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Preface

This book provides a systematic study of spectral and scattering theory for many-body Schrödinger operators at two-cluster thresholds. While the two-body problem (reduced after separation of the centre of mass motion to a one-body problem at zero energy) is a well-studied subject, the literature on many-body threshold problems is sparse. However, our analysis covers for example the system of three particles interacting by Coulomb potentials and restricted to a small energy region to the right of a fixed nonzero two-body eigenvalue. In general, we address the question: How do scattering quantities for the many-body atomic and molecular models behave in the limit when the total energy approaches a fixed two-cluster threshold? This includes mapping properties and singularities of the limiting scattering matrix, asymptotics of the total scattering cross-section and absence of transmission from one channel to another in the small inter-cluster kinetic energy region. Our principal tools are the Feshbach–Grushin dimension reduction method and spectral analysis based on a certain Mourre estimate. Additional topics (of independent interest) are the limiting absorption principle, microlocal resolvent estimates, Rellich- and Sommerfeld-type theorems and asymptotics of the limiting resolvents at thresholds. While these features are fairly well-understood for two-body Schrödinger operators, they are poorly understood in the many-body case, even for two-cluster thresholds. It is the goal of the book to remedy this point. The mathematical physics field under study is very rich, and there are many open problems, several of them stated explicitly in the book for the interested reader.

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Contents

Chapter 1
Introduction

1.1 Scope and Results

The spectral and scattering theory for the quantum mechanical one-body problem at zero energy is a well-studied subject. The classical theory [6, 36, 38, 39, 48] involves a real potential $V(x)$ on $\mathbb{R}^n$ decaying at least like $\mathcal{O}(|x|^{-\rho})$ for some $\rho > 2$, referred to throughout this book as a 'very short-range' potential. The slowly decaying case for which the decay rate $\rho \in (0, 2)$ requires additional conditions, roughly sign conditions [15, 16, 21, 47, 72, 73]. The critical case is defined by $V(x) \approx C|x|^{-2}$, possibly with angular dependence, and the results depend on the coupling constant [62, 70]. The obtained results for the above models are highly model and case sensitive, and they depend explicitly on the dimension if the potential is very short-range. In general, for very short-range or critically decaying potentials, zero-energy resonance states may appear. The possible presence of zero-energy resonance and/or bound states is the main difficulty for threshold spectral analysis. An interesting issue is the zero-energy resolvent asymptotics which leads to various applications in Quantum Mechanics, for example the asymptotics of the scattering matrix and phase shifts, cf. Levinson's theorem [36, 48]. Resonance states are often called *half-bound states* in the physics literature, for the reason that for very short-range potentials in $\mathbb{R}^3$ they contribute by $1/2$ in the classical Levinson's theorem which relates the total variation of the scattering phase to the number of bound states (plus $1/2$ if zero resonance is present). More generally, for critically decaying potentials or on asymptotically conical Riemannian manifolds of dimension n, there possibly exist for (arbitrary numbers) $\nu \in [0, 1]$ so-called *zero-energy resonance states* which slightly abusively may also be called ν-*bound states*. They are solutions to the stationary Schrödinger equation for zero energy behaving like $\mathcal{O}(|x|^{-\frac{n-2}{2}-\nu})$ as $|x|$ tends to infinity. The ν-bound states give rise to terms of order $z^{-\nu}$ in a zero-energy resolvent expansion (corrected by logarithm terms in z when $\nu = 0, 1$) which leads to $t^{-(1-\nu)}$-behaviour of wave functions when $|t| \to \infty$. Moreover the quantity ν contributes to the generalized Levinson's theorem [9, 41, 69, 70].

Thresholds of an N-body Schrödinger operator are eigenvalues of the sub-Hamiltonians. There exists much less literature on threshold spectral analysis for the N-body problem. We can only mention the work [67] on the resolvent expansion in a special case of the lowest threshold which is the bottom of the essential spectrum. The goal of the present work is to present a systematic study of spectral and scattering theory for the quantum mechanical N-body problem at any negative two-cluster threshold λ_0, i.e. λ_0 is an eigenvalue of (possibly several) sub-Hamiltonians associated with two-cluster decomposition, but not of those with three or more clusters. These restrictions on the nature of the considered threshold exclude the presence of the Efimov effect there. So for example for the (dynamical nuclei physics) 3-body problem, the threshold zero is excluded from our analysis, while all other thresholds for this model are negative and of two-cluster type. (We shall later give precise definitions.) Philosophically, the two-cluster threshold problem is amenable to simplification in terms of an effective one-body problem by the Feshbach–Grushin dimension reduction method. This is indeed realized in [67] for very short-range pair potentials in dimension three for the case of the lowest threshold $\lambda_0 = \Sigma_2$, the bottom of the essential spectrum, assumed to be a unique two-cluster threshold (i.e. an eigenvalue of exactly one sub-Hamiltonian, this being of two-cluster type). However, in the present work we extend the framework considerably, so that it covers the usual atom physical models (see Sects. 2.1.1 and 2.2.1) for which the slowly decaying nature of the Coulomb pair potentials in dimension three requires refined analysis. Also we include the cases where the two-cluster threshold $\lambda_0 > \Sigma_2$ as well as multiple two-cluster and degenerate eigenvalue cases, which also call for refined analysis, in particular microlocal analysis.

One main ingredient which enables us to attain the goal of spectral analysis at any two-cluster threshold is the Mourre's estimate for the Hamiltonian with one threshold removed. For a given two-cluster threshold λ_0, the restriction of the total Hamiltonian onto the orthogonal complement of the associated spectral subspace is a non-local N-body Hamiltonian for which λ_0 is no longer a threshold. We essentially prove the Mourre's estimate at λ_0 for this reduced Hamiltonian and deduce the limiting absorption principles and microlocal resolvent estimates. The limiting absorption principles are used to construct an appropriate Grushin problem such that we can reduce the two-cluster problem to an effective one-body problem near an arbitrary two-cluster threshold.

The main example of this book is the dynamical nuclei physical model, H, obtained by removal of mass centre from the total Hamiltonian

$$\widetilde{H} = -\sum_{j=1}^{N} \frac{1}{2m_j} \Delta_{x_j} + \sum_{1 \le i < j \le N} q_i q_j |x_i - x_j|^{-1}, \quad x_j \in \mathbb{R}^3, \qquad (1.1)$$

where x_j, m_j and q_j denote the position, mass and charge of the jth particle. Let a two-cluster decomposition $a = (C_1, C_2)$ of N particles be given (see Sect. 2.1.1 for more information on the notation). We then write the full Hamiltonian as

$$H = H^{C_1} \otimes 1 \otimes 1 + 1 \otimes H^{C_2} \otimes 1 + 1 \otimes 1 \otimes p_a^2 + I_a,$$

where H^{C_k}, $k = 1, 2$, are cluster-Hamiltonians (defined as for H with the mass centre of cluster C_k removed), p_a^2 is the inter-cluster kinetic energy Hamiltonian and I_a is the *inter-cluster potential*. Suppose $\lambda_a = \lambda_0$ is an eigenvalue of the sub-Hamiltonian $H^a = H^{C_1} \otimes 1 + 1 \otimes H^{C_2}$ (λ_0 being of two-cluster type, see (2.20)). Picking a corresponding orthonormal basis $\varphi_1^a, \ldots \varphi_m^a \in \ker(H^a - \lambda_0) \subset L^2(\mathbf{X}^a)$, $m = m_a$, the *effective inter-cluster potential* is the $m \times m$ matrix-valued function in the relative position variable of the two clusters, viz. $R = R_1 - R_2$,

$$V(R)_{kl} := \langle \varphi_k^a, I_a \varphi_l^a \rangle_{L^2(\mathbf{X}^a)} = Q_1 Q_2 \delta_{kl} |R|^{-1} + Q_{kl}(\widehat{R}) |R|^{-2} + \mathcal{O}(|R|^{-3}). \quad (1.2)$$

Here Q_1 and Q_2 are the total charge of the particles in the clusters C_1 and C_2, respectively, and δ_{kl} is the Kronecker symbol. In addition we denote by Q_a the matrix-valued homogeneous potential (Q_{kl}) and $\widehat{R} = R/|R|$. (The operator Q_a depends on the total charges and dipole moments, cf. (2.8).) Let P^a denote the orthogonal (rank m) projection onto $\ker(H^a - \lambda_0)$ in $L^2(\mathbf{X}^a)$. Then obviously $\Pi^a = P^a \otimes 1$ projects onto the span of functions of the form $\varphi^a \otimes f_a$, $\varphi^a \in \ker(H^a - \lambda_0)$, in $L^2(\mathbf{X})$.

In terms of (1.2) a relevant classification reads:

Case 1 (slowly decaying case) $\quad Q_1 Q_2 \neq 0$.
Case 2 (critically decaying case) $\quad Q_1 Q_2 = 0$ and the function $Q_a \neq 0$.
Case 3 (very short-range case) $\quad Q_1 Q_2 = 0$ and the function $Q_a = 0$.

This means that in the simpler case where λ_0 is eigenvalue of exactly one two-cluster sub-Hamiltonian, the N-body Coulomb Hamiltonian may be modelled by a one-body effective Hamiltonian with a slowly decaying, a critically decaying or a very short-range potential according to the indicated properties of the product $Q_1 Q_2$ and Q_a.

In general, λ_0 may be a multiple two-cluster threshold. Let $\widetilde{A}$ be the set of cluster decompositions a for which $\lambda_0 \in \sigma_{\mathrm{pp}}(H^a)$. For each $a \in \widetilde{A}$ and $a = (C_1^a, C_2^a)$, denote Q_j^a the total charge in cluster C_j^a, $j = 1, 2$. The computation of (1.2) naturally suggests that we split $\widetilde{A}$ into $\widetilde{A} = \mathcal{A}_1 \cup \mathcal{A}_2 \cup \mathcal{A}_3$ specified as follows.

$\mathcal{A}_1$: the effective inter-cluster interaction is to leading order attractive Coulombic, i.e. $Q_1^a Q_2^a < 0$.
$\mathcal{A}_2$: the effective inter-cluster interaction is to leading order repulsive Coulombic, i.e. $Q_1^a Q_2^a > 0$.
$\mathcal{A}_3$: the effective inter-cluster interaction is $\mathcal{O}(|x_a|^{-2})$, i.e. $Q_1^a Q_2^a = 0$.

Clearly the elements of $\mathcal{A}_1 \cup \mathcal{A}_2$ are classified as Case 1, while the elements of $\mathcal{A}_3$ are classified either as Case 2 or Case 3. This motivates the splitting $\mathcal{A}_3 = \mathcal{A}_3^{\mathrm{cd}} \cup \mathcal{A}_3^{\mathrm{vs}}$ by specifying

$$\mathcal{A}_3^{\mathrm{cd}} = \{a \in \mathcal{A}_3 \mid Q_a \neq 0\} \text{ and } \mathcal{A}_3^{\mathrm{vs}} = \{a \in \mathcal{A}_3 \mid Q_a = 0\}$$

corresponding to Case 2 and Case 3, respectively. Therefore there are several cases to discuss for a general two-cluster threshold.

Let us now state some main results (here simplified) for the N-body Coulomb Hamiltonian with particles in $\mathbb{R}^3$ which are in fact special cases of the results proved in this work for generalized N-body Schrödinger operators. For any $a \in \mathcal{A}_3$, one will see that there are computable numbers $s_a \geq 1$ and $d_a \in \mathbb{N}_0$ determined by spectral properties of the vector-valued Schrödinger operator on the unit-sphere $\mathbb{S}^2$ with the matrix-valued potential Q_a (see Sect. 5.3). One of the main results concerns the expansion of locally H^1-solutions for $(H - \lambda_0)u = 0$ in terms of standard weighted L^2-space and weighted Sobolov-space notation (see Sect. 2.4 for a complete list of definitions), referring here to our most general result (see Sect. 5.3).

Theorem 1.1 *For any two-cluster threshold λ_0 and $a \in \widetilde{\mathcal{A}}$, let m_a be the dimension of $\ker(H^a - \lambda_0)$ in $L^2(\mathbf{X}^a)$ and Π^a the associated orthogonal projection defined as before. Then one has:*

(1) The space of locally H^1 solutions to $(H - \lambda_0)u = 0$ in

$$\sum_{a \in \mathcal{A}_1} \Pi^a L^2_{-3/4} + \sum_{a \in \mathcal{A}_2} \Pi^a L^2_{(-3/2)^+} + \sum_{a \in \mathcal{A}_3} \Pi^a L^2_{(-\min\{3/2,\, s_a\})^+} + L^2_{-1/2}, \quad (1.3a)$$

say denoted by $\mathcal{E}$, has finite dimension.
(2) If $\mathcal{A}_3 = \emptyset$, then $\mathcal{E} \subset H^1_\infty$.
(3) The dimension of the space of resonance states

$$n_{\text{res}} = \dim \left(\mathcal{E} / \ker(H - \lambda_0)_{|H^1} \right) \leq \sum_{a \in \mathcal{A}_3} d_a.$$

(4) The numbers $s_a = 3/2$ and $d_a = m_a$ for any $a \in \mathcal{A}_3^{\text{vs}}$. In particular, if $\mathcal{A}_3^{\text{cd}} = \emptyset$, then (1.3a) simplifies as

$$\sum_{a \in \mathcal{A}_1} \Pi^a L^2_{-3/4} + \sum_{a \in \mathcal{A}_2 \cup \mathcal{A}_3^{\text{vs}}} \Pi^a L^2_{(-3/2)^+} + L^2_{-1/2}, \quad (1.3b)$$

and 3 reads

$$n_{\text{res}} \leq \sum_{a \in \mathcal{A}_3^{\text{vs}}} m_a.$$

Here we used the notation $L^2_{s+} = \cup_{t>s} L^2_t$ and $L^2_t = L^2(\mathbf{X}; \langle x \rangle^{2t} dx)$ for $s, t \in \mathbb{R}$.

If $\widetilde{\mathcal{A}} = \mathcal{A}_3^{\text{vs}} = \{a\}$ and $\lambda_0 = \Sigma_2$ the lowest threshold, then one has $d_a = m_a = 1$, (1.3a) reads as $\Pi^a L^2_{(-3/2)^+} + L^2_{-1/2}$ and the space of resonance states is of dimension $n_{\text{res}} \leq 1$. This is a natural extension of the results of [JK] on zero resonance and the relevant null-space at zero energy for a one-body Hamiltonian with a very short-range potential in dimension three. However, Theorem 1.1 is very general and covers a

variety of situations. One may also view Theorem 1.1 as a version of the well-known Rellich theorem for non-threshold energies [2, Theorem 1.4] (see also Theorem 4.12), although the above analogue at a two-cluster threshold is considerably more complex. For example, the analogue of (1.3a) and (1.3b) in the continuous spectrum away from thresholds reads $L^2_{-1/2}$, and we note that for almost all (probably valid for all) such energies the space of generalized eigenfunctions in $L^2_{-1/2-\epsilon}$ (for any $\epsilon > 0$) has infinite dimension [59]. In comparison, in the context of Theorem 1.1 with $\widetilde{\mathcal{A}} = \mathcal{A}_1 = \{a\}$ we show that the space of generalized eigenfunctions at λ_0 in $\Pi^a L^2_{-3/4-\epsilon} + L^2_{-1/2-\epsilon}$ is infinite-dimensional (see Theorem 7.13 2).

The proof of Theorem 1.1 is complicated; in fact we give a full proof only under the Direct Sum Condition (5.68a) and the Auxiliary Regularity Condition (5.68b), treating the general case in a somewhat sketchy fashion. Although we shall not elaborate on these conditions in this introduction we believe that (5.68a) is always fulfilled for the regular many-body Schrödinger operator discussed here (see Example 3.6 for a partial justification). For many-body Schrödinger operators with infinite mass nuclei the Direct Sum Condition may not be fulfilled (see Sect. 3.5 for an example). The Auxiliary Regularity Condition (5.68b) has a more technical flavour in that it is a spectral condition for an auxiliary operator of the Grushin method. As a general feature the conditions (5.68a) and (5.68b) simplify proofs, and therefore we prefer to (and will) impose them in several contexts.

One of the threshold phenomena indicated by Theorem 1.1 is the possible existence of resonance states combined freely with the possible existence of L^2-eigenfunctions at the two-cluster threshold λ_0. This is completely analogous to the situation for the one-body problem in dimension three for very short-range potentials [36] (exhibiting a somewhat similar sophisticated Rellich theorem at zero energy). Therefore we distinguish as in [36] between four cases for λ_0: Regular Case where λ_0 is neither an eigenvalue nor a resonance of H and Exceptional Cases 1, 2 and 3 according to whether λ_0 is a resonance but not an eigenvalue, an eigenvalue but not a resonance or both an eigenvalue and a resonance of H, respectively (see Sect. 6.1.1.1). The resolvent asymptotics at zero energy for the one-body problem is determined by this classification. It is a separate issue for us to obtain similar resolvent asymptotics at λ_0 in the present framework. However, our analysis is not complete, mainly due to lack of strong decay of Coulomb potentials hampering the analysis. Of course the Regular Case is the easiest case and we shall actually treat this with $\widetilde{\mathcal{A}} = \mathcal{A}_1 \cup \mathcal{A}_2 \cup \mathcal{A}_3^{\mathrm{vs}}$ (see Theorem 6.44). For the Exceptional Cases 1 and 3 (defined by the presence of a resonance) we show the following result.

Theorem 1.2 (Exceptional point of 1st or 3rd kind) *Let λ_0 be any two-cluster threshold for which $n_{\mathrm{res}} \geq 1$, i.e. λ_0 is a resonance of H. Suppose the conditions (5.68a) and (5.68b) (referred to above),*

$$\mathrm{ran}\, \Pi_H \subset L^2_t \text{ for some } t > 3/2, \tag{1.4}$$

where Π_H is the orthogonal projection onto $\ker(H - \lambda_0)$ (i.e. the eigenprojection if λ_0 is an eigenvalue of H and zero otherwise), and suppose

$$\widetilde{\mathcal{A}} = \mathcal{A}_2 \cup \mathcal{A}_3^{\text{vs}}. \tag{1.5}$$

Then the following asymptotics hold for $R(\lambda_0 + z) = (H - \lambda_0 - z)^{-1}$ as an operator from H_s^{-1} to H_{-s}^1, $s > 1$, for $z \to 0$ in $\mathcal{Z}_\pm = \{\text{Re } z \geq 0, \, \pm \text{Im } z > 0\}$ and for some $\epsilon = \epsilon(s) > 0$:

$$R(\lambda_0 + z) = -z^{-1}\Pi_H + \frac{\mathrm{i}}{\sqrt{z}} \sum_{j=1}^{n_{\text{res}}} \langle u_j, \cdot \rangle u_j + \mathcal{O}(|z|^{-\frac{1}{2}+\epsilon}). \tag{1.6}$$

Here $\{u_1, \ldots, u_{n_{\text{res}}}\} \subset H_{(-1/2)^-}^1$ is a basis of resonance states of H being independent of the choice of the sign of $\mathcal{Z}_\pm$.

Among the above conditions (1.4) is the 'unpleasant one'. It is an implicit (possibly redundant) condition appearing as an artifact of our methods. If λ_0 is exceptional point of 1st kind, (1.4) is obviously fulfilled since then $\Pi_H = 0$. Our Theorem 6.44 as well as Theorem 1.2 above require explicitly $\mathcal{A}_3^{\text{cd}} = \emptyset$. For generalized N-body Schrödinger operators, similar resolvent expansions are obtained without condition (1.4), but with faster decay assumption on the intercluster potential. In this case, the $z^{-\frac{1}{2}}$-term of (1.6) contains some additional terms resulting from interactions between resonance states and threshold energy L^2-eigenfunctions and these terms disappear once (1.4) is satisfied.

Under a spectral condition for certain elements of $\mathcal{A}_3^{\text{cd}}$ (those for which (1.10) is violated) oscillatory behaviour of the resolvent near the two-cluster threshold is expected. This is thanks to arguments of [62].

Let us now briefly outline our main applications in N-body threshold scattering. One of our results concerns the following generalization of a result from [15, 16].

Theorem 1.3 *Suppose that $\lambda_0 = \Sigma_2$ is a two-cluster threshold and the conditions (5.68a) and (5.68b). Suppose*

$$\widetilde{\mathcal{A}} = \mathcal{A}_1, \tag{1.7}$$

and that λ_0 is not an eigenvalue of H (i.e. assume the Regular Case). Let $\mathcal{C}$ denote the set of scattering channels $\alpha = (a, \lambda_0, \varphi_\alpha)$ with $a \in \widetilde{\mathcal{A}}$ (note that λ_0 is a simple eigenvalue of H^a). Then for any $\alpha, \beta \in \mathcal{C}$:

(1) The element of the scattering matrix $S_{\beta\alpha}(\lambda)$ (modelled after [15, 16]) is well-defined for λ slightly above λ_0 and possesses a strong limit as $\lambda \to (\lambda_0)_+$.

(2) The singular support of the limiting element $S_{\beta\alpha}(\lambda_0)$ (which is, by definition, the complement of the largest open set in which the distributional kernel of $S_{\beta\alpha}(\lambda_0)$ is smooth) fulfils

$$\text{sing supp } S_{\beta\alpha}(\lambda_0) \quad \begin{cases} \subset \{(\omega, \omega') \mid \omega \cdot \omega' = -1\} & \text{for } \beta = \alpha, \\ = \emptyset & \text{for } \beta \neq \alpha. \end{cases} \tag{1.8}$$

Condition (1.7) means that for any two-cluster decomposition $a \in \widetilde{A}$ the charges of the clusters of a have opposite sign, hence the effective inter-cluster potential is to leading order attractive Coulombic. It is a remarkable consequence of (1.8) that the distributional kernel of $S_{\beta\alpha}(\lambda_0)$, $\beta = \alpha$, is smooth at the forward direction of scattering $\{\omega \cdot \omega' = 1\}$. The proof of Theorem 1.3 may be considered as an extension of the one used in [15, 16] to obtain a similar 'semi-classical' result on the scattering matrix $S_{\mathrm{cou}}(E)$ for the one-body problem with an attractive Coulomb potential. See [11, 12, 64, 65] for some refined studies of N-body scattering matrices in the short-range case.

Another result under (1.7) concerns the difference

$$S_{\alpha\alpha}(\lambda) - S_{\mathrm{cou}}(\lambda - \lambda_0); \quad \alpha \in \mathcal{C} \text{ and } \lambda \in [\lambda_0, \lambda_0 + \delta].$$

Under conditions, in particular including the non-multiple property $\#\widetilde{\mathcal{A}} = 1$ (primarily used to simplify the presentation) covering the case where the two-cluster threshold $\lambda_0 > \Sigma_2$, we show that this difference is a 'partial smoothing operator' (see Theorem 7.10 and Remark 7.11 3). Yet another result is a characterization of the limiting element $S_{\alpha\alpha}(\lambda_0)$ given by asymptotics in terms of appropriate 'channel quasi-modes' (see Theorem 7.13 2).

This leads to another subject of interest, more precisely *non-transmission* at λ_0. This is a geometric concept amounting to the mathematically precise feature

$$\|1 - S_{\alpha\alpha}(\lambda)^* S_{\alpha\alpha}(\lambda)\| \longrightarrow 0 \text{ for } \lambda \longrightarrow (\lambda_0)_+. \tag{1.9}$$

Note that non-transmission has the clean physics interpretation that asymptotically (as $\lambda \to (\lambda_0)_+$) only elastic scattering occurs for the incoming channel α, hence 'rearrangement' or 'breakup' are asymptotically excluded phenomena of the scattering process. We derive a formula under (1.7) (see Corollary 7.15) indicating that on the contrary transmission does occur in this case if $\lambda_0 > \Sigma_2$ (see also Remarks 7.16 and 8.2 4).

In contrast to the attractive slowly decaying case we do prove non-transmission in the following three cases (assuming as above in all cases the non-multiple property $\#\widetilde{\mathcal{A}} = 1$):

(I) Effective repulsive Coulombic case, i.e. $\widetilde{\mathcal{A}} = \mathcal{A}_2$.
(II) $I_a(x^a = 0) = 0$, 'above the Hardy limit' case and λ_0 is regular.
(III) $I_a(x^a = 0) = 0$ and very short-range case, i.e. $\widetilde{\mathcal{A}} = \mathcal{A}_3^{\mathrm{vs}}$, and λ_0 is 'maximally exceptional of 1st kind'.

A special case of (II) is that $\widetilde{\mathcal{A}} = \mathcal{A}_3^{\mathrm{vs}}$ and λ_0 is neither an eigenvalue nor a resonance. The notions in (II) and (III) are in general given as follows (see also Sect. 8). The phrase 'above the Hardy limit' refers to a spectral property of the vector-valued Schrödinger operator on the unit-sphere $\mathbb{S}^2$ with the matrix-valued potential Q_a (writing $\widetilde{\mathcal{A}} = \{a\}$), more precisely

$$\inf \sigma\big(-\Delta_\theta + Q_a(\theta)\big) > -1/4. \tag{1.10}$$

Here $\theta \in \mathbb{S}^2$ and $-\Delta_\theta$ is the Laplacian on $\mathbb{S}^2$. For III) the potential $Q_a = 0$ and 'maximally exceptional of 1st kind' refers to Exceptional Case 1 and the condition $n_{\text{res}} = m_a = \dim \ker(H^a - \lambda_0)$. We note for comparison that if $m_a > 1$ and $n_{\text{res}} = \{1, \ldots, m_a - 1\}$ then indeed transmission can occur if λ_0 is exceptional of 1st kind (see Sect. 8.5).

The last subject of interest concerns *total cross-sections* for atom–ion scattering (see Sect. 9). It is an observed physical phenomenon at the very beginning of the era of Quantum Mechanics that when there is no dipole moment for the atom, the total cross-sections are finite. A mathematical proof for this physics folklore is subtle and is given in [34]. The operator under consideration is a special case of the dynamical nuclei physical model from Sect. 2.1.1 with the particle dimension $n = 3$. We assume $\lambda_0 = \Sigma_2$ is a two-cluster threshold, the conditions (5.68a) and (5.68b), (1.4) and $\widetilde{\mathcal{A}} = \mathcal{A}_3^{\text{ys}}$. It is known from [34] that for any channel $\alpha = (a, \lambda_0, \varphi_\alpha)$, $a \in \widetilde{\mathcal{A}}$, and any incident direction $\omega \in \mathbb{S}^2$,

$$\text{the total cross-section } \sigma_\alpha(\lambda, \omega) \text{ is finite}$$

for non-threshold λ's above λ_0. In the present work we derive bounds and asymptotics of this quantity as $\lambda \to (\lambda_0)_+$. The result depends on whether λ_0 is regular or exceptional of 2nd kind (yielding bounded asymptotics, see Theorem 9.6) or if λ_0 is exceptional of 1st or 3rd kind (yielding $(\lambda - \lambda_0)^{-1}$ type unbounded asymptotics, see Theorem 9.7). In the case where $\lambda_0 = \Sigma_2$ is exceptional of 1st kind (a resonance but not an eigenvalue), the atom–ion total cross-section exhibits the (partially universal) behaviour given by

$$\sigma_\alpha(\lambda, \omega) = \frac{1}{\lambda - \lambda_0}(4\pi c + o(1)), \quad \text{as } \lambda \longrightarrow (\lambda_0)_+.$$

Here $c \leq 1$, and $c = 1$ in the maximally exceptional case (in particular in the non-multiple case $\#\widetilde{\mathcal{A}} = 1$). Our proof relies on the derivation of Theorem 1.2.

1.2 Prerequisites and Organization of the Book

This book is a research monograph on two-cluster threshold scattering in the N-body problem with most of the results appearing for the first time. A general framework of reduction at an arbitrary two-cluster threshold is presented and several applications are given. Still many questions remain open in two-cluster threshold scattering, we believe that the presented methods may be useful for those who want to solve some of them.

We hope that this book can be useful not only to experts, but also to young researchers and PhD students who are interested in mathematical problems arising from quantum physics. The background requirement is knowledge on functional analysis, spectral theory and pseudodifferential operators. The reader can find these

materials in the textbooks [51], the monograph [74] on abstract quantum scattering and [25, Chap. XVIII] on PsDOs. The books [14, 30] furnish panoramic accounts on N-body scattering and also contain necessary prerequisites for the present monograph. In particular [30, Sects. 3.1–3.3] provides a thorough introduction to cluster decompositions, Jacobi-coordinates, N-body Hamiltonians, etc. Chapter 2 of the present book also gives some preliminaries of this sort, although it is not a complete exposition.

On the other hand, Chap. 3 is written in a self-contained way and sets forward a general framework for reduction of the N-body problem near a two-cluster threshold to the study of an effective Schrödinger operator with a non-local matrix-valued potential. Chapters 2 and 3 are helpful for understanding the philosophy of dimension reduction in two-cluster scattering, and in addition the developed Grushin reduction method is vital for all later analysis in the book. The subsequent chapters are all rather technical and need more advanced tools which are mentioned and developed in the context. Chapter 4 is devoted to spectral theory of an auxiliary N-body Hamiltonian with a non-local potential appearing in the Grushin method, while Chaps. 5 and 6 are devoted to Rellich-type theorems (including Theorem 1.1) and resolvent expansions (including Theorem 1.2), respectively. Finally in Chaps. 7–9 we study applications to N-body threshold scattering. Almost all of Chap. 7 is devoted to the study of elastic scattering in the presence of a attractive slowly decaying effective potential (for the physical models corresponding to the condition $\widetilde{\mathcal{A}} = \mathcal{A}_1$). In general, elastic scattering might not be the only occurring scattering process in this case. This is in contrast to the issue of Chap. 8 where we indeed provide criteria for elastic scattering asymptotically being the only occurring scattering process, slightly above a given two-cluster threshold λ_0 (for example the criterion $\widetilde{\mathcal{A}} = \mathcal{A}_2$ mentioned above). Our concept of non-transmission is related, although in a disguised form, to the issue of Chap. 9, where we derive asymptotics of the total cross-sections for an atom–ion (with the conditions $\lambda_0 = \Sigma_2$ and $\widetilde{\mathcal{A}} = \mathcal{A}_3^{\mathrm{vs}}$).

Chapter 2
Many-Body Schrödinger Operators, Conditions and Notation

There are several classes of many-body Schrödinger operators. All of them may be put into the form of generalized N-body Schrödinger operators introduced in [14].

2.1 Regular N-Body Schrödinger Operators

Regular N-body Schrödinger operator H is the many-body Schrödinger operator obtained by the removal of the centre of mass from the total Hamiltonian

$$\widetilde{H} = -\sum_{j=1}^{N} \frac{1}{2m_j} \Delta_{x_j} + \sum_{1 \le i < j \le N} V_{ij}(x_i - x_j), \quad x_j \in \mathbb{R}^n, \qquad (2.1)$$

where N is the number of particles, x_j and m_j denote the position and mass of the jth particle. The pair potentials V_{ij} are assumed to be real and relatively compact with respect to $-\Delta$ in $L^2(\mathbb{R}^n)$, and they satisfy for some $\rho > 0$ the condition

$$|V_{ij}(y)| \le C_{ij}|y|^{-\rho} \text{ for } y \in \mathbb{R}^n \text{ with } |y| > R,$$

for some $R > 0$. However, we shall need some extra regularity. It is convenient to use the following condition.

Condition 2.1 There exists $\rho > 0$ such that for all pair potentials V_{ij} there is a splitting $V_{ij} = V_{ij}^{(1)} + V_{ij}^{(2)}$, where

(1) $V_{ij}^{(1)}$ is smooth and
$$\partial_y^\alpha V_{ij}^{(1)}(y) = \mathcal{O}\big(|y|^{-\rho - |\alpha|}\big). \qquad (2.2)$$

(2) $V_{ij}^{(2)}$ is compactly supported and

$$V_{ij}^{(2)}(-\Delta + 1)^{-1} \text{ is compact on } L^2(\mathbb{R}_y^n). \tag{2.3}$$

The Hamiltonian H is regarded as a self-adjoint operator on $L^2(\mathbf{X})$, where $\mathbf{X}$ is the $n(N-1)$-dimensional real vector space $\mathbf{X} := \{\sum_{j=1}^N m_j x_j = 0\}$. For $1 \le k \le N$, a k-cluster decomposition of the N-particle system labelled by $\{1, \dots, N\}$ is a partition

$$a = (C_1, \dots, C_k) \text{ with } \cup_{j=1}^k C_j = \{1, \dots, N\}, \quad C_i \cap C_j = \emptyset \text{ if } i \ne j.$$

Let $\mathcal{A}$ denote the set of all cluster decompositions of the N-particle system. The notation $a_{\max}$ and $a_{\min}$ refers to the 1-cluster and N-cluster decompositions, respectively. Let for $a \in \mathcal{A}$ the notation $\#a$ denote the number of clusters in a. For $i, j \in \{1, \dots, N\}, i < j$, we denote by (ij) the $(N-1)$-cluster decomposition given by letting $C = \{i, j\}$ form a cluster and all other particles $l \notin C$ form 1-particle clusters. We write $(ij) \subset a$ if i and j belong to the same cluster in a. More general, we write $b \subset a$ if each cluster of b is a subset of a cluster of a. If a is a k-cluster decomposition, $a = (C_1, \dots, C_k)$, we let

$$\mathbf{X}^a = \{x \in \mathbf{X} \mid \sum_{l \in C_j} m_l x_l = 0, j = 1, \dots, k\} = \mathbf{X}^{C_1} \oplus \dots \oplus \mathbf{X}^{C_k},$$

and

$$\mathbf{X}_a = \{x \in \mathbf{X} \mid x_i = x_j \text{ if } i, j \in C_m \text{ for some } m \in \{1, \dots, k\}\}.$$

Note that $a \subset b \Leftrightarrow \mathbf{X}^a \subset \mathbf{X}^b$. Moreover $\mathbf{X}^a$ and $\mathbf{X}_a$ give an orthogonal decomposition for $\mathbf{X}$ equipped with the quadratic form

$$q(x) = \sum_j 2m_j |x_j|^2, \qquad x \in \mathbf{X}.$$

For $x \in \mathbf{X}$, we have the corresponding orthogonal decomposition: $x = x^a + x_a$ with $x^a = \pi^a x \in \mathbf{X}^a$ and $x_a = \pi_a x \in \mathbf{X}_a$.

With this notation, the N-body Schrödinger operator H introduced above can be written in the form

$$H = H_0 + V,$$

where $H_0 = p^2$ is (minus) the Laplace–Beltrami operator on the Euclidean space $(\mathbf{X}, q)$ and $V = V(x) = \sum_{a=(ij) \in \mathcal{A}} V_a(x^a)$ with $V_a(x^a) = V_{ij}(x_i - x_j)$ for the $(N-1)$-cluster decomposition $a = (ij)$. More precisely, for example,

$$x^{(12)} = \left(\frac{m_2}{m_1 + m_2}(x_1 - x_2), -\frac{m_1}{m_1 + m_2}(x_1 - x_2), 0, \dots, 0 \right).$$

We note the following geometric properties for $N \geq 3$: For all $a, b \in \mathcal{A}$ with $\#a = 2, \#b = N - 1$ and $b \not\subset a$

$$\text{ran} \left(\pi^b \pi^a \right) = \text{ran } \pi^b, \tag{2.4a}$$

$$\pi^b : \mathbf{X}_a \longrightarrow \mathbf{X}^b \text{ is bijective.} \tag{2.4b}$$

Remark 2.2 Let us recall that there exist several coordinate systems such as Jacobi coordinates, atomic coordinates, clustered Jacobi coordinates. See [51, XI.5, Vol. III] or [30, Sect. 3.3]. For example, the Jacobi coordinates measure the jth particle from the mass centre of particles $\{1, \ldots, j - 1\}, j = 2, \ldots, N$. Concretely, set

$$y_j = x_{j+1} - \frac{1}{\sum_{k=1}^{j} m_k} \sum_{k=1}^{j} m_k x_k, \quad j = 1, \ldots, N - 1. \tag{2.5}$$

Then in coordinates $y = (y_1, \ldots, y_{N-1}) \in \mathbb{R}^{n(N-1)}$, the regular N-body operator H can be written as $H = H_0 + \sum_{1 \leq i < j \leq} V_{ij}(x^{ij})$ where

$$H_0 = \sum_{j=1}^{N-1} -\frac{1}{2\mu_j} \Delta_{y_j}, \quad \mu_j^{-1} = m_{j+1}^{-1} + (\sum_{k=1}^{j} m_k)^{-1}$$

and $x^{ij} = x_i - x_j$ expressed in y variables. In N-body scattering theory, for a given cluster decomposition $a = (C_1, \ldots, C_k)$, it is convenient to use the clustered Jacobi coordinates [51, XI.5, Vol. III] which consists in taking Jacobi coordinates for each subsystem C_j to form an intra-cluster coordinates system x^a and the Jacobi coordinates for the cluster mass centres to form an inter-cluster variables x_a. However, such explicit computation in coordinates is often not necessary. In this work we use mostly geometric properties of an abstract N-body configuration (cf. Sect. 2.3) rather than concrete coordinates systems, except though for the last chapter on atom–ion scattering, where clustered atomic coordinates are used. See also Example 3.6.

2.1.1 Principal Example, Dynamical Nuclei

Consider a system of N particles interacting by Coulomb forces. The Hamiltonian then reads

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j} \Delta_{x_j} + \sum_{1 \leq i < j \leq N} q_i q_j |x_i - x_j|^{-1}, \quad x_j \in \mathbb{R}^n, n \geq 3, \tag{2.6}$$

where x_j, m_j and q_j denote the position, mass and charge of the jth particle, respectively. H is regarded as a self-adjoint operator in $L^2(\mathbf{X})$ (with mass centre removed).

Let us consider a two-cluster decomposition $a = (C_1, C_2)$. For convenience assume $C_1 = \{1, \ldots, J\}$ and $C_2 = \{J + 1, \ldots, N\}$. We can write

$$H = H^1 \otimes 1 \otimes 1 + 1 \otimes H^2 \otimes 1 + 1 \otimes 1 \otimes p_a^2 + I_a,$$

where H^k, $k = 1, 2$, are cluster-Hamiltonians (defined similarly in their centre of mass frames) and

$$I_a = \sum_{i \in C_1, \, j \in C_2} q_i q_j |x_i - x_j|^{-1}.$$

To expand I_a we let for $k = 1, 2$

$$Q_k = \sum_{j \in C_k} q_j, \ M_k = \sum_{j \in C_k} m_j,$$

$$R_k = R_k(x) = \sum_{j \in C_k} \tfrac{m_j}{M_k} x_j, \ \widetilde{Q}_k = \widetilde{Q}_k(x^{C_k}) = \sum_{j \in C_k} q_j(x_j - R_k),$$

$$M = M_1 + M_2, \ R = R_1 - R_2,$$

and we decompose for all $x \in \mathbf{X}$

$$x = x^{C_1} + x^{C_2} + x_a,$$
$$x^{C_1} = (x_1 - R_1, \ldots, x_J - R_1, 0, \ldots, 0) \in \mathbf{X}^{C_1},$$
$$x^{C_2} = (0, \ldots, 0, x_{J+1} - R_2, \ldots, x_N - R_2) \in \mathbf{X}^{C_2},$$
$$x_a = \left(\tfrac{M_2}{M} R, \ldots, \tfrac{M_2}{M} R, -\tfrac{M_1}{M} R, \ldots, -\tfrac{M_1}{M} R \right) \in \mathbf{X}_a.$$

Note that indeed the centre of charge $\widetilde{Q}_k$ is a function of x^{C_k}.

Consequently we can expand for $i \in C_1$ and $j \in C_2$

$$|x_i - x_j|^{-1} = |R|^{-1} - \tfrac{R}{|R|^3} \cdot \left((x_i - R_1) - (x_j - R_2) \right) + \mathcal{O}\big(|R|^{-3}\big)|x^a|^2.$$

This is in the regime $|R| \to \infty$ and $|x_i - R_1| + |x_j - R_2| \leq \tfrac{1}{2}|R|$.

Hence in turn we obtain for $|R| \to \infty$

$$I_a = Q_1 Q_2 |R|^{-1} + \tfrac{R}{|R|^3} \cdot \left(Q_1 \widetilde{Q}_2(x^{C_2}) - Q_2 \widetilde{Q}_1(x^{C_1}) \right) + \mathcal{O}\big(|R|^{-3}\big)|x^a|^2, \quad (2.7)$$

which leads to various cases. We use the notation φ^k, $k = 1, 2$, to denote a cluster bound state (for the cluster Hamiltonian H^k) and $\langle \cdot, \cdot \rangle_k$ to denote the corresponding cluster inner product. The *effective potential*

$$V(R) := \langle \varphi^1 \otimes \varphi^2, I_a \varphi^1 \otimes \varphi^2 \rangle_{L^2(\mathbf{X}^a)}.$$

Case 1 $V \approx |R|^{-1}$: $Q_1 Q_2 \neq 0$.
Case 2 $V \approx |R|^{-2}$:
Subcase 2a $Q_1 \neq 0$, $Q_2 = 0$ and $\langle \varphi^2, \widetilde{Q}_2 \varphi^2 \rangle_2 \neq 0$.
Subcase 2b $Q_2 \neq 0$, $Q_1 = 0$ and $\langle \varphi^1, \widetilde{Q}_1 \varphi^1 \rangle_1 \neq 0$.
Case 3 $V = \mathcal{O}(|R|^{-3})$:
Subcase 3a $Q_1 = Q_2 = 0$.
Subcase 3b $Q_1 \neq 0$, $Q_2 = 0$ and $\langle \varphi^2, \widetilde{Q}_2 \varphi^2 \rangle_2 = 0$.
Subcase 3c $Q_2 \neq 0$, $Q_1 = 0$ and $\langle \varphi^1, \widetilde{Q}_1 \varphi^1 \rangle_1 = 0$.

By exchanging the clusters the Subcases 2b and 3c correspond to the Subcases 2a and 3b, respectively. Note also that for Subcases 2a, 3a and 3b, assuming sufficient decay of the cluster bound states, the effective potential

$$V(R) = \langle \varphi^1 \otimes \varphi^2, I_a \varphi^1 \otimes \varphi^2 \rangle_{L^2(\mathbf{X}^a)} = Q_1 \frac{R}{|R|^3} \cdot \langle \varphi^2, \widetilde{Q}_2 \varphi^2 \rangle_2 + \mathcal{O}(|R|^{-3}). \quad (2.8)$$

Hence indeed $V \approx |R|^{-2}$ at infinity in Subcase 2a, while $V = \mathcal{O}(|R|^{-3})$ in Subcases 3a and 3b. Note also that $|R|^{-2}$ is the critical decay rate for threshold analysis, cf. [62]. Consequently in Case 2 the effective potential V is said to be *critically decaying*. In Case 1 the potential $V \approx |R|^{-1}$, and V is said to be *slowly decaying*. For $Q_1 Q_2 < 0$ and $Q_1 Q_2 > 0$ the one-body results of [21, 47, 73] will be useful, respectively. In Case 3 the effective potential is said to be *very short-range*, and other one-body results/techniques will be useful, cf. for example [36]. Case 2 (the critically decaying case) is different and rather 'rich'.

A detailed analysis of the structure of a class of generalized eigenfunctions at a two-cluster threshold, possibly a multiple and/or a non-simple two-cluster threshold, will be carried out for physical models in Sect. 5.3. (See (2.20) for the definition of a 'two-cluster threshold'.)

From the derivation follows the possibility that the second term $\mathcal{O}(|R|^{-3})$ of (2.8) actually has homogeneity -3 at infinity. For example this happens for Subcase 3a exactly when the moments $\widetilde{R}_1 := \langle \varphi^1, \widetilde{Q}_1 \varphi^1 \rangle_1 \neq 0$ and $\widetilde{R}_2 := \langle \varphi^2, \widetilde{Q}_2 \varphi^2 \rangle_2 \neq 0$ due to the computation for this case,

$$\mathcal{O}(|R|^{-3}) = |R|^{-5} (|R|^2 \widetilde{R}_1 \cdot \widetilde{R}_2 - 3(R \cdot \widetilde{R}_1)(R \cdot \widetilde{R}_2)) + \mathcal{O}(|R|^{-4}).$$

If certain 'moments' vanish for Subcases 3a and 3b, the order of the second term of (2.8) is of the form $\mathcal{O}(|R|^{-4})$, cf. [34, Appendix A]. In Chap. 6 we shall obtain leading order resolvent expansions for Case 3 without distinguishing between whether the homogeneous -3 term vanishes or not. In Sect. 9 we shall study a case where in fact the effective potential is (at least) of order $\mathcal{O}(|R|^{-4})$. In the same section an explicit calculation of the Hamiltonian is given in terms of so-called clustered atomic coordinates.

Strictly speaking, the distinction between Cases 2 and 3 as defined above makes best sense for a simple two-cluster threshold and we will not use this classification in the non-simple case. Rather in the general possibly non-simple case one needs

the following (slightly) different definition, see Sect. 5.3 for further details. Let λ_a be a non-threshold eigenvalue of the sub-Hamiltonian $H^a = H^1 \otimes 1 + 1 \otimes H^2$ (more precisely, we will need $\lambda_a \in \mathcal{T}_2$, see (2.20)). Picking an orthonormal basis $\varphi_1^a, \ldots \varphi_m^a \in L^2(\mathbf{X}^a)$, $m = m_a$ (being one or possibly bigger), in the range of the corresponding eigenprojection, the *effective potential* is the $m \times m$-matrix-valued function in the variable $R = R_1 - R_2$,

$$V(R)_{kl} := \langle \varphi_k^a, I_a \varphi_l^a \rangle_{L^2(\mathbf{X}^a)} = Q_1 Q_2 \delta_{kl} |R|^{-1} + Q_{kl}(\widehat{R})|R|^{-2} + \mathcal{O}\big(|R|^{-3}\big). \quad (2.9)$$

Here δ_{kl} is the Kronecker symbol and $\widehat{R} = R/|R|$. Stated in terms of (2.9) by using the notation $Q_a = (Q_{kl})$ for the matrix-valued function defined by the second terms, the more general (and correct) classification reads:

Case 1 (slowly decaying case) $Q_1 Q_2 \neq 0$.
Case 2 (critically decaying case) $Q_1 Q_2 = 0$ and $Q_a = (Q_{kl}) \neq 0$.
Case 3 (very short-range case) $Q_1 Q_2 = 0$ and $Q_a = (Q_{kl}) = 0$.

2.2 N-Body Schrödinger Operators with Infinite Mass Nuclei

In the case of $M \geq 1$ infinite mass nuclei located at $R_m \in \mathbb{R}^n$, $m = 1, \ldots, M$, the Hamiltonian reads

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j} \Delta_{x_j} + \sum_{1 \leq i < j \leq N} V_{ij}(x_i - x_j) + \sum_{1 \leq j \leq N,\, 1 \leq m \leq M} V_{jm}^{\mathrm{ncl}}(x_j - R_m),$$

(2.10)

where we impose similar conditions on V_{jm}^{ncl} as for V_{ij} in Condition 2.1. The one-body problem $N = 1$ is included in (2.10) (the middle term is absent in that case). The configuration space reads $\mathbf{X} = \mathbb{R}^{nN}$, and we use the metric g as before. The 'electron-electron' interaction $V_{ij}(x_i - x_j)$ takes as before the form $V_a(x^a)$ where $x^a = \pi^a x$, $a = (ij)$, is the orthogonal projection of x onto an n-dimensional subspace. Similarly the 'electron–nuclei' interaction $\sum_{1 \leq m \leq M} V_{jm}^{\mathrm{ncl}}(x_j - R_m)$ takes the form $V_a(x^a)$ where again $x^a = \pi^a x$, $a = a(j)$, is the orthogonal projection of x onto an n-dimensional subspace (let $x^a = (0, \ldots, 0, x_j, 0, \ldots, 0)$, i.e. all other coordinates than the jth are put equal to zero). Rather than using the cluster decompositions to label a family of 'subspaces of internal motion' $\{\mathbf{X}^a\}$ similar to those considered in Sect. 2.1 we prefer henceforth to appeal to abstract labelling. Precisely, we consider the smallest finite family $\{\mathbf{X}^a \mid a \in \mathcal{A}\}$ of subspaces of $\mathbf{X}$ which is stable under addition and which contains $\{0\}$ and the n-dimensional subspaces discussed above. See Sect. 2.3, and see [14, Sect. 5.1] for a discussion of the abstract N-body problem. On the other hand, there is a concrete description of the index set $\mathcal{A}$ and this family $\{\mathbf{X}^a \mid a \in \mathcal{A}\}$ which can be useful to have in mind: Consider $a = (C_1, \ldots, C_p)$

where the sets C_q are disjoint subsets of $\{1, \ldots, N\}$. For $p \geq 2$ and $q < p$ we have $\#C_q \geq 2$ and we let $\mathbf{X}^{C_q} = \{x \in \mathbf{X} \mid x_j = 0 \text{ if } j \notin C_q \text{ and } \sum_{i \in C_q} m_i x_i = 0\}$. Either similarly $\mathbf{X}^{C_p} = \{x \in \mathbf{X} \mid x_j = 0 \text{ if } j \notin C_p \text{ and } \sum_{i \in C_p} m_i x_i = 0\}$ (in that case we have $\#C_p \geq 2$) or $\mathbf{X}^{C_p} = \{x \in \mathbf{X} \mid x_j = 0 \text{ if } j \notin C_p\}$. In both cases let correspondingly $\mathbf{X}^a = \mathbf{X}^{C_1} \oplus \cdots \oplus \mathbf{X}^{C_p}$. Moreover we supplement by writing $\mathbf{X}^{a_{\min}} = \{0\}$ where, for example, $a_{\min} := \emptyset$. This is a concrete labelling of the family of subspaces of internal motion.

The ordering of subspaces yields an ordering of the abstract set of indices $\mathcal{A}$, by definition $a \subset b \Leftrightarrow \mathbf{X}^a \subset \mathbf{X}^b$. We denote $\mathbf{X} = \mathbf{X}^{a_{\max}}$ and $\mathbf{X}^a + \mathbf{X}^b = \mathbf{X}^{a \cup b}$. The orthogonal complement of $\mathbf{X}^a$ is denoted by $\mathbf{X}_a$. To have a uniform language we refer to the indices $a \in \mathcal{A}$ as 'cluster decompositions'. The length of a chain of cluster decompositions $a_1 \subsetneq \cdots \subsetneq a_k$ is the number k. This chain is said to connect $a = a_1$ and $b = a_k$. The maximal length of all chains connecting a given $a \in \mathcal{A} \setminus \{a_{\max}\}$ and $a_{\max}$ is denoted by $\#a$. We define $\#a_{\max} = 1$ and note that $\#a_{\min} = N + 1$. We say $a \in \mathcal{A}$ is k-cluster if $\#a = k$.

We note the following geometric properties for $N \geq 2$: For all $a, b \in \mathcal{A}$ with $\#a = 2$, $\#b = N$ and $b \not\subset a$

$$\operatorname{ran}\left(\pi^b \pi^a\right) = \{0\} \text{ or } \operatorname{ran}\left(\pi^b \pi^a\right) = \operatorname{ran} \pi^b, \tag{2.11a}$$

$$\pi^b : \mathbf{X}_a \longrightarrow \mathbf{X}^b \text{ is bijective.} \tag{2.11b}$$

2.2.1 Principal Example, Fixed Nuclei

Consider a system of N n-dimensional particles, $n \geq 3$, interacting by Coulomb forces. The Hamiltonian (2.10) then reads

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j} \Delta_{x_j} + \sum_{1 \leq i < j \leq N} q_i q_j |x_i - x_j|^{-1} + \sum_{1 \leq j \leq N, 1 \leq m \leq M,} q_j q_m^{\text{ncl}} |x_j - R_m|^{-1}, \tag{2.12}$$

where x_j, m_j and q_j denote the position, mass and charge of the jth 'electron', and R_m and q_m^{ncl} are the position and charge of the mth 'nucleus'.

Consider the two-cluster decomposition $a = (C)$, $C = \{1, \ldots, N-1\}$, meaning $\mathbf{X}^a = \{x = (x_1, \ldots, x_N) \in \mathbf{X} = \mathbb{R}^{nN} \mid x_N = 0\}$. Letting $R = x_N$ we write $H = H^1 \otimes 1 + 1 \otimes p_R^2 + I_a$ where H^1 is the cluster-Hamiltonian (i.e. the Hamiltonian for the first $N - 1$ electrons) and

$$I_a = \sum_{1 \leq i \leq N-1} q_i q_N |x_i - R|^{-1} + \sum_{1 \leq m \leq M,} q_N q_m^{\text{ncl}} |R - R_m|^{-1}.$$

Introducing

$$Q = \sum_{1 \leq j \leq N-1} q_j + \sum_{1 \leq m \leq M} q_m^{\text{ncl}},$$

$$\widetilde{Q} = \widetilde{Q}(x^a) = \sum_{1 \le j \le N-1} q_j x_j,$$

$$\widetilde{Q}^{\mathrm{ncl}} = \sum_{1 \le m \le M} q_m^{\mathrm{ncl}} R_m,$$

the asymptotics of I_a for $|R| \to \infty$ reads

$$I_a = q_N Q |R|^{-1} + q_N \frac{R}{|R|^3} \cdot \left(\widetilde{Q}(x^a) + \widetilde{Q}^{\mathrm{ncl}} \right) + \mathcal{O}\big(|R|^{-3}\big)\big(1 + |x^a|^2\big). \tag{2.13}$$

For the expectation in a cluster bound state $\varphi = \varphi^a(x^a)$ with sufficient decay we consequently obtain the asymptotics for $|R| \to \infty$,

$$\langle \varphi, I_a \varphi \rangle_{L^2(\mathbf{X}^a)} = q_N Q |R|^{-1} + q_N \frac{R}{|R|^3} \cdot \left(\langle \varphi, \widetilde{Q}\varphi \rangle_{L^2(\mathbf{X}^a)} + \widetilde{Q}^{\mathrm{ncl}} \right) + \mathcal{O}\big(|R|^{-3}\big). \tag{2.14}$$

This leads to various cases.

Case 1 $q_N Q \ne 0$.
Case 2 $q_N \langle \varphi, \widetilde{Q}\varphi \rangle_{L^2(\mathbf{X}^a)} \ne -q_N \widetilde{Q}^{\mathrm{ncl}}$ and $Q = 0$.
Case 3 $q_N = 0$, or $q_N \ne 0$, $Q = 0$ and $\langle \varphi, \widetilde{Q}\varphi \rangle_{L^2(\mathbf{X}^a)} = -\widetilde{Q}^{\mathrm{ncl}}$.

Case 1 is the *slowly decaying case*, Case 2 is the *critically decaying case* and Case 3 is the *very short-range case*. Strictly speaking this classification makes best sense for φ being unique, i.e. for the simple case; in the non-simple case one needs a slightly different terminology, see Sects. 2.1.1 and 5.3.

2.3 Generalized N-Body Schrödinger Operators

Motivated by Sects. 2.1 and 2.2 we discuss the abstract N-body problem, cf. [14, Sect. 5.1]. Let $\mathbf{X} \ne \{0\}$ be a real finite-dimensional vector space with an inner product q. We consider a finite family $\{\mathbf{X}^a \mid a \in \mathcal{A}\}$ of subspaces of $\mathbf{X}^a \subset \mathbf{X}$ which is stable under addition and which contains $\{0\}$ and $\mathbf{X}$. The ordering of subspaces yields an ordering of the abstract set of indices $\mathcal{A}$, $a \subset b \Leftrightarrow \mathbf{X}^a \subset \mathbf{X}^b$. We denote $\{0\} = \mathbf{X}^{a_{\min}}$, $\mathbf{X} = \mathbf{X}^{a_{\max}}$ and $\mathbf{X}^a + \mathbf{X}^b = \mathbf{X}^{a \cup b}$. The orthogonal complement of $\mathbf{X}^a$ is denoted by $\mathbf{X}_a$. We refer to the indices $a \in \mathcal{A}$ as 'cluster decompositions'. The *length* of a chain of cluster decompositions $a_1 \subsetneq \cdots \subsetneq a_k$ is the number k. This chain is said to connect $a = a_1$ and $b = a_k$. The maximal length of all chains connecting a given $a \in \mathcal{A} \setminus \{a_{\max}\}$ and $a_{\max}$ is denoted by $\#a$. We define $\#a_{\max} = 1$ and denoting $\#a_{\min} = N + 1$ we say the family $\{\mathbf{X}^a \mid a \in \mathcal{A}\}$ is of N-body type. Note that for the setup of Sects. 2.1 and 2.2 these examples are of $(N-1)$-body type and of N-body type, respectively. This terminology might appear slightly misleading for Sect. 2.1. Henceforth we shall treat the generalized N-body framework only. This would consequently apply