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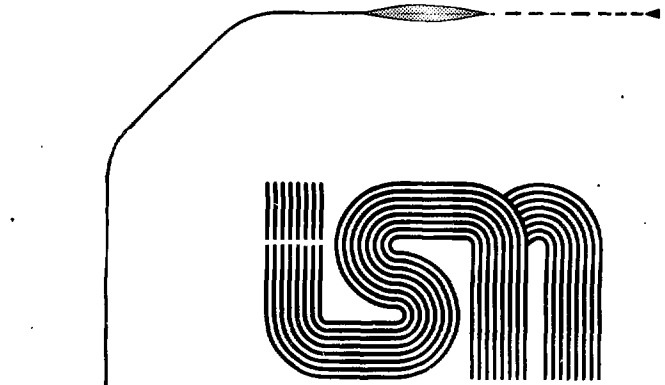

THE RESONATING GROUP METHOD IN AN HARMONIC OSCILLATOR BASIS

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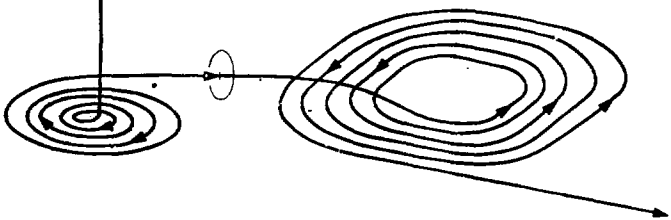

THE RESONATING GROUP METHOD IN AN HARMONIC OSCILLATOR BASIS

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Abstract . The scattering states for a general many body system is formulated within the resonating group method. The resulting Lippman-Schwinger equation is solved in an harmonic oscillator basis for which a number of advantages are emphasized. The analytical formula giving the free propagator in that basis is fully derived.

THE RESONATING GROUP METHOD

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1. Introduction

For various types of atomic or nuclear physics situations one is lead to solve scattering problems for which one searches transition rates from a state consisting of two clusters towards a state consisting of a new (or the same) partition for the two clusters.

The exact solution for such a problem is presently not feasible once the number of particles exceeds four. Among the approximate methods introduced to solve the general problem, the resonating group method proposed by Wheeler (1937) is very attractive and powerful. The N-body problem is transformed into a system of coupled channel equations for the wave functions relative to the various partitions defining the clusters. The coupling potentials between distinct channels are strongly non local.

The solution for the scattering Schrödinger equation in configuration space is a set of coupled integro-differential equations, with appropriate boundary conditions. Numerically one needs to discretise the space on a mesh and one has to solve the resulting linear system. If n_c is the number of channels and n_R the number of points on the mesh, the dimension for the system is $n_c \times n_R$ and one easily sees that for typical values of $n_R \sim 100$ the computational task is quite heavy.

On the other hand, the integro-differential equations can be cast into a system of coupled integral equations for which the boundary conditions are already included. The resulting equations, in momentum representation, are the well known Lippman-Schwinger equations (see Newton 1966) which relate the transition matrix T (which contains all the physical information for the scattering) to the potential matrix

$$T = V + V G_0^+ T \qquad (1)$$

Again, one can solve the equations by a discretisation on the p - axis. So doing one encounters difficulties because the free propagator G_o^+ has a pole and it is not easy to deal with it. On the other hand, the Lippman-Schwinger formalism is well suited because most of the coupling potentials can be developed on separable operators in an appropriate converging way.

In this paper we propose to solve the scattering problem resulting from a resonating group treatment with an harmonic oscillator (H.O.) basis. Of course, this basis is not intended to be used for an expansion of the scattering wave (this would be very bad because of the oscillating behaviour of this function) but rather to express the transition operator T. In that case we are faced to the new problem of getting the matrix elements of the free propagator G_o^+ in the H.O. basis. Once this last problem is solved, one is left with a linear system, without poles, whose dimension is now $n_c \times n_\ell$ where n_ℓ^2 is the number of separable operators appropriate for expanding the coupling potentials. Typically $n_\ell \sim 3$ or 4 is a very good approximation.

In the next section the resonating group method is reviewed and the corresponding Lippman-Schwinger equation is expressed on the H.O. basis. The cross sections or phase shifts are then derived and the unitary relation is given. In the third section the analytical expression for the free propagator matrix elements within this basis is demonstrated. The conclusions are drawn in the last section.

2. Resonating group method with harmonic oscillator basis

In the following we will consider a system of N interacting particles - identical or not - and suppose that a non relativistic treatment is a good approximation for reality. Thus the Schrödinger equation is the correct equation which

describes the state of our system. Nevertheless the many body problem is very complicated. In principle the actual potential is a sum of two body terms, but also of 3, 4 ... and N-body interactions. The introduction of these many-body contributions is out of the scope of a correct microscopic calculation and usually one forgets about them arguing that their effects can be simulated by using effective renormalised two-body interactions instead of the true bare ones. Despite this crude assumption the many-body problem remains still a terrible task and is untractable in practice for general situations. In most of the microscopic many-body systems (atomic, nuclear or particle physics) the interacting particles are identical and the Pauli principle must be fulfilled. On the other hand, the total Hamiltonian is translationnally invariant and can be decomposed in two terms : the center of mass kinetic energy and the intrinsic Hamiltonian. The total wave function can be separated in a similar way as the product of a center of mass plane wave and an intrinsic wave function which depends only on the intrinsic degrees of freedom (Jacobi coordinates). One says that the center of mass motion is correctly treated. However, the translationnal invariance and the Pauli principle are hardly reconcilable. The point is that, under permutations, the Jacobi coordinates transform all together through orthogonal rotations which are not easy to be dealt with. Only for small systems can this correct treatment be undertaken seriously. For large systems the second quantization approach is very elegant and powerful to fulfil Pauli principle but violates translationnal invariance and introduces spurious center of mass motions. In this paper we shall be interested only in the former correct description. Hence in the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \qquad (2)$$

H, $|\Psi\rangle$ and E stand for intrinsic quantities. A correct and satisfactory treatment of (2) is presently achieved only for very small systems (N = 2, 3 or 4). For larger ones ($N \geq 5$) one must rely on some approximations. Among these the cluster theory (see Wildermuth et al 1966, 1977, Kukulin et al 1983) has proven to be very efficient. The basic idea is to partition the system into two (or may be more) subsystems (1) and (2) with N_1 and N_2 particles respectively and to express the total wavefunction as a superposition of outer products of eigenmodes for each subsystem. This new basis is in principle complete and even overcomplete but the cluster approximation restricts it to few dominant eigenmodes. This is a truncation in the original Hilbert space and in a good choice of the clusters and their eigenmodes - the cleverness of the physicist relies mainly on that point - results the accuracy of the approximations. The price to be paid is the non orthogonality of the basis. Among the technical methods proposed in cluster theory the generator coordinate method (GCM) and the resonating group method (RGM) are widely used. In the following we shall be concerned only in the RGM because in our opinion it is proper and best suited for scattering problems. The RGM is already an old method since it was proposed first by Wheeler in 1937. It has been employed for scattering problems in atomic and nuclear physics and recently (see Oka, Yazaki 1984) for hadron-hadron scattering in terms of quarks. However it can describe as well bound state properties. The trial RGM wave function looks like

$$|\Psi(1,2,\cdots N)\rangle = \sum_c \mathcal{A}\,|\Phi_c(1,2,\cdots N)\rangle$$
$$= \sum_c \mathcal{A}\Big\{\Big[\Psi_{c_1}(1,2,\cdots N_1)\,\Psi_{c_2}(N_1+1,\cdots,N)\Big]_c\,\chi_c(1,2,\cdots N)\Big\}\rangle \qquad (3)$$

where the sum runs over the various channels c defined by the chosen eigenmodes c_1 and c_2 for the clusters as well the various intrinsic couplings (color, spin,

isospin...) symbolically denoted by [ ] and the total angular momentum coupling denoted by { } necessary to insure good irreducible representations for the various symmetry groups of the Hamiltonian. The eigenmodes $|\Psi_{c_1}\rangle$ and $|\Psi_{c_2}\rangle$ are assumed to be correctly antisymmetrised for identical particles but the antisymmetriser $\mathcal{A}$ is introduced in order to fulfil the Pauli principle for identical particles within two different clusters. The relative wave function $|\chi_c(1,2,\ldots N)\rangle$ is expressed simply in configuration space since it is assumed to depend only through the particular combination of $\vec{r}_i$ which represents the intercluster Jacobi coordinate

$$b\vec{R} = \frac{1}{M_1}\sum_{i\in(1)} m_i \vec{r}_i - \frac{1}{M_2}\sum_{i\in(2)} m_i \vec{r}_i \qquad (4)$$

In that formula and in all what follows b is the lenght unit; in practice it is the size parameter for the harmonic oscillator basis. The rotational invariance is preserved for most of physical problems and it is natural to express the angular part of $|\chi_c\rangle$ on spherical harmonics. The resulting angular momentum LM is included in the channel definition and it is convenient to expand the radial part of $|\chi_c\rangle$ on a given basis which may be discrete or continuous. Generally speaking $|\chi_c\rangle$ will be expressed in terms of a basis $|u\ L\ M\rangle$. In practice we will use two types of basis :

- the separation basis which is continuous and where u represents the relative distance Ro for the clusters

$$\langle \vec{R} | u=R_0, LM\rangle = \frac{\delta(R-R_0)}{R} Y_{LM}(\hat{R}) \qquad (5)$$

- the harmonic oscillator basis (HO) which is discrete and where u represents the number of nodes n for the radial HO

$$\langle \vec{R} | u=n, LM\rangle = \varphi_{nLM}(\vec{R}) = \frac{u_{nL}(R)}{R} Y_{LM}(\hat{R}) \qquad (6)$$

Φ_{nLM} is the HO wave function defined precisely in the next section and $u_{nL}(R)$ its radial part.

The basis wavefunctions for the RGM are then

$$\mathcal{A}\,|\,\Phi_c(u)\rangle = \mathcal{A}\left\{\left[\Psi_{c_1}\Psi_{c_2}\right]_c\,|uLM\rangle\right\} \qquad (7)$$

and the Schrödinger equation can be rewritten, in that basis, as an Hill-Wheeler (1953) equation (HW) which fulfils, if no approximation is assumed, a variational principle

$$\sum_{c',u'}\left[E\,N_{cu,c'u'} - H_{cu,c'u'}\right]\chi_{c'u'} = 0 \qquad (8)$$

($\sum_{u'}$ must be understood as $\int dRo$ in case of basis $|Ro\ LM\rangle$). The basis functions(7) are not orthogonal and this explains the presence of a norm kernel different from unity. Here $\chi_{cu} = \langle u|\chi_c\rangle$ is the expansion coefficient of $\mathcal{A}\,|\Phi_c\rangle$ on the basis (7) and N and H the norm and energy kernels for our system. Owing to the property $\mathcal{A}^\dagger = \mathcal{A}$, $\mathcal{A}^2 = \mathcal{A}$ and $[H,\mathcal{A}] = 0$, these can be written

$$\begin{matrix} N_{cu,c'u'} \\ H_{cu,c'u'} \end{matrix} = \langle \Phi_c(u)\,|\,\mathcal{A}\,\begin{matrix} 1 \\ H \end{matrix}\,|\,\Phi_{c'}(u')\rangle \qquad (9)$$

Depending on the system, the antisymmetriser can include a huge number of terms. However one can exploit the fact that the clusters themselves are already antisymmetrised to greatly reduce this number because several terms give the same contribution. In practice $\mathcal{A}$ can be replaced (up to a constant

multiplicative factor which is unimportant) by $\mathbb{1} + \mathcal{S}$ giving rise for the kernels to two different contributions : the direct kernels coming from the terms of $\mathcal{H}$ which behaves like $\mathbb{1}$ and the exchange kernels coming from all other contributions

$$N_{\alpha u,\alpha' u'} = N^{(D)}_{\alpha u,\alpha' u'} + N^{(E)}_{\alpha u,\alpha' u'}$$
$$H_{\alpha u,\alpha' u'} = H^{(D)}_{\alpha u,\alpha' u'} + H^{(E)}_{\alpha u,\alpha' u'} \qquad (10)$$

In a second step, we write the total Hamiltonian H so as to get explicitly the natural separation into two clusters

$$H = \sum_i \frac{\vec{P}_i^2}{2m_i} + \sum_{i<j} V_{ij} = K + H_1 + H_2 + V_{12} \qquad (11)$$

In this formula H_i is the intrinsic Hamiltonian for cluster i, K the relative kinetic energy and V_{12} the intercluster potential. The interesting point is that the cluster wavefunctions $|\Psi_{\alpha i}\rangle$ have been built in order to be mainly eigenstates of the i subsystems

$$H_i |\Psi_{\alpha i}\rangle = E_{\alpha i} |\Psi_{\alpha i}\rangle \qquad (12)$$

and consequently

$$(H_i)_{\alpha u,\alpha' u'} = E_{\alpha i} N_{\alpha u,\alpha' u'} \qquad (13)$$

The effect of $H_1 + H_2$ is thus to replace the total energy E in the HW equation

by the relative kinetic energy $\mathcal{E}_{c'} = E - E_{c_1'} - E_{c_2'}$. This is precisely the kinetic energy for the scattering of the two clusters c_1 and c_2 in channel c'. Let us take into account the following properties .

$$N^{(D)}_{cu,c'u'} = \delta_{cc'}\,\delta_{uu'}$$
$$K^{(D)}_{cu,c'u'} = \delta_{cc'}\,K^{(c)}_{uu'} \qquad (14)$$

Strictly speaking the discrete norm is rigorously equal to unity only if there is no particle rearrangement when passing from channel c to channel c'. If it is not so the resulting non diagonal terms may be included in $N^{(E)}$.

Then the HW equation (8) can be cast into the more convenient form

$$\sum_{u'} \left[\mathcal{E}_c\,\delta_{uu'} - K^{(c)}_{uu'}\right] \chi_{cu'} = \sum_{c'u'} V_{cu,c'u'}\,\chi_{c'u'} \qquad (15)$$

with

$$V_{cu,c'u'} = K^{(B)}_{cu,c'u'} + V^{(D)}_{12\,cu,c'u'} + V^{(E)}_{12\,cu,c'u'} - \mathcal{E}_{c'}\,N^{(E)}_{cu,c'u'} \qquad (16)$$

Considering χ_{cu} as the component of the relative function $|\chi_c\rangle$ on the basis vectors $|u\rangle$ the equation of motion (15) looks like

$$\left[\mathcal{E}_c - K^{(c)}\right] |\chi_c\rangle = \sum_{c'} V_{cc'}\,|\chi_{c'}\rangle \qquad \forall c \qquad (17)$$

This form is quite similar to a Schrödinger equation with coupled channels; there

are however a number of differences

i) $V_{cc'}$ is not strictly speaking a potential; it reflects fully all the complications due to Pauli principle and non orthogonality as is transparent from (16)

ii) $|\chi_o\rangle$ does not represent a probability amplitude; this is also related to the non orthogonality of the basis.

We shall see below how to manage this drawback.

Most of the time the direct potential $V^{(D)}$ is local ($V^{(D)}_{cc'}(R_o, R'_o)$ is proportionnal to $\delta(R_o - R'_o)$); on the other hand, the exchange terms are non local and it is by no means trivial (and may be not justified either) to construct an equivalent local potential. However, because the exchange kernels of two bound states (which consequently are spatially localized) are expected to vanish rapidly once the clusters do not overlap, the exchange kernels ($V^{(E)}_{cc'}(R_o, R'_o)$ for instance) fall off very quickly to zero - at least exponentially - when Ro or R'o tend to infinity. The same property holds when the exchange kernels are expressed in the HO basis; they drop rapidly to zero when the number of nodes tends to infinity. The calculation of the exchange kernels is in general very complicated and tedious. However, if the cluster wave functions Ψ_{ci} are themselves expanded on an HO basis (the convergence is in general very fast), the exchange kernels in the HO basis can be computed exactly and with a finite number of terms with the help of generalized Brody-Moshinsky coefficients (Silvestre-Brac 1985). This is one of the advantages of using HO wave functions in the resonating group method. As already stated another interesting point is that the exchange kernels ($V^{(E)}_{cn,c'n'}$ for instance) tend rapidly to zero when n or l and $n' \to \infty$.

For our method to work very well, we shall suppose that the same

property holds for the direct term i.e. $V^{(D)}_{12\,cn,c'n'}$ tends rapidly to zero when n or n' $\to \infty$. This is obviously the case when $V^{(D)} \equiv 0$. Indeed, this last circumstance occurs quite often : for instance in the interaction of two neutral clusters via electromagnetic forces or the interaction of two colourless objects via chromodynamical forces etc... All the preceding remarks were intended to emphasize that the right hand part of (15) is rapidly convergent when V is expanded on an HO basis (in practical cases, n = 0, 1, 2 are enough to insure a good convergence). On the contrary for scattering problems $\chi_c(R)$ in open channels has an oscillating behaviour and an HO expansion of $|\chi_c\rangle$ in the left hand part of (15) is expected to be very bad. Thus the essence of our method is to treat $|\chi_c\rangle$ in the configuration space for the direct kinematic part(left hand side of (15)) but in the HO basis for the exchange kernels (right hand side of (15)). Let us be more precise.

For the rest of this section, in order to simplify the notations, we will write all the lenghts in unit b, the wave numbers in unit b^{-1} and the energies in unit $\hbar^2/(2\mu_c b^2)$ (μ_c is the reduced mass for the channel c). Thus ε_c must be understood as $2\mu_c b^2 \varepsilon_c/\hbar^2$, k_c as $b\,k_c$, $V_{cc'}$ as $2\frac{\mu_c b^2}{\hbar^2} V_{cc'}$ and hence for instance $\varepsilon_c = k_c^2$. The equation of motion (17) is quite general and is applied as well for bound and scattering states. We discuss first the scattering problem. The physical energy E is an input. All the channels with $k_c^2 > 0$ are open and the system can make a transition from a given incoming channel c_0 to any of the open channels c. However the closed channels also influence in principle the wave function for the open channels. One can put the general equation (17) in the following form

$$|\chi_c\rangle = \delta_{cc_0}|k_{c_0}\rangle + \sum_{c'} G_0^+(\varepsilon_c) V_{cc'} |\chi_{c'}\rangle \qquad (18)$$

Here we have introduced the free propagator $G_0^+(E) = \lim_{\varepsilon \to 0} (E+i\varepsilon - K)^{-1}$ describing outgoing spherical waves and $|k_{c_0}\rangle$ the incoming spherical wave

corresponding to the incident physical channel c_o (solution of the homogeneous equation (17) for $c = c_o$). The asymptotic behaviour of $|\chi_c\rangle$ in the configuration space is well known

$$\langle R|\chi_c\rangle = \chi_c(R) \sim \delta_{cc_o} R j_{L_c}(k_c R) - T_{cc_o} R h^+_{L_c}(k_c R) \qquad (19)$$

where L_c means the relative angular momentum for the clusters (recall $\langle \vec{R}|\chi_c\rangle = \frac{\chi_c(R)}{R} Y_{LM}(\hat{R})$)

Although $\chi_c(R)$ is not a probability amplitude its asymptotic behaviour indeed represents such an amplitude because as already stated $N^{(\epsilon)}_{cc'}(R,R') \to 0, R \to \infty$) and thus the basis functions $|\Phi_c(R)\rangle$ are orthogonal. T_{cc_o} is a constant which is in fact the matrix elements of the T operator and the cross section for the scattering $c_o \to c$ is obtained by standard formulae from T_{cc_o}. The physically interesting problem is thus the calculation of T_{cc_o}. Once the incoming channel c_o is given the resulting wave function $|\chi_c\rangle$ depends also on c_o and in (18) $|\chi_c\rangle$ should read $|\chi_c(c_o)\rangle$.

Defining the transition matrix T through the following equation

$$\sum_{c'} V_{cc'}|\chi_{c'}(c_o)\rangle = |T_c(c_o)\rangle = T_c|k_{c_o}\rangle \qquad (20)$$

it is easy from (18) to get the Lippman Schwinger equation allowing the determination of $|T_c(c_o)\rangle$ namely

$$\sum_{c'} (\mathbb{1} - V G_o^+)_{cc'} |T_{c'}(c_o)\rangle = |T^o_c(c_o)\rangle \qquad (21)$$

with $$|T^o_c(c_o)\rangle = V_{cc_o}|k_{c_o}\rangle \qquad (22)$$

representing the Born term. Assuming that $|T_c(c_0)\rangle = |T_c^0(c_0)\rangle$ is known as the Born approximation.

In our method, we propose to solve the Lippman-Schwinger equation in the HO basis because, as we already pointed out, $V_{cn,c'n'}$ is exactly calculable and moreover tends rapidly to zero when the number of nodes n (or n') increases. Thus the expansion of $|T_c(c_0)\rangle$ on the HO is rapidly convergent and we need only very few terms in the expansion of (21) : the maximum number of nodes n_ℓ can be restricted to 2 or 3 with a good accuracy. Our method imposes to calculate the propagator $G^{c+}_{cn,c'n'} = \delta_{cc'} G^{o+}_{nn'L}(\varepsilon_c)$ (G^{o+} depends on c uniquely through the relative angular momentum L of the clusters) in the HO basis. This problem is discussed in detail in the following section. The matrix $\mathbb{1} - VG^{o+}$ is then easily computed. It is not difficult to write the inhomogeneous term if one remarks that the amplitude of the spherical wave $|k_c\rangle$ in an HO basis is proportional to $U_{nL}(k_c)$ Precisely :

$$T^0_{cn}(c_0) = \sum_{n_0} V_{cn,c_0 n_0} (-1)^{n_0} \sqrt{\frac{\pi}{2}} \frac{U_{n_0 L_0}(k_{c_0})}{k_{c_0}} \qquad (23)$$

and after that, by solving the linear system (21) one gets $T_{cn}(c_0)$ The matrix elements T_{cc_0} for the T matrix giving the probability amplitude to make a transition from the channel c_0 to the channel c are obtainable by

$$T_{cc_0} = \langle k_c | T_c | k_{c_0} \rangle = \sum_n (-1)^n \sqrt{\frac{\pi}{2}} U_{nL}(k_c) T_{cn}(c_0) \qquad (24)$$

The scattering problem is entirely solved now. It is possible to check the

unitary relation which can be written in our case

$$\sum_{c \text{ open}} \frac{|T_{cc_0}|^2}{k_c} = \mathrm{Im}\ \frac{T_{c_0c_0}}{k_{c_0}} \qquad (25)$$

Concerning the bound state problem, the things are a bit different. First, the energy E is no longer an input but is the output of our calculation. Secondly, the asymptotic behaviour for $|\chi_c\rangle$ does not include the incoming wave $|k_{c_0}\rangle$ in (18); consequently the inhomogeneous Born term is absent from (21). The equation which allows the determination of the bound state energy is reduced to :

$$\det\left[1 - V(E)\, G_0(E)\right] \qquad (26)$$

(in that case G_0 is real and there is no multiple determination).

When all the channels but one are closed only elastic scattering occurs and it is traditionnal to introduce the phase shift δ_{c_0} between the incoming and the outcoming waves. It is easily calculated with the help of (24) and through the definition

$$T_{c_0c_0} = e^{i\delta_{c_0}} \sin\delta_{c_0} \qquad (27)$$

In that case the asymptotic behaviour of χ_c is

$$\chi_{c_0}(R) \sim k_{c_0}^{-1} \sin\left(k_{c_0}R - \frac{l\pi}{2} + \delta_{c_0}\right) \qquad (28)$$

It is also possible to get the phase shift by computing the logarithmic derivative of $\chi_{c_0}(R)$ at large distances.

Let us remark another advantage of our method. It is possible to obtain directly $\chi_c(R)$ by solving (15) in the configuration space. In that case we need to discretise the problem and to define a mesh of n_R points. If n_c denotes the number of channels taken into account, it is necessary to solve a linear system whose dimension $n_c \times n_R$ may be quite large. In our method for the corresponding equation (21), the dimension of our matrices is $n_c \times n_\ell$ which is in general a small number. For a deeper treatment on this point see for instance (Gignoux and Silvestre-Brac 1986).

3. Green function in the harmonic oscillator basis

In this section our purpose is to evaluate the free Green function in an harmonic oscillator basis since it was a basic ingredient for the method discussed previously. As far as we know the analytical expression that we obtain was never published.

Thus we are faced with the problem of evaluating

$$G^{o+}_{nn'\ell}(E,b) = \lim_{\varepsilon \to 0} \langle \varphi_{n\ell m}(b) | (E+i\varepsilon - K)^{-1} | \varphi_{n'\ell m}(b) \rangle \qquad (29)$$

The kinetic energy operator $K = \frac{\vec{p}^2}{2\mu}$ is invariant under rotation and it is the same angular momentum ℓm which appears in the bra and in the ket. Let b be the size parameter for the harmonic oscillator wave function; it is more convenient to define the space vectors r in unit of b $\vec{x} = \vec{r}/b$ and the wave vectors $\vec{k}$ in unit of b^{-1}, $\vec{q} = b\vec{k}$. The HO wave functions are defined in the configuration space with the usual Moshinsky (1959) phase conventions

$$\langle \vec{x} \mid n\ell m \rangle = \frac{U_{n\ell}(x)}{x} Y_{\ell m}(\hat{x}) = \varphi_{n\ell m}(\vec{x})$$

$$U_{n\ell}(x) = \left[\frac{2(n!)}{\Gamma(n+\ell+3/2)}\right]^{1/2} x^{\ell+1} e^{-\frac{x^2}{2}} L_n^{\ell+1/2}(x^2) \qquad (30)$$

$$L_n^{\ell+1/2}(x^2) = \sum_{s=0}^{n} (-1)^s \frac{\Gamma(n+\ell+3/2)}{(n-s)!\,\Gamma(s+\ell+3/2)} \frac{x^{2s}}{s!}$$

are the Laguerre polynomials.

In the momentum representation $|\vec{q}\rangle$ the HO wave functions (Fourier transform of $\varphi_{n\ell m}(\vec{x})$) have the same form as in the coordinate representation but differ by an important phase factor. Explicitly

$$\langle \vec{q} \mid n\ell m \rangle = (2\pi)^{-3/2} \int e^{-i\vec{q}\cdot\vec{x}} \varphi_{n\ell m}(\vec{x})\, d\vec{x} = (-i)^{2n+\ell} \varphi_{n\ell m}(\vec{q}) \qquad (31)$$

It is more convenient to use the momentum representation to evaluate the Green function. For typographical reasons we will omit the (+) (outgoing propagator) and (0) (free propagator) superscript indices in all what follows having always in mind that we calculate the free outgoing wave function One can write

$$G_{nn'\ell}(E,b) = (+)^{nn'} \frac{2\mu b^2}{\hbar^2} \lim_{\varepsilon \to 0} \int \varphi^*_{n\ell m}(\vec{q})\, \varphi_{n'\ell m}(\vec{q}) \left[q_0^2 - q^2 + i\varepsilon\right] d\vec{q} \qquad (32)$$

with $$q_0^2 = \frac{2\mu b^2 E}{\hbar^2}$$

The integration over angles is trivial and we are left with the radial integration

$$A = \lim_{\varepsilon \to 0} \int_0^\infty U_{nl}(q)\, U_{n'l}(q) \left[q_0^2 - q^2 + i\varepsilon\right]^{-1} dq \qquad (33)$$

Using the well known property

$$\lim_{\varepsilon \to 0} \left[q_0^2 - q^2 + i\varepsilon\right] = P.P\,(q_0^2 - q^2)^{-1} - i\pi\delta(q_0^2 - q^2) \qquad (34)$$

the Green function can be split in two parts . the real part G^R coming from the P.P and the imaginary part G^I (present only for scattering problems $q_0^2 > 0$) coming from the δ functions. The imaginary part is quite easy to be evaluated; the real part is more involved. One has to calculate the following integral

$$R = P.P \int_0^\infty e^{-q^2} q^{2l+2} L_n^{l+1/2}(q^2)\, L_{n'}^{l+1/2}(q^2) \left[q^2 - q_0^2\right]^{-1} dq \qquad (35)$$

Let us remark that $L_n^{l+1/2}(q^2)\, L_{n'}^{l+1/2}(q^2) = P_N(q^2)$ is a polynomial of degree $N = n + n'$. The trick is thus to isolate the singularity of (35) in a much simpler integral. Explicitly

$$R = R_1 + R_2$$

with

$$R_1 = P.P \int_0^\infty e^{-q^2} \left[q^{2l+2} P_N(q^2) - q_0^{2l+2} P_N(q_0^2)\right] \left[q^2 - q_0^2\right]^{-1} dq \qquad (36)$$

and

$$R_2 = q_0^{2l+2} P_N(q_0^2)\; P.P \int_0^\infty e^{-q^2} \left[q^2 - q_0^2\right]^{-1} dq$$

In R1 the pole disappears and the resulting integrals are standard. We are left with a polynomial in q_o^2 whose coefficients are purely geometrical and can be computed and tabulated once for all.

The integral contained in R2 is related to the complex error function erf (z) (see for instance Abramowitz 1970). After some manipulations one gets

$$P.P\int_0^\infty e^{-q^2}\left[q^2-q_o^2\right]^{-1}dq = \frac{i\pi}{2q_o}\,e^{-q_o^2}\,erf(iq_o) = -\frac{\sqrt{\pi}}{q_o}\,F(q_o) \tag{37}$$

where $F(x) = e^{-x^2}\int_0^x e^{t^2}dt$ is the real Dawson's integral.

Now everthing is complete. Let us summarize the results

$$G_{nn'\ell}(E,b) = G^R_{nn'\ell}(E,b) + iG^I_{nn'\ell}(E,b) \tag{38}$$

$$G^I_{nn'\ell}(E,b) = (-1)^{\frac{n+n'+1}{2}}\frac{2\mu b^2}{\hbar^2}\frac{\pi}{2q_o}\,U_{n\ell}(q_o)\,U_{n'\ell}(q_o) \tag{39}$$

$$G^R_{nn'\ell}(E,b) = (-1)^{\frac{n+n'+1}{2}}\frac{2\mu b^2}{\hbar^2}\left\{\frac{i\sqrt{\pi}}{2q_o}\,U_{n\ell}(q_o)\,U_{n'\ell}(q_o)\,erf(iq_o) + \sum_{k=0}^{\ell+n+n'} b_k(n,n',\ell)\,q_o^{2k}\right\} \tag{40}$$

with

$$b_k(n,n',\ell) = 2^{2k+1-n-n'}\left[\frac{n!\,n'!\,(2n+2\ell+1)!\,(2n'+2\ell+1)!}{(n+\ell)!\,(n'+\ell)!}\right]^{1/2} \times \sum_{p=0}^{n}\sum_{\substack{p'=0 \\ p+p'\geq k-\ell}}^{n'}(-1)^{p+p'}\frac{(2\ell+2p+2p'-2k)!\,(p+\ell)!\,(p'+\ell)!}{(p+p'+\ell-k)!\,(2p+2\ell+1)!\,(2p'+2\ell+1)!\,(n-p)!\,(n'-p')!\,p!\,p'!} \tag{41}$$

The geometrical coefficients $b_k(n,n',\ell)$ fulfil the relations

$$b_k(n,n',\ell) = b_k(n',n,\ell) \tag{42}$$

$$b_k(n,n',\ell) = 0 \qquad \text{if} \quad k > n+n'+\ell$$

and q_o is given by (32).

4. Conclusions

In this paper we propose an approach to solve the scattering problem in an harmonic oscillator basis. The method can be applied in a resonating group treatment of cluster theory; it is specially best suited when the direct energy potential kernel $V^{(D)}$ cancels or when it is rapidly convergent on an HO basis. The formalism is general enough to include an arbitrary number n_c of coupled channels and to allow non local potentials. There are two main advantages of this method as compared to the traditional approach in the configuration space. First of all the exchange kernels N^E and H^E of the Hill-Wheeler equation, which are by far the most complicated and the most time consuming terms, can be calculated exactly in an HO basis and it is not necessary to reconvert them in the R representation. The second point is certainly the most interesting, at least from the numerical point of view. In practical situations the direct potential V^D is either absent or local while the exchange kernels are always non local. The usual method which discretises eq. (15) in the separation basis needs to handle a linear system of order $n_c \times n_R$ (n_R is the number of points in the coordinate mesh). To insure a good accuracy in the results, one must take n_R sufficiently large - typically around 100 - and this restricts severely the number of channels one can include in our treatment. On the other hand, the method

proposed here needs to solve a linear system of order $n_c \times n_\ell$ where n_ℓ is the maximum number of nodes in the HO basis taken into account. The exchange kernels are so rapidly converging in the HO basis that $n_\ell \sim$ 3 or 4 is a very good approximation. One can thus hope to increase drastically the number of channels considered in physical examples. This argument holds from storage numerical considerations. However, it must be relativised from computing time reasons. The exchange kernels N^E and H^E are very time consuming and this time roughly increases as n_c^2 (but it was also true in the first method). In the method proposed in this paper one also needs the calculation of the free Green function in the HO basis. An analytical expression, which we never saw before, is given which allows a very fast and accurate computation of G_0^+ : it mainly consists in computing the Dawson integral which is available in any good code libraries and a polynomial in the energy whose coefficients are purely geometrical and can be tabulated once for all.

This method was applied with success in several problems we tackled for instance the nucleon-nucleon interaction in term of quarks (Silvestre-Brac et al 1986), $QQ\bar{q}\bar{q}$ multiquarks (Zouzou et al 1986) or the dilambda system (Silvestre-Brac et al 1987). Spurious wave functions which could occur because of the non orthogonality of the RGM basis can be removed quite easily (Valliser 1986) within this frame.

During this work was completed, we received a thesis from Dr Bicudo (1986) in which similar approaches were developed.

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