \rangle = h^a$ in $C_0^\infty(a) \otimes C_0^\infty(\Omega^a)$, (A.12) then follows.

Because $\varphi_N(x^a) \to \varphi(x^a)$ $(N \to \infty)$ and $\|\varphi_N(x^a)\|^2 \le \|\varphi(x^a)\|^2$ Lebesgue's theorem implies

$$\begin{aligned}
\lim_N \|\varphi_N - \varphi\|^2 &= \lim_N \textstyle\int dx^a \|\varphi_N(x^a) - \varphi(x^a)\|^2\\
&= \textstyle\int dx^a \lim_N \|\varphi_N(x^a) - \varphi(x^a)\|^2 \quad = 0\ .
\end{aligned}$$

Using $\langle \alpha_n | \alpha_m \rangle = \delta_{nm}$ we find for $N > M$

$$\langle \varphi_N - \varphi_M | 1 \otimes H^a | \varphi_N - \varphi_M \rangle = \sum_{n=M+1}^{N} \langle \beta_n | H^a | \beta_n \rangle\ .$$

This converges to 0 for $N, M \to \infty$ if $\sum_n |\langle \beta_n | H^a | \beta_n \rangle|$ is finite. But

$$\begin{aligned}
2 \textstyle\sum_n \langle \beta_n | T^a | \beta_n \rangle &= \textstyle\sum_n \|\nabla^a \beta_n\|^2 = \sum_n \int dx^a |\langle \alpha_n | \nabla^a \varphi(x^a) \rangle|^2\\
&= \textstyle\int dx^a \|\nabla^a \varphi(x^a)\|^2 = \langle \varphi | -\Delta^a \varphi \rangle \qquad < \infty\ ,
\end{aligned}$$

where we interchanged sum and integral in the third expression and then summed up. Similarly $\sum_n \langle \beta_n | V_\pm^a | \beta_n \rangle = \langle \varphi | V_\pm^a | \varphi \rangle < \infty$. This completes the proof. ▮

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