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V.V.Pupyshev, S.A.Rakityansky

SEMIANALYTICAL METHOD OF SOLUTION OF THE N-BODY BOUND-STATE PROBLEM WITHIN THE HYPERSPHERICAL APPROACH

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Demands on the high-accuracy calculations revive (after more than 20 years of intense attention to the pure computer calculations) interest in analytical or semianalytical methods in quantum mechanics. In particular, the necessity of them arises in consideration of the weakly bound systems where the traditional numerical approaches meet serious difficulties /1/.

Being based on the two earlier suggested ideas, namely, the application of the variable-phase approach to the hyperspherical one /2/ and the solution of the Schroedinger equation by representing the wave-function as series /3,4/ factorized in energy and radius, we develop here a method for constructing a many-body Jost-matrix semianalytical-expression with explicit analytical dependence on the total energy. This dependence allows us to find easily the bound states as zeros of the Jost-matrix determinant in the complex-energy plane.

In the framework of the hyperspherical approach /5/ the N-body bound-state wave-function is approximated by the finite series

$$\Psi_{\rho}^{\alpha}(\vec{r}) \approx r^{2-3N/2} \sum_{[L]=[L_{min}]}^{[L_{max}]} \mathcal{U}_{[L]}^{\alpha}(\rho,r)\, Y_{[L]}(\hat{\vec{r}}), \quad (1)$$

where the hyperradial functions $\mathcal{U}_{[L]}^{\alpha}(\rho,r)$ obey the system of equations

$$[\partial_r^2 + \rho^2 - \lambda(\lambda+1)/r^2]\,\mathcal{U}_{[L]}^{\alpha}(\rho,r) = \sum_{[L']} v_{[L][L']}(r)\,\mathcal{U}_{[L']}^{\alpha}(\rho,r). \quad (2)$$

Here multi-index $[L]$ involves the hypermomentum L and all other nonconserved quantum numbers allowed by the set $\{\alpha\}$ of the well defined numbers; the momentum ρ is conjugated to the hyperradius r and related to the total energy E by $\rho^2 = 2E$; $\lambda = L+3(N-2)/2$; and the elements of matrix v are defined as hyperangle integrals

$$\mathcal{V}_{[L][L']}(r) = 2\int d\hat{\vec{r}}\, Y^*_{[L]}(\hat{\vec{r}})\, V(\vec{r})\, Y_{[L']}(\hat{\vec{r}}) \tag{3}$$

of the sum V of the 2-body potentials assuming each to be more rapidly decreasing at large r and less singular at $r=0$ than the centrifugal one.

To make all subsequent formulae more clear we omit some indices and arguments and use the behaviour

$$\mathcal{V}_{[L][L']}(r) \underset{r\to 0}{\sim} \alpha_{[L][L']}/r^{2-\varepsilon}, \quad \varepsilon > 0 \tag{4}$$

while all our results are valid in a more general case $\lim\limits_{r\to 0} r^2 \mathcal{V}(r) = 0$.

Considering (2) as a matrix equation [6], we see that it has as many independent regular (at $r=0$) column-solutions as the column dimension. All these linear independent columns we combine in the square matrix ϕ^{α}. As one knows, the N-body scattering problem leads to the same hyperradial equation (2). Therefore, any physical solution may, in principle, be constructed as linear combination of columns of the fundamental matrix $\| \phi^{\alpha}_{[L][L']} \|$ of regular solutions with the coefficients $A^{\alpha}_{[L']}$ defined by appropriate physical boundary conditions at $r \neq 0$. In our bound-state problem, the condition $\mathcal{U}_{[L]}(\rho,\infty) = 0$ imposed on the function

$$\mathcal{U}_{[L]}(\rho,r) = \sum_{[L']} \phi_{[L][L']}(\rho,r) A_{[L']}(\rho), \tag{5}$$

implies the homogeneous algebraic system

$$\sum_{[L']} \phi_{[L][L']}(\rho,\infty) A_{[L']}(\rho) = 0 \tag{6}$$

defining the weight-coefficients $A_{[L']}$ with the exception of a common norm factor. The homogeneous system (6) has nontrivial solutions if and only if

$$\det \| \phi_{[L][L']}(\rho,\infty) \| = 0. \tag{7}$$

The zeros of (7) correspond to the bound state energies $E = \rho^2/2$ we are looking for. Thus, the above scheme reduces the initial problem, concerning with equation (2), to the construction of the basic functions $\phi_{[L][L']}(\rho,r)$.

Since, $r=0$ is a singular point [6] of (2), we have to supply the regularity condition $\phi(\rho,0) = 0$ with an explicit behavious of ϕ with $r \to 0$. Since the investigations by Bartlett et al. [7] and Fock [8], such a behaviour is intensively explored with-

in various approaches (see, for example, the reviews [9,10] and recent works [11]). As it is known [12], the potentials of the type (4) with integer ε cause the diagonal matrix elements of $\| \phi_{[L][L']} \|$ near $r=0$ behave like $r^{\lambda+1}$ while the nondiagonal ones like $r^{\lambda'+1+\varepsilon}$. Formally, to define uniquely the linear independent regular column-solutions for the slightly singular ($\lim\limits_{r\to 0} r^2 \mathcal{V}(r) = 0$) potentials it is enough [13] to put the boundary conditions

$$\lim_{r\to 0} \phi_{[L][L']}(\rho,r)/r^{\lambda'+1} = \delta_{[L][L']}. \tag{8}$$

But for practical calculations one also needs, at least, the leading terms of all the matrix elements. We assume (8) and derive these terms below.

To solve the boundary problem (2), (8) we apply the variable constant method [6] which is equivalent to a linear version of the variable phase approach [14]. Within this method we look for ϕ as

$$\phi_{[L][L']}(\rho,r) = j_\lambda(\rho r)\, c_{[L][L']}(\rho,r) - y_\lambda(\rho r)\, s_{[L][L']}(\rho,r) \tag{9}$$

where j_λ and y_λ are the Rikkati-Bessel and Rikkati-Neumann functions [15] being regular and irregular solutions of (2) when $\mathcal{V} \equiv 0$. Then, instead of (2), we arrive at the following equations for the matrices c and s :

$$\partial_r c = -y\mathcal{V}(jc - ys)/\rho, \quad \partial_r s = -j\mathcal{V}(jc - ys)/\rho, \tag{10a}$$

where $j = \| j_\lambda \delta_{[L][L']} \|$ and $y = \| y_\lambda \delta_{[L][L']} \|$ are the diagonal matrices. We can fulfil (8) with the conditions

$$\lim_{r\to 0} j_\lambda(\rho r)\, c_{[L][L']}(\rho,r)/r^{\lambda'+1} = \delta_{[L][L']},$$
$$\lim_{r\to 0} y_\lambda(\rho r)\, s_{[L][L']}(\rho,r)/r^{\lambda'+1} = 0, \tag{10b}$$

which therefore serve as the boundary ones for (10a). Considering (10a) near $r=0$, we can replace $y_\lambda(\rho r) \sim \tau_\lambda (\rho r)^{-\lambda}$, $j_\lambda(\rho r) \sim \sigma_\lambda (\rho r)^{\lambda+1}$, $\mathcal{V}_{[L][L']}(r)$ and $(jc - ys)$ by their leading terms and perform the integration explicitly. As a result, we obtain the leading terms of c and s :

$$c_{[L][L']}(\rho,r) \underset{r\to 0}{\sim} \frac{\delta_{[L][L']}}{\sigma_\lambda \rho^{\lambda+1}} - \frac{\tau_\lambda \alpha_{[L][L']}}{(\lambda'-\lambda+\varepsilon)\rho^{\lambda+1}}\, r^{\lambda'-\lambda+\varepsilon}, \tag{11a}$$

$$\mathcal{S}_{[L][L']}(\rho,r) \underset{r\to 0}{\sim} -\frac{\sigma_\lambda \alpha_{[L][L']}}{\lambda+\lambda'+1+\varepsilon}\rho^\lambda r^{\lambda+\lambda'+1+\varepsilon}, \qquad (11b)$$

which are to be used in practical calculations instead of (10b).

Further, applying the Rikkati-Hankel functions[15] $h_\lambda^{(\pm)}=j_\lambda \pm i y_\lambda$ and introducing the notation $\mathcal{F}^{(\pm)}=C\pm i\mathcal{S}$, we rewrite (9) as

$$\Phi_{[L][L']}(\rho,r)=\frac{1}{2}\{h_\lambda^{(+)}(\rho r)\mathcal{F}^{(+)}_{[L][L']}(\rho,r)+h_\lambda^{(-)}(\rho r)\mathcal{F}^{(-)}_{[L][L']}(\rho,r)\} \qquad (12)$$

and by analogy with the 2-body case [16] call $\| f^{(\pm)}_{[L][L']}(\rho)\| = \lim_{r\to\infty}\| \mathcal{F}^{(\pm)}_{[L][L']}(\rho,r)\|$ the Jost matrices. Then, taking into account the asymptotic behaviour [15]

$$h_\lambda^{(\pm)}(z) \underset{|z|\to\infty}{\sim} \mp i \exp[\pm i(z-\lambda\pi/2)],$$

we can reformulate (7) and (6), defining the bound-state energies $E_b=-\rho_b^2/2 \quad (\rho_b>0)$ and the weight-factors $A_{[L]}$ as

$$\det \| f^{(-)}_{[L][L']}(i\rho_b)\| = 0, \qquad (13)$$

$$\sum_{[L']} f^{(-)}_{[L][L']}(i\rho_b)A_{[L']}=0. \qquad (14)$$

We also note, if zero of the Jost-matrix determinant is placed under the real positive half-axis of the complex ρ-plane, then it is possible to find such weight-factors $\widehat{A}_{[L]}$ which retain in the physical solution asymptotics only the outgoing hyperspherical waves. In some cases the last may be identified [17] with N-body resonance states.

Thus, explicitly extracting the Bessel functions in (9) or (12), we have reduced the problem (2), (8) to (10), (11) for $C(\rho,r)$ and $\mathcal{S}(\rho,r)$ which are expected to be smoother functions of r. But they yet remain implicitly dependent on ρ, while to use (13) an explicit ρ-dependence is more desirable.

As we will show below, one can easily achieve the last under the conditions $r\leqslant r_{max}$, $|\rho| r_{max} \ll 1$ by expanding C and $\mathcal{S}$ in series.

In this way, we apply the well known[15] series representations of the Bessel and Neumann functions. Introducing an arbitrary hyperradial parameter R and using the identity $\ln(\rho r/2) \equiv \ln(\rho R/2)+\ln(r/R)$, we can separate ρ and r

in the only nonfactorized term of the Rikkati-Neumann function expansion arising for a half-integer λ. This enables us to rewrite the known spherical and cylindrical function representations in the uniform way:

$$j_\lambda(\rho r)=\rho^{\lambda+1}\sum_{n=0}^{\infty}\rho^{2n}f_n^{(\lambda)}(r),$$
$$y_\lambda(\rho r)=\rho^{-\lambda}\sum_{n=0}^{\infty}\rho^{2n}g_n^{(\lambda)}(r)+h(\rho)j_\lambda(\rho r), \qquad (15)$$

where $h(\rho)\equiv 0$ for integer λ and $h(\rho)=\frac{2}{\pi}\ln(\rho R/2)$ for half-integer λ, and $g_n^{(\lambda)}$ in the last case gets the R-dependence.

The structure of (10a), (11) and (15) stimulates us to try the expansions

$$C_{[L][L']}(\rho,r)=\rho^{-(\lambda+1)}\sum_{n=0}^{\infty}\rho^{2n}C_{n[L][L']}(r)+h(\rho)\mathcal{S}_{[L][L']}(\rho,r),$$
$$\mathcal{S}_{[L][L']}(\rho,r)=\rho^{\lambda}\sum_{n=0}^{\infty}\rho^{2n}\mathcal{S}_{n[L][L']}(r). \qquad (16)$$

Inserting (15), (16) into (10a) and comparing (16) with (10b) and (11), we get the initial value problem for the matrix elements of C_n and $\mathcal{S}_n$ depending only on r:

$$\begin{cases}\partial_r C_{n[L][L']}=-\sum'_{ijk[L'']} g_i^{(\lambda)}V_{[L][L'']}\left(f_j^{(\lambda'')}C_{k[L''][L']}-g_j^{(\lambda'')}\mathcal{S}_{k[L''][L']}\right), \\ \partial_r \mathcal{S}_{n[L][L']}=-\sum'_{ijk[L'']} f_i^{(\lambda)}V_{[L][L'']}\left(f_j^{(\lambda'')}C_{k[L''][L']}-g_j^{(\lambda'')}\mathcal{S}_{k[L''][L']}\right),\end{cases} \qquad (17a)$$

$$\begin{cases}C_{n[L][L']}(r) \underset{r\to 0}{\sim} \delta_{n0}\{\sigma_\lambda^{-1}\delta_{[L][L']}-(\lambda'-\lambda+\varepsilon)^{-1}\tau_\lambda\alpha_{[L][L']}r^{\lambda'-\lambda+\varepsilon}\}, \\ \mathcal{S}_{n[L][L']}(r) \underset{r\to 0}{\sim} -\delta_{n0}(\lambda+\lambda'+1+\varepsilon)^{-1}\sigma_\lambda\alpha_{[L][L']}r^{\lambda+\lambda'+1+\varepsilon},\end{cases} \qquad (17b)$$

where $\sum'$ denotes sum over the indices obeing the condition $i+j+k=n$. Thanks to this condition the system (17a) is of the recurrent type, i.e. the equations for C_0 and $\mathcal{S}_0$ involve only their own matrix elements, the equations for C_1 and $\mathcal{S}_1$ involve the previous and the own ones, and so on. Therefore, at every n-th recurrent step we have as unknown only the elements of the matrices C_n and $\mathcal{S}_n$.

Exploring convergence of expansions (16) we have shown by the method of contracting mappings [13] that these series asymptotically $(|\rho| r\to 0)$ converge to $C(\rho,r)$ and $\mathcal{S}(\rho,r)$ in the vicinity of the origin of complex ρ-plane, when $r \in [0, r_{max}]$ and $|\rho r_{max}| \ll 1$. Therefore, using (16) we can write $\mathcal{F}^{(\pm)}_{[L][L']}$ as

$$\mathcal{F}^{(\pm)}_{[L][L']}(\rho,r) = \rho^{-(\lambda+1)}\{Q^{(M\pm)}_{[L][L']}(\rho,r) + O(|\rho r|^{2M+2})\}, \tag{18}$$

$$Q^{(M\pm)}_{[L][L']}(\rho,r) \equiv \sum_{n=0}^{M} \rho^{2n}\{c_{n[L][L']}(r) \pm \rho^{2\lambda+1}[h(\rho)\pm i]\, s_{n[L][L']}(r)\}$$

with any $M < \infty$ provided that $|\rho r| \ll 1$. As in the standard variable-phase approach [14], if $v(r) \equiv 0$ for $r \geqslant r_{max}$, then according to (10a) our c, s and therefore $\mathcal{F}^{(\pm)}$ are invariable beyond r_{max}. Hence, if the matrix $v(r)$ is cut off at large enough $r = r_{max}$ (as it is usually done in practice), then owing to (18) equations (13), (14) are reduced to

$$\det \| Q^{(M-)}_{[L][L']}(i\rho_b, r_{max}) + O(|\rho_b r_{max}|^{2M+2}) = 0, \tag{19}$$

$$\sum_{[L']} \{ Q^{(M-)}_{[L][L']}(i\rho_b, r_{max}) + O(|\rho_b r_{max}|^{2M+2})\} A_{[L']}(i\rho_b) = 0. \tag{20}$$

One sees, the bound-state energy may finally be found with any given accuracy on a sufficiently small interval $\rho_b \in [0, \rho_{max}]$ as a zero of $\det Q^{(M-)}(i\rho_b, r_{max})$ which is an explicit polynomial function of ρ and $h(\rho)$ with the numerical coefficients $c_{n[L][L']}(r_{max})$ and $s_{n[L][L']}(r_{max})$ defined by (17). In every concrete N-body problem these ρ-independent equations are to be solved only once. Then, for each zero $\rho = i\rho_b$ of (19) and for all $r \leqslant r_{max}$, $M < \infty$, provided that $\rho_b \leqslant \rho_{max}$ and $|\rho_{max} r_{max}| \ll 1$, we can, by using (5), (9), (15) and (16), express (1) semianalytically:

$$\Psi_p(\vec{r}) \approx r^{2-3N/2} \sum_{[L],[L']=[L_{min}]}^{[L_{max}]} Y_{[L]}(\hat{\vec{r}})\, \phi_{[L][L']}(p,r) A_{[L']}(p), \tag{21}$$

$$\phi_{[L][L']}(p,r) = \sum_{n=0}^{M} p^{2n} \sum_{i+j=n} [f_i^{(\lambda)}(r) c_{j[L][L']}(r) - g_i^{(\lambda)}(r) s_{j[L][L']}(r)] + O(|pr|^{2M+2}) \tag{22}$$

We should like to note one undoubted virtue of the developed recipe. In fact, solving (17) we obtain much more than desired initially. Along with the bound-state function (21) for the discrete values of ρ we simultaneously construct the fundamental matrix of regular solutions (22) for any complex ρ of the circle $|\rho| \leqslant \rho_{max}$. In principle, this matrix may be considered as a full solution of the N-body problem within the above constraints, for any physical wave function is a superposition of columns of the fundamental matrix.

Expressions (21) and (22) may be useful in various quantum mechanical problem ranging from quantum chemistry to nuclear astrophysics where typical energies are of small absolute values.

In conclusion, we stress the following: first, $L \leqslant L_{max}$ and $r \leqslant r_{max}$ are standard restrictions of practical calculations within the hyperspherical approach; second, an important question about the behaviour of $\mathcal{F}^{(\pm)}(\rho, r)$ with $\rho \to 0$ and $r \to \infty$ remains still open; and at last, the above suggested method seems to be perspective for weakly bound systems. Some ideas related to adaptation of the method to the systems with the Coulomb forces and to the scattering problems were sketched in our previous publications [18].

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