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Conditions for the absence of bound states for three-body systems

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Abstract. We combine operator inequalities with the Feshbach formalism and recently derived functional inequalities and obtain a condition for the absence of three-body bound states in the case where one particle is assumed to be fixed.

1. Introduction

Although there exist some methods for estimating the number of two-body bound states (Simon 1976), no general procedures are known for more complicated systems. For calculating scattering length and phases especially it is necessary to have some knowledge about the number of bound states. In this paper we consider a three-particle system, where one particle has infinite mass, the two others are attracted by the centre but repel each other ($2m = 1$):

$$H = p_1^2 - V(x_1) + p_2^2 - V(x_2) + V_{12}(|x_1 - x_2|) \equiv H_0 + V_{12}. \tag{1}$$

It turns out that the potentials may even be non-central.

H should be a self-adjoint operator (Simon 1972, Reed and Simon 1972) defined on a domain $\mathscr{D}$ dense in $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$, $\mathscr{H}_i = L^2(\mathrm{d}^3x_i)$. All that we require is:

(*a*) the existence of some L^p-norm estimates;

(*b*) a knowledge of the ground state wavefunction ϕ and the first two energy levels ϵ_0, ϵ_1 of the two particle system;

(*c*) if the spectrum of H_0 is given by $2\epsilon_0$, $\epsilon_0 + \epsilon_1, \ldots, \epsilon_0, 2\epsilon_1, \ldots$ the essential spectrum‡ of H should start at ϵ_0, as one would expect physically for potentials going to zero at infinity;

(*d*) $\epsilon_0 < 2\epsilon_1$ (assumed for simplicity);

(*e*) in the following we will project one particle in the ground state, the other will see an effective potential. The number of two-body bound states within that potential should be zero (see equation (6)).

It is known that assumption (*c*) is valid for a large class of potentials (Hunziker 1966). According to (*c*) we will investigate states below ϵ_0.

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‡ There are different ways of breaking up the spectrum of an operator A (Reed and Simon 1972, pp 230–7): $\lambda \in \sigma_{\mathrm{ess}}$ if and only if the spectral projection operator on the interval $(\lambda - \epsilon, \lambda + \epsilon)$: $P_{(\lambda-\epsilon,\lambda+\epsilon)}(A)$ is infinite for all $\epsilon > 0$.

The well known projection operator formalism cannot be used directly to prove the absence of bound states. For Coulomb-like potentials especially one has to raise an infinity of bound states of H_0 up to the beginning of the continuum. Moreover, to deal with such situations we will combine the Feshbach formalism with operator inequalities.

2. Presentation of the inequality

Our starting point will be an equation similar to the Feshbach equation of nuclear physics. To formulate it we will need two lemmas.

Lemma 1. Let $P^2 = P = P^+$, $Q = 1 - P$, then

$$P(Ph^{-1}P)^{-1}P = PhP - PhQ(QhQ)^{-1}QhP \qquad (2)$$

if the inverse operators exist on the appropriate subspaces.

Proof. $1 - (1-P)hQ(QhQ)^{-1}Q = P$; multiplying from the left by Ph^{-1} and from the right by hP gives

$$P + Ph^{-1}PhQ(QhQ)^{-1}QhP = Ph^{-1}PhP$$

which proves (2).

Lemma 2. Let h be a self-adjoint operator on $\mathscr{H}$:

$$\sigma_{\mathrm{ess}}(h) = [\epsilon_0, \infty) \qquad \sigma_{\mathrm{d}}(h) = \{E_i | E_i < \epsilon_0\},†$$

let P be an orthogonal operator $P^2 = P = P^+$, denote $Q = 1 - P$ and assume that the inverse of $Q(h - E)Q$ exists on $Q\mathscr{H}$; then $E \in \sigma_{\mathrm{d}}(h) \leftrightarrow \exists\, P\psi \in P\mathscr{H}$, so that

$$\{P(h-E)P - PhQ[Q(h-E)Q]^{-1}QhP\}\psi = 0. \qquad (3)$$

Proof. (*a*) $E \in \sigma_{\mathrm{d}}(h)$, $(h-E)\psi = 0$. Projecting onto $P\mathscr{H}$ and $Q\mathscr{H}$ gives

$$P(h-E)(P+Q)\psi = 0, \qquad Q(h-E)(P+Q)\psi = 0.$$

Since we assumed the existence of the inverse of $Q(h-E)Q$ we obtain from the second part

$$Q\psi = -[Q(h-E)Q]^{-1}QhP\psi.$$

Insertion into the first part gives (3).

(*b*) Let E be a solution of (3), $E \notin \sigma_{\mathrm{d}}(h)$ then $P(h-E)^{-1}P$ exists and has an inverse on $P\mathscr{H}$; using lemma 1 contradicts (3).

Now take for h in lemma 2 our Hamiltonian and for the projection $P_2 = 1_1 \otimes R_2$ where $R_2 = |\phi(x_2)\rangle\langle\phi(x_2)|$ should project onto the ground state of $p_2^2 - V(x_2)$ and define

$$h_1 = P_2(H-E)P_2 - P_2V_{12}Q_2[Q_2(H-E)Q_2]^{-1}Q_2V_{12}P_2 \equiv P_2(H-E)P_2 - V_{\mathrm{opt}}. \qquad (4)$$

Lemma 2 tells us that the number of bound states of H below ϵ_0 equals the number of bound states of h_1 defined on $P_2\mathscr{H}$ with $E < \epsilon_0$. The last part of h_1, usually called the

† σ_{d} denotes the discrete spectrum, which is the part of the spectrum consisting of isolated points of finite multiplicity: $\lambda \in \sigma_{\mathrm{d}}$ if and only if $P_{(\lambda-\epsilon, \lambda+\epsilon)}(A)$ is finite dimensional for some $\epsilon > 0$.

optical potential, includes the influence of excited states. The assumption that $Q(H-E)Q$ has an inverse will be further specified in equation (6).

Lemma 3. Let $A \geqslant B$ be two self-adjoint operators on $\mathscr{H}$, a_i, b_i their eigenvalues, then $a_i \geqslant b_i$.

This ordering theorem, a well known consequence of the minimum–maximum principle will be used together with lemma 4 to construct a lower bound operator on the optical potential.

Lemma 4. Let $v \geqslant 0$, $P = P^2 = P^+$, then $v \geqslant P(Pv^{-1}P)^{-1}P$.

The proof and applications have been given several times (W Thirring, T7 Quantenmechanik, Lecture Notes, University of Vienna, Grosse *et al* 1976). To proceed, we observe that replacing E in $V_{\rm opt}$ by ϵ_0 gives a lower bound; furthermore applying lemma 4 gives

$$\begin{aligned} &h_1 \geqslant h_2 = P_2(H-E)P_2 - P_2 V_{12} Q_2[Q_2(H_0 + P_1 v_2^{\rm L} - \epsilon_0)Q_2]^{-1} Q_2 V_{12} P_2 \\ &P_1(P_1 V_{12}^{-1} P_1)^{-1} P_1 \equiv P_1 v_2^{\rm L}, \qquad P_1 = R_1 \otimes 1_2. \end{aligned} \tag{5}$$

Since in general $Q_2(H_0 + P_1 v_2^{\rm L} - \epsilon_0)Q_2$ will not be bounded by a positive c-number we proceed as follows.

Observing that $[P, h] = 0$ implies

$$h^{-1} = P(PhP)^{-1}P + Q(QhQ)^{-1}Q,$$

we may divide $V_{\rm opt}$ into two parts choosing $P = R_1 \otimes 1_2$, $R_1 = |\phi(x_1)\rangle\,\langle\phi(x_1)|$; for the second part we may use the c-number bound

$$Q_1 Q_2 (H_0 - \epsilon_0) Q_1 Q_2 \geqslant (2\epsilon_1 - \epsilon_0) Q_1 Q_2 \equiv \delta\epsilon Q_1 Q_2 > 0$$

so that we obtain

$$\begin{aligned} &h_2 \geqslant h_3 P_2 \\ &h_3 = p_1^2 - V(x_1) + \langle \phi_2 V_{12} \phi_2 \rangle - V_{\rm opt}^{\rm I}(x_1) - \frac{1}{\delta\epsilon} V_{\rm opt}^{\rm II}(x_1) \\ &V_{\rm opt}^{\rm I} = \langle \phi_2 V_{12} P_1 Q_2 (Q_2 H_2^{\rm L} Q_2)^{-1} Q_2 V_{12} \phi_2 \rangle \\ &V_{\rm opt}^{\rm II} = \langle \phi_2 V_{12} Q_1 Q_2 V_{12} \phi_2 \rangle \\ &H_2^{\rm L} = p_2^2 - V_2(x_2) + v_2^{\rm L}(x_2) \equiv p_2^2 - V_{\rm eff}(x_2). \end{aligned}$$

Now we can state our condition for the absence of bound states.

Theorem 1. Let H be given as described in § 1. Assume that there exists a p such that

$$N_p(V_{\rm eff}) > 0 \qquad N_p(V) \equiv c_p - \|r^{(2p-3)/p} V^-\|_p \qquad c_p = \frac{p}{p-1}\left(\frac{(p-1)\Gamma^2(p)}{\Gamma(2p)}\right)^{1/p} \tag{6}$$

and $p \geqslant 1$ if $V_{\rm eff}$ is radial symmetric, $p \geqslant 3/2$ otherwise, then under the condition that

$$N_{\bar p}(V_\Sigma) \geqslant \frac{1}{\delta\epsilon}\|r^{(2\bar p-3)/2\bar p}\phi V_{\rm e}\|^2_{2\bar p/(\bar p+1)} + \inf_{r,t,q} K^2_{r,s,t}\frac{\|V_{12}\|_s^2}{N_q(V_{\rm eff})}\|r^{(2q-3)/2q}\phi\|_\sigma^2\|r^{(2\bar p-3)/2\bar p}\phi\|_\tau^2 \tag{7}$$

$$1+\frac{2}{\sigma}=\frac{2}{r}+\frac{1}{q}, \qquad 1+\frac{2}{\tau}=\frac{2}{t}+\frac{1}{\bar{p}}, \qquad 2=\frac{1}{r}+\frac{1}{s}+\frac{1}{t}, \qquad 1\leqslant q, \bar{p}, r, s, t\leqslant\infty$$

$$V_{\mathrm{e}}(x_1)=\langle\phi_2 V_{12}\phi_2\rangle$$

$$V_{\Sigma}(x_1)=V(x_1)-V_{\mathrm{e}}(x_1)+\frac{1}{\delta\epsilon}(\langle\phi_2 V_{12}^2\phi_2\rangle-\langle\phi_2 V_{12}\phi_2\rangle^2)$$

for some $\bar{p}\geqslant 3/2$, there exists no three-body bound state.

Remarks. Condition (6) guarantees the absence of two-body bound states for V_{eff}; such a condition has been derived by Glaser *et al* (1976). V^- always denotes the negative part of the potential. The constants $K_{r,s,t}\leqslant 1$ enter through Young's inequality and will be specified below.

Proof. We will show that the functional which corresponds to h_3:

$$h_3(\chi)=\int|\nabla\chi|^2+\int|\chi|^2\left(V_{\mathrm{e}}-V-V_{\mathrm{opt}}^{\mathrm{I}}-\frac{1}{\delta\epsilon}V_{\mathrm{opt}}^{\mathrm{II}}\right) \tag{8}$$

is positive under the stated conditions.

As an application of lemma 4 we first note that

$$\langle\chi V_{\mathrm{opt}}^{\mathrm{I}}\chi\rangle=\sup_{\substack{\rho_2\in\mathcal{H}_2\\ \rho_2\perp\phi_2}}\frac{|\langle\chi_1\phi_2 V_{12}\phi_1\rho_2\rangle|^2}{\langle\rho_2 H_2^{\mathrm{L}}\rho_2\rangle} \tag{9}$$

since (6) implies that $H_2^{\mathrm{L}}>0$.

Next we make use of a result derived by Glaser *et al* (1976):

$$\int|\nabla\rho|^2\geqslant c_p\left(\int r^{p'-3}\rho^{2p'}\right)^{1/p'} \qquad \frac{1}{p}+\frac{1}{p'}=1 \tag{10}$$

where ρ has to be from a suitable chosen space of functions (e.g. C^{∞}) such that the norms exist. Using Hölder's inequality in the denominator and the recently derived sharp form of Young's inequality (Brascamp and Lieb 1976, Beckner 1975):

$$\int \mathrm{d}^n x\,\mathrm{d}^n y\, f(x)g(x-y)h(y)\leqslant K_{r,s,t}\|f\|_r\|g\|_s\|h\|_t$$

$$K_{r,s,t}=\tilde{c}_r\tilde{c}_s\tilde{c}_t, \qquad \tilde{c}_\alpha=\left(\frac{\alpha^{1/\alpha}}{\alpha'^{1/\alpha'}}\right)^{n/2}, \qquad \frac{1}{\alpha}+\frac{1}{\alpha'}=1,$$

$$1\leqslant r, s, t\leqslant\infty, \qquad 2=\frac{1}{r}+\frac{1}{s}+\frac{1}{t}$$

for the numerator, and adjusting the L^p norms so that the ρ dependence drops out, an upper bound to (9) is obtained:

$$\langle\chi V_{\mathrm{opt}}^{\mathrm{I}}\chi\rangle\leqslant K_{r,s,t}^2\frac{\|V_{12}\|_s^2}{N_p(V_{\mathrm{eff}})}\|\phi\chi\|_r^2\|r^{(2p-3)/2p}\phi\|_\tau^2\equiv Z_{\mathrm{I}}(\chi) \tag{11}$$

$$1+\frac{2}{\tau}=\frac{2}{t}+\frac{1}{p}.$$

The second term of the optical potential describing the influence of states from $Q_1Q_2\mathcal{H}$ can be bounded in the following way:

$$\langle\chi V_{\text{opt}}^{\text{II}}\chi\rangle \leqslant \langle\chi_1(\langle\phi_2 V_{12}^2\phi_2\rangle - \langle\phi_2 V_{12}\phi_2\rangle^2)\chi_1\rangle + |\langle\chi_1\phi_1 V_e(1)\rangle|^2 = Z_{\text{II}}(\chi). \tag{12}$$

Putting these all together and using (10) again yields

$$h_3(\chi) \geqslant \|r^{(p'-3)/2p'}\chi\|_{2p'}^2 c_p - Z_{\text{I}}(\chi) - \frac{Z_{\text{II}}(\chi)}{\delta\epsilon} + \langle\chi|V_e - V|\chi\rangle. \tag{13}$$

With the help of Hölder's inequality and assumption (6) the positivity of the functional $h_3(\chi)$ is proved.

3. Remarks

(*a*) To illustrate condition (6) for the absence of two-body bound states we remark that for $p = \frac{3}{2}$, $c_{3/2}^{3/2} = 3\pi\sqrt{3}/16$ and $(\|V\|_{3/2}/c_{3/2})^{3/2} = (8/\sqrt{3})V_{\text{ps}} \equiv \tilde{V}_{\text{ps}}$ where V_{ps} denotes the classical phase space volume

$$V_{\text{ps}} = \int \frac{d^3x\, d^3p}{(2\pi)^3} |(p^2 - V)^-| = \frac{1}{6\pi^2}\int d^3x |V^-|^{3/2}$$

so that (6) reads $\tilde{V}_{\text{ps}} < 1$. Actually a generalization is valid: the total number of two-body bound states N is bounded by $N \leqslant cV_{\text{ps}}$, and goes asymptotically for $V = \lambda v$, $\lambda \to \infty$ like $N \sim V_{\text{ps}}$ (Glaser *et al* 1976).

(*b*) To illustrate (7) we note that for $\bar{p} = p = q = \frac{3}{2}$ a weaker condition results (since $K \leqslant 1$):

$$c_{3/2} - \|V_{\bar{2}}\|_{3/2} \geqslant \frac{1}{\delta\epsilon}\|\phi V_e\|_{6/5}^2 + \frac{\|V_{12}\|_{3/2}^2}{c_{3/2} - \|V_{\text{eff}}\|_{3/2}}. \tag{7a}$$

Considering the case where excited states give small contributions (7*a*) implies the absence of three-body bound states if the potential $-V(1) + \langle\phi_2 V_{12}\phi_2\rangle$, corrected by a contribution coming from the ground state of H_0 as intermediate state, has no two-body bound states.

(*c*) For Coulomb-like repulsive potentials $V_{12} = \alpha/r_{12}$ condition (7) is always violated since $1/r_{12}$ is in no L^p space. A way out will be the use of Sobolev's inequality (Reed and Simon 1975) instead of Young's inequality in the derivation. We did not include this since the usual proofs of Sobolev's inequality give no numerical constants for the bound.

(*d*) In addition to (*c*) a further problem arises for the H^- atom where $\alpha = 1$. The effective potential

$$V_{\text{eff}}(x_1) = -\frac{1}{x_1} + \frac{1}{x_1 + (4/x_1) - e^{-x_1}[(4/x_1) + 1]}$$

actually has one bound state, so condition (6) is violated. In other words by projecting one particle into the ground state the infinite number of bound states below ϵ_0 is lifted into the continuum except for one state. A way out may be to restrict the Hamiltonian to $(1 - P_1 \otimes P_2)\mathcal{H}$ and noting that

$$(1 - P_1 \otimes P_2)h(1 - P_1 \otimes P_2) \geqslant \epsilon_0(1 - P_1 \otimes P_2)$$

would imply, that the number of three-body bound states of h is less than or equal to one.

(e) One should add that recently it has been proved by a different method, that exactly one bound state exists for the H^- atom (Hill 1976).

(f) The condition $2\epsilon_1 - \epsilon_0 > 0$ can be relaxed by introducing a sum of appropriate projection operators. If one restricts oneself to the subspace of antisymmetric wavefunctions, $\delta\epsilon$ can be replaced by $\epsilon_2 + \epsilon_3 - \epsilon_1$.

(g) Note that in general $\inf_\rho \langle \rho H_2^L \rho \rangle$ will be zero, so that our division of V_{opt} is necessary.

(h) Although we formulated our condition for identical particle interactions, the generalization to other cases is obviously possible.

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