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Inversion procedure for a certain class of nonspherically symmetric potentials

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Abstract. An iterative inversion procedure is studied for a particular class of nonspherically symmetric interactions. This class consists of the potentials whose Fourier transform is a product of two factors: a function of the magnitude of the transform-space vector and a function of its direction only. The input data required for the inversion procedure are the amplitude for backward scattering for all the directions of incident momentum (with respect to some specified axis) at a fixed energy, and the value of the spherical average of the interaction, which is assumed to be known.

Conditions are established for the convergence of the inversion procedure, and for the existence and uniqueness of a solution of the above-mentioned factorizable form. The results are extended to the much wider class of potentials which can be represented as a sum of N factorizable interaction terms. The inversion method then requires knowledge of the backward scattering amplitude at N different energies. These results have potential applications to the determination of intermolecular forces from scattering data. In this case the spherical average of the potential, knowledge of which is required as input for the above procedure, can itself be determined from scattering data by presently available inversion methods.

1. Introduction

The recent highly accurate measurements of elastic differential cross sections of interatomic and intermolecular collisions, have led to an increased interest in the problem of inversion of scattering data to obtain the potential (Buck and Pauly 1971, Vollmer 1969, Olson and Mueller 1967). For spherically symmetric potentials, rigorous, quantum-mechanical inversion procedures are available (Newton 1966, Sabatier 1972), and also semiclassical inversion methods were given for such forces (Buck 1971, Miller 1971). However, all this is sufficient for dealing with interatomic potentials only, for molecule–molecule interactions are generally not spherically symmetric. Unfortunately, no systematic and rigorous method is available yet for solving the inversion problem for nonspherically symmetric forces. A formal iterative inversion procedure for such interactions was proposed by Prosser (1969). However, so far no proof has been given that this procedure converges and that the solution it yields is unique. The purpose of the present article is to describe some results on the questions of convergence and uniqueness in Prosser's method, and thus to provide a sounder mathematical basis for its application. Because of the difficulty in establishing conditions for convergence in the general case, we shall confine our considerations to a limited class of nonspherically symmetric interactions which will be defined below. Whereas the questions that we shall study are mathematical in nature, it will be useful to keep in mind a physical system to which our

results can perhaps be applied. Consider the elastic scattering of an atom by a molecule. Suppose that one can represent the interaction between the collision partners to a good approximation by a potential function $U(\boldsymbol{r})$ which depends only upon $\boldsymbol{r}$, the distance between the atom and the centre of mass of the molecule. For a fixed molecular orientation the interaction will clearly depend upon the direction of $\boldsymbol{r}$ with respect to the molecular orientation as well as upon the distance $r \equiv |\boldsymbol{r}|$, thus $U(\boldsymbol{r})$ will be nonspherically symmetric in general. Consider, however, as is the case in most molecular beam experiments, a molecule free to rotate in the absence of external fields. Suppose for simplicity that the collision takes place at extremely low energies, so that the rotation of the molecule is much faster than the relative translational motion of the collision partners. To a good approximation one can then regard the incoming atom as experiencing an effective potential equal to the average of $U(\boldsymbol{r})$ over all orientations of the molecule. This effective potential $\bar{U}(r) = \langle U(\boldsymbol{r})\rangle_{\Omega(\boldsymbol{r})}$ is spherically symmetric. We shall confine ourselves in this article to the cases where the nonaveraged interaction $U(\boldsymbol{r})$ has the following property:

$$\tilde{U}(\boldsymbol{k}) \equiv \frac{2m}{\hbar^2}\int \mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{r}}U(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = g(k)\gamma(\hat{k}) \tag{1}$$

where $\hat{k}$ denotes a unit vector in the direction of $\boldsymbol{k}$, and m stands for the reduced mass of the collision partners. The constant factor $2m/\hbar^2$ in equation (1) was introduced to make some of the forthcoming expressions more compact. Whereas the factorization assumption (1) constitutes a severe restriction on the interactions considered, it is nevertheless possible that some realistic intermolecular forces can be approximated by a function having this property. It is easy to show from the properties of the Fourier transform that the effect of free molecular rotation on the interaction in Fourier space $\tilde{U}(\boldsymbol{k})$ is to produce an average $\langle\tilde{U}(\boldsymbol{k})\rangle_{\Omega(\boldsymbol{k})}$ over all directions in $\boldsymbol{k}$ space. From equation (1) we have:

$$\langle\tilde{U}(\boldsymbol{k})\rangle_{\Omega(\boldsymbol{k})} \equiv \bar{\tilde{U}}(k) = g(k)\bar{\gamma}. \tag{2}$$

$\bar{\gamma}$, the average of $\gamma(\hat{k})$ over all possible directions of $\hat{k}$ is just a number. The interaction $\bar{\tilde{U}}(k)$ is spherically symmetric, and one can therefore determine, in principle, this function from scattering data by any of the existing inversion methods for spherically symmetric potentials. Suppose that in addition to a scattering experiment in which the molecule is free to rotate one does also another experiment in which the orientation of the scattering molecule is kept fixed by an external field. The question now arises whether one can, from the scattering data of the second experiment combined with knowledge of $g(k)$ determined from the first experiment, find $\gamma(\hat{k})$ by a systematic procedure. This provides some physical motivation for the mathematical questions that we shall now consider.

2. The inversion procedure

The model that we shall consider is the scattering of a particle of mass m by a potential $U(\boldsymbol{r})$ assumed to have the property (1). The T matrix for the scattering process satisfies the Lippmann–Schwinger equation which can be written in the form (see, for instance, Watson and Nuttall 1967, p 14)

$$\langle\boldsymbol{k}'|T|\boldsymbol{k}\rangle = \langle\boldsymbol{k}'|U|\boldsymbol{k}\rangle + \int \frac{\langle\boldsymbol{k}'|U|\boldsymbol{k}''\rangle\langle\boldsymbol{k}''|T|\boldsymbol{k}\rangle\,\mathrm{d}\boldsymbol{k}''}{E_k - E_{k''} + \mathrm{i}\epsilon} \tag{3}$$

where $\boldsymbol{k}$, $\boldsymbol{k}'$ denote respectively the initial and the final wavevector, and $E_k = \hbar^2|\boldsymbol{k}|^2/2m$

is the energy of the system. Repeated iterations of equation (3) yield the familiar Born series for $\langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle$. Let us assume that this series converges for the energy E_k. Later we shall justify this assumption under the conditions we shall impose for establishing the validity of the inversion procedure described below. Meanwhile we just mention the well known result (Zemach and Klein 1958) that at a sufficiently high energy E_k the Born series converges for any potential which satisfies the weak conditions:

$$I(r) \equiv \int \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}|U(\boldsymbol{r}')|\,\mathrm{d}\boldsymbol{r}' < M, \qquad I(r) \sim \mathrm{O}\left(\frac{1}{r}\right) \qquad \text{as } r \to \infty,$$

where M is constant.

Written in the momentum (or wavevector) representation, the Born series for $T(\boldsymbol{k}', \boldsymbol{k})$ has the form:

$$\frac{2m}{\hbar^2}\langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle = \tilde{U}(\boldsymbol{k}'-\boldsymbol{k}) + \sum_{s=1}^{\infty} \int\int \cdots \int \mathrm{d}\boldsymbol{k}_1 \ldots \mathrm{d}\boldsymbol{k}_s \tilde{U}(\boldsymbol{k}_1-\boldsymbol{k}')\frac{1}{k^2-k_1^2+\mathrm{i}\epsilon}\tilde{U}(\boldsymbol{k}_2-\boldsymbol{k}_1)\ldots$$
$$\times \frac{1}{k_s^2-k^2+\mathrm{i}\epsilon}\tilde{U}(\boldsymbol{k}-\boldsymbol{k}_s) \tag{4}$$

where $\tilde{U}(\boldsymbol{q})$ is defined in equation (1), and $k_i \equiv |\boldsymbol{k}_i|$. Setting $\boldsymbol{k}' = -\boldsymbol{k}$ and substituting the expression (1) for $\tilde{U}(\boldsymbol{q})$ into the above equation we obtain:

$$\gamma(\hat{k}) = -4\pi\frac{f(-\boldsymbol{k}, \boldsymbol{k})}{g(2k)} - \sum_{s=1}^{\infty} \int\int \cdots \int \mathrm{d}\Omega_1\, \mathrm{d}\Omega_2 \ldots \mathrm{d}\Omega_s L_s(\boldsymbol{k}, \hat{q}_1, \hat{q}_2 \ldots \hat{q}_s) \prod_{i=1}^{s+1} \gamma(\hat{q}_i) \tag{5}$$

$f(-\boldsymbol{k}, \boldsymbol{k}) = -(m/2\pi\hbar^2)\langle -\boldsymbol{k}|T|\boldsymbol{k}\rangle$ is the backward scattering amplitude, $\mathrm{d}\Omega_i$ denotes integration over all directions of $\hat{k}_i \equiv \boldsymbol{k}_i/k_i$ and the following definitions are used:

$$\hat{q}_1 = \frac{\boldsymbol{k}-\boldsymbol{k}_1}{|\boldsymbol{k}-\boldsymbol{k}_1|}, \qquad \hat{q}_2 = \frac{\boldsymbol{k}_2-\boldsymbol{k}_1}{|\boldsymbol{k}_2-\boldsymbol{k}_1|}, \ldots, \qquad \hat{q}_s = \frac{\boldsymbol{k}_s-\boldsymbol{k}_{s-1}}{|\boldsymbol{k}_s-\boldsymbol{k}_{s-1}|}, \qquad \hat{q}_{s+1} = \frac{\boldsymbol{k}-\boldsymbol{k}_s}{|\boldsymbol{k}-\boldsymbol{k}_s|} \tag{6}$$

$$L_s(\boldsymbol{k}, \hat{q}_1, \ldots, \hat{q}_s) = \frac{1}{g(2k)}\int_0^{\infty} \mathrm{d}k_1 k_1^2 \int_0^{\infty} \mathrm{d}k_2 k_2^2 \ldots \int_0^{\infty} \mathrm{d}k_s k_s^2 g(|\boldsymbol{k}_1+\boldsymbol{k}|)\frac{1}{k^2-k_1^2+\mathrm{i}\epsilon}$$
$$\times g(|\boldsymbol{k}_2-\boldsymbol{k}_1|)\ldots\frac{1}{k_s^2-k^2+\mathrm{i}\epsilon}g(|\boldsymbol{k}-\boldsymbol{k}_s|). \tag{7}$$

Equation (5) is essentially the same as the basic equation employed by Prosser (1969), but is specialized to interactions with the factorization property (1), and simplified accordingly. Following the discussion of § 1, we shall assume that $g(k)$ is known as a function of k. Thus, taking again the example of atom–molecule scattering, this tacitly implies supposition of the availability of scattering data for an experiment in which the molecule is not prepared in any state of orientation, as well as for an experiment in which the molecule does have a definite orientation in space. From the results of the first experiment the spherically averaged atom–molecule potential

$$V(r) = \frac{\hbar^2\bar{\gamma}}{2m(2\pi)^3}\int g(k)\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\,\mathrm{d}\boldsymbol{k}$$

can be determined by any of the presently available inversion methods for spherically symmetric forces. We are left with the task of determining $\gamma(\hat{k})$ from the experiment in which orientation is involved. Assuming that $f(-\boldsymbol{k}, \boldsymbol{k})$ is known at a fixed energy for

all the directions of $\boldsymbol{k}$, we can attempt to calculate $\gamma(\hat{k})$ from equation (5). It is natural to try an iterative solution:

$$\gamma_{n+1}(\hat{k}) = -4\pi\frac{f(-\boldsymbol{k},\boldsymbol{k})}{g(2k)} - \sum_{s=1}^{\infty}\int\int\ldots\int \mathrm{d}\Omega_1\ldots\mathrm{d}\Omega_s L_s(\boldsymbol{k},\hat{q}_1,\ldots,\hat{q}_s)\prod_{i=1}^{s+1}\gamma_n(\hat{q}_i) \tag{8}$$

with $\gamma_0(\hat{k}) \equiv 0$.

The convergence properties of this iterative process, as well as the related questions of existence and uniqueness of a solution of equation (5) will be investigated in the next section.

3. Convergence of the iterations and the existence of a unique solution

Throughout the discussion below, $k = |\boldsymbol{k}|$ will be kept fixed.

Proposition 1. Suppose that one can find a constant $\alpha(k)$ such that $g(q)$ which we assumed known as a function of $q = |\boldsymbol{q}|$, obeys the following inequality:

$$|L_s(\boldsymbol{k},\hat{q}_1,\ldots,\hat{q}_s)| \leqslant \alpha(k) < \frac{1}{8\pi} \tag{9}$$

for all s. L_s, a functional of $g(q)$, is defined by equation (7). Suppose further that the given scattering data satisfy the condition:

$$\left|\frac{f(-\boldsymbol{k},\boldsymbol{k})}{g(2k)}\right| < \frac{1}{8\pi}M(k), \qquad M(k) = \text{a constant} \tag{10}$$

and that one can find a value of $M(k)$ which in addition to satisfying (10) also obeys the inequality:

$$M(k) \leqslant \frac{1}{4\pi}(1-8\pi\alpha(k)). \tag{11}$$

Then all the iterates $\gamma_n(\hat{k})$ are uniformly bounded functions of k:

$$|\gamma_n(\hat{k})| < M(k). \tag{12}$$

The proof is obvious and proceeds by induction. For $n = 1$ it is trivial to verify from (5) and (10) that inequality (12) is obeyed. Assuming (12) to hold for $n = p$, we find from (5), (10) and (9):

$$\begin{aligned}|\gamma_{p+1}(\hat{k})| &\leqslant 4\pi\left|\frac{f(-\boldsymbol{k},\boldsymbol{k})}{g(2k)}\right| + \left|\sum_{s=1}^{\infty}\int \mathrm{d}\Omega_1\ldots\int \mathrm{d}\Omega_s L_s(\boldsymbol{k},\hat{q}_1,\ldots,\hat{q}_s)\prod_{i=1}^{s+1}\gamma_p(\hat{q}_i)\right| \\ &< \frac{1}{2}M + \sum_{s=1}^{\infty}(4\pi)^s M^{s+1}\alpha < \frac{1}{2}M + \frac{M^2 4\pi}{1-4\pi M}\alpha\end{aligned} \tag{13}$$

which together with condition (11) readily leads to $|\gamma_{p+1}(\boldsymbol{k})| < M$, establishing the result that we sought to prove.

Proposition 2. Suppose that conditions (9)–(11) are satisfied and that, in addition

$$J = 8\pi\alpha M\frac{|1-2\pi M|}{(1-4\pi M)^2} < 1. \tag{14}$$

Then the sequence of iterates $\{\gamma_n(\hat{k})\}$ converges uniformly, that is, $\lim_{n\to\infty}\gamma_n(\hat{k})$ exists for all $\hat{k}$.

Proof. Subtracting the expression (8) for the $(n+1)$th iterate from the corresponding expression for the nth iterate and using the inequality (9) one gets:

$$|\gamma_{n+1}(\hat{k})-\gamma_n(\hat{k})| \leqslant \alpha \sum_{s=1}^{\infty} \int d\Omega_1 \dots \int d\Omega_s \left| \prod_{i=1}^{s+1} \gamma_n(\hat{q}_i) - \prod_{i=1}^{s+1} \gamma_{n-1}(\hat{q}_i) \right|. \tag{15}$$

Using the inequality (11) it can easily be shown that:

$$\left| \prod_{i=1}^{s+1} \gamma_n(\hat{q}_i) - \prod_{i=1}^{s+1} \gamma_{n-1}(\hat{q}_i) \right| \leqslant (s+1)(M(k))^s \max_{\hat{q}} |\gamma_n(\hat{q})-\gamma_{n-1}(\hat{q})|. \tag{16}$$

The proof proceeds by induction and is straightforward, so we shall not give it here.

Substituting the above inequality into (15) one obtains:

$$|\gamma_{n+1}(\hat{k})-\gamma_n(\hat{k})| \leqslant \alpha \sum_{s=1}^{\infty} (s+1)(4\pi M)^s \max_{\hat{q}} |\gamma_n(\hat{q})-\gamma_{n-1}(\hat{q})|. \tag{17}$$

Carrying out the obvious summation of the series which appears in (17) yields:

$$|\gamma_{n+1}(\hat{k})-\gamma_n(\hat{k})| \leqslant J \max_{\hat{q}} |\gamma_n(\hat{q})-\gamma_{n-1}(\hat{q})| \tag{18}$$

where J is defined in (14). (18) is valid for all values of $\hat{k}$, so in particular we must have:

$$\max_{\hat{k}} |\gamma_{n+1}(\hat{k})-\gamma_n(\hat{k})| \leqslant J \max_{\hat{k}} |\gamma_n(\hat{k})-\gamma_{n-1}(\hat{k})|. \tag{19}$$

From the definition of γ_1 and γ_0 together with condition (10) we have:

$$\max_{\hat{k}} |\gamma_1(\hat{k})-\gamma_0(\hat{k})| < \tfrac{1}{2}M.$$

By repeated application of (19) we get:

$$\max_{\hat{k}} |\gamma_2(\hat{k})-\gamma_1(\hat{k})| < \tfrac{1}{2}MJ; \max_{\hat{k}} |\gamma_3(\hat{k})-\gamma_2(\hat{k})| < \tfrac{1}{2}MJ^2; \max_{\hat{k}} |\gamma_n(\hat{k})-\gamma_{n-1}(\hat{k})| < \tfrac{1}{2}MJ^{n-1}. \tag{20}$$

Since $\gamma_0 \equiv 0$, we have:

$$\lim_{n\to\infty} \gamma_n(\hat{k}) = \sum_{n=1}^{\infty} (\gamma_n(\hat{k})-\gamma_{n-1}(\hat{k})). \tag{21}$$

By (20), the series on the right-hand side of (21) can be majorized by:

$$\left| \sum_{n=1}^{\infty} (\gamma_n(\hat{k})-\gamma_{n-1}(\hat{k})) \right| \leqslant \sum_{n=1}^{\infty} \max_{\hat{k}} |\gamma_n(\hat{k})-\gamma_{n-1}(\hat{k})| < \frac{1}{2}M \sum_{n=1}^{\infty} J^{n-1}. \tag{22}$$

The majorizing series converges under condition (14), $J < 1$. Thus, also the series on the left-hand side of (22) converges, and $\lim_{n\to\infty}\gamma_n(\hat{k})$ exists.

We note here that the above result, and also the propositions below, can be proved more compactly if use is made of the contraction mapping principle from the abstract theory of equations in Banach spaces (see, for instance, Wouk 1964). We prefer, however, to use simpler techniques.

Proposition 3. Assume again that conditions (9)–(11), (14) hold. Then

$$\gamma(\hat{k}) \equiv \lim_{n\to\infty} \gamma_n(\hat{k}) \tag{23}$$

is a solution of the nonlinear integral equation (5). We shall briefly sketch the proof.

For any function $\beta(\hat{k})$ of $\hat{k}$, we define

$$K\beta(\hat{k}) \equiv -4\pi \frac{f(-\boldsymbol{k}, \boldsymbol{k})}{g(2k)} - \sum_{s=1}^{\infty} \int \mathrm{d}\Omega_1 \ldots \int \mathrm{d}\Omega_s L_s(\hat{k}, \hat{q}_1, \ldots, \hat{q}_s) \prod_{i=1}^{s+1} \beta(\hat{q}_i). \tag{24}$$

The domain of the nonlinear operator K consists of the functions $\beta(\hat{k})$ for which the right-hand side of (24) converges. Note that $\gamma(\hat{k})$ is included in this domain: since by (12) all the iterates are bounded by M, also their limit $\gamma(\hat{k})$ will satisfy $|\gamma(\hat{k})| \leqslant M$ where M obeys (10) and (11) (the equality sign cannot be ruled out here). Using this relation, convergence of the right-hand side of (24) for $\beta(\hat{k}) = \gamma(\hat{k})$ can be established by the same argument which was used to majorize the series in (13). Consider now the following inequality, which holds for any of the iterates (8):

$$|K\gamma - \gamma| \leqslant |K\gamma - K\gamma_n| + |K\gamma_n - \gamma| = |K\gamma - K\gamma_n| + |\gamma_{n+1} - \gamma|. \tag{25}$$

Using the inequality $|\gamma(\hat{k})| \leqslant M$ together with conditions (9)–(11), (14), and proceeding in the same way as in the proof of proposition 2, it is easy to show that

$$\max_{\hat{k}} |K\gamma - K\gamma_n| \leqslant J \max_{\hat{k}} |\gamma(\hat{k}) - \gamma_n(\hat{k})|. \tag{26}$$

From (26) and (23) it is obvious that the right-hand side of (25) tends to zero as $n \to \infty$. Thus we must have:

$$\gamma(\hat{k}) = K\gamma(\hat{k}), \tag{27}$$

that is, the limit (23) of the iterates satisfies equation (5). We have thus shown that there exists a factorizable solution of the type (1) for the inversion problem under the conditions (9)–(11), (14).

We shall now consider the question of the uniqueness of the solution.

Proposition 4. Let $\gamma_A(\hat{k})$, $\gamma_B(\hat{k})$ be two bounded solutions of equation (5), and suppose that conditions (9)–(11), (14) are satisfied. Also, assume that M of condition (8) is an upper bound on the magnitudes of $\gamma_A(\hat{k})$, $\gamma_B(\hat{k})$. Then:

$$\gamma_A(\hat{k}) = \gamma_B(\hat{k}). \tag{28}$$

Subtracting the equation satisfied by $\gamma_A(\hat{k})$ from that which is obeyed by $\gamma_B(\hat{k})$ and following the same procedure as in the proof of proposition 2, we obtain the inequality

$$|\gamma_A(\hat{k}) - \gamma_B(\hat{k})| \leqslant J \max_{\hat{q}} |\gamma_A(\hat{q}) - \gamma_B(\hat{q})|.$$

This holds for every $\hat{k}$, so in particular:

$$\max_{\hat{k}} |\gamma_A(\hat{k}) - \gamma_B(\hat{k})| \leqslant J \max_{\hat{k}} |\gamma_A(\hat{k}) - \gamma_B(\hat{k})|.$$

But this inequality is consistent with the condition $J < 1$ only when

$$\max_{\hat{k}} |\gamma_A(\hat{k}) - \gamma_B(\hat{k})| = 0,$$

hence (28) follows.

Finally, a comment is due on the assumption made at the outset of the treatment, that the Born series converges for the energy which pertains to the wavenumber k. It was with the aid of this assumption that (5) was derived. The question arises if the conditions (9)–(11), (14) that were imposed on the known function $g(q)$ and on the scattering amplitude do, in fact, imply convergence of the Born series. What one has to show is that the series on the right-hand side of (5) converges. This was, however,

already proved tacitly earlier, since we established that the right-hand side of (24) converges for $\beta(\hat{k}) = \gamma(\hat{k})$.

The connection between the convergence properties of the inversion procedure and that of the Born series implies that it is best for the sake of fast convergence to apply the inversion scheme at an energy as high as the availability of scattering data permits. This is not in any contradiction with the fact that other, low energy experiments may be the best input source for inversion procedures that seek to determine the spherical average of the interaction from scattering data. We have already argued in § 1 that spherically-averaged intermolecular forces can be obtained from low energy scattering data. The results of such an inversion procedure combined with the scattering amplitude measured at relatively high energies can serve as input information in the present scheme which yields the anisotropy of the intermolecular force.

4. Extension to more general interactions

The main limitation of the results of the previous sections, is that they are confined to a very restricted class of potentials. It is not clear whether interactions of that form can provide a reasonable approximation for, say, realistic intermolecular forces. We shall give here an extension of the results of § 3 to a much wider class of potentials.

We assume that $U(\boldsymbol{k})$ can be expanded in the form:

$$\tilde{U}(\boldsymbol{k}) = \sum_{i=1}^{N} g_i(k)\gamma^i(\hat{k}) \tag{29}$$

where the functions $g_i(k)$ are taken to be known. One can think about (29) as an expansion in some basis set of functions of k. This expansion is, of course, not unique and depends upon the basis we choose. The most unsatisfactory feature of this approach is that one has to postulate *a priori* that the expansion series terminates after a certain number of terms. For a wide subclass of potentials of the form (29), the integer N can be determined from scattering data: consider again the example of atom–molecule scattering, and recall that we can determine from experimental data the spherically averaged potential

$$\langle \tilde{U} \rangle_{\Omega(\boldsymbol{k})} = \sum_{i=1}^{N} g_i(k)\bar{\gamma}^i.$$

If we restrict ourselves to the class of potentials for which $\bar{\gamma}^i \neq 0$ for all i, and if the $g_i(k)$ are taken to be an orthonormal set, then the number of terms N in (29) will just be the number of functions $g_i(k)$ which are not orthogonal to the function $\langle \tilde{U} \rangle_{\Omega(\boldsymbol{k})}$. The postulate that $\bar{\gamma}^i \neq 0$ for all i is, however, highly undesirable since it cannot be checked from given scattering data at the outset of the inversion scheme.

Suppose that the backward scattering amplitude $f(-\boldsymbol{k}, \boldsymbol{k})$ is known at N different energies, with k^i denoting the wavenumber which corresponds to the energy E_i. Let $D = \{d_{ij}\}$ be the matrix which is the inverse of $G = \{g_{ij} \equiv g_i(k_j)\}$ (assuming that the inverse exists). Substitution of (29) into equation (4) leads, after trivial manipulations, to the following set of coupled nonlinear integral equations for the $\gamma^l(k)$:

$$\gamma^l(\hat{k}) = V_l(\hat{k}) - \sum_{s=1}^{\infty} \sum_{i_1=1}^{N} \cdots \sum_{i_{s+1}}^{N} \int \mathrm{d}\Omega_1 \cdots \int \mathrm{d}\Omega_s L^{sl}_{i_1 \ldots i_{s+1}}(\hat{k}, \hat{q}_1, \ldots, \hat{q}_s)\gamma^{i_1}(\hat{q}_1) \cdots \gamma^{i_{s+1}}(\hat{q}_{s+1}) \tag{30}$$

for $1 = 1, 2, \ldots, N$. The $\hat{q}_i$ are defined as in § 2 and:

$$V_l(\hat{k}) = -4\pi \sum_j^N d_{lj} f(-\boldsymbol{k}_j, \boldsymbol{k}_j)$$

$$L^{sl}_{i_1 \ldots i_{s+1}} = \sum_{j=1}^N d_{lj} \int_0^\infty \mathrm{d}k_1 k_1^2 \int_0^\infty \mathrm{d}k_2 k_2^2 \ldots \int_0^\infty \mathrm{d}k_s k_s^2 g_{i_1}(|\boldsymbol{k}_1 + \boldsymbol{k}^j|)$$

$$\times \frac{1}{(k^j)^2 - k_1^2 + i\epsilon} g_{i_2}(|\boldsymbol{k}_2 - \boldsymbol{k}_1|) \ldots \frac{1}{k_s^2 - (k^j)^2 + i\epsilon} g_{i_{s+1}}(|\boldsymbol{k}_s - \boldsymbol{k}^j|). \tag{31}$$

Suppose now that there exists a constant $\alpha < 1/8\pi$ such that

$$\max_s \max_{\hat{q}_i} \max_l \left| \sum_{i_1=1}^N \ldots \sum_{i_{s+1}}^N L^{sl}_{i_1 \ldots i_{s+1}}(\hat{q}_1, \ldots, \hat{q}_s) \right| \leqslant \alpha \tag{32}$$

and that one can find a constant M such that

$$|V_l(\hat{k})| < M \qquad \text{(for all } l\text{)}. \tag{33}$$

Moreover, assume that

$$M \leqslant \frac{1}{4\pi}(1 - 8\pi\alpha); \qquad J = 8\pi\alpha M \frac{|1 - 2\pi M|}{(1 - 2\pi M)^2} < 1. \tag{34}$$

Then it is a straightforward, although rather tedious matter, to extend the results of § 3 to the present case. One can thus show that: (i) iterations of the coupled equations (30) converge to yield a set of N functions $\gamma^i(\hat{k})$ which are solutions of these equations; (ii) the solutions so obtained for the $\gamma^i(\hat{k})$ are unique under the above conditions.

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