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On Description of Nuclear and Atomic Extended States

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Abstact: In this Report one discusses various types of spatial extended nuclear and atomic states: nuclear halo states, coulombian and kinematical threshold states, vibrational states involved in fission phenomena, atomic Rydberg states. These states are related to non-polarizing peripheral interactions (acting outside of a core). In the present approach for a spatial extended state, the (inner space) core is represented by R-matrix while the peripheral region and the phenomena occurring there are represented by logarithmic derivative of a single channel reaction model.

INTRODUCTION

Most of the nuclear properties, both for structure and for reactions, can be described in terms of short-range interacting potentials, e.g. [1]. For example, many global nuclear structure properties are described by the potentials with a "sharp-edge" finite radius as harmonic oscillator, rectangular well or Woods-Saxon potentials. For describing global aspects of scattering states one can use the folding potentials which present a radial dependence similar with that of a "sharp-edge" finite radius, e.g. [2]. In addition to bound and scattering states one has to mention resonant states which are quasi-stationary states of positive energy and which are coupled to external nuclear region via scattering states; in fact they modulate in amplitude the scattering states, e.g. [3]. These facts result into the conclusion that most of the nuclear aspects could be described in terms of the short range potentials which act in the "internal part" of the configuration space. The interaction in the "external part" of the configuration space is assumed simple in nature and, in some cases, it reduces to the coulombian one, e.g. [4]. There are however "peculiar" spatial extended nuclear states which ask for specific peripheral interactions. One can mention in this respect neutron halo states, e.g. [5], threshold states, e.g. [6], vibrational states involved in fission, e.g. [7]; also atomic Rydberg states, e.g. [8]. For every case there is a specific theoretical model related to peculiarity of the corresponding peripheral interaction. In this work a structure and reaction theoretical approach to spatial extended states, based on R-matrix, is presented.

The nuclear halo states are neutron states, spatially extended outside of the nuclear radius; it appears that their mechanism is a complicated problem of effective interactions. As energy they are located near the threshold, which is transition point between bound discrete states and the continuum spectrum. The nuclear profile of the halo neutron states is given by an extended dilute wave function tail. This is in contrast to profile of normal nuclei, whose surface is very well defined. One defines for one-neutron halo *s*-state the external wave function as $\exp(-r/\rho)/r$ where the decay length ρ [9]

$$\rho = \hbar / \sqrt{2mS_n}$$

is given in terms of reduced mass m and the neutron separation energy S_n. By evaluating the moments $\langle r^n \rangle$ as a function of separation energy S_n (decreasing towards to zero) it was found that these moments are finite provided $n < 2l - 1$. By defining the halo by the divergent second moment, as a function of S_n, one obtains halo only for s and p - states. The numerical calculations done with a square-well potential support this property, namely the neutron halo are related only to $l = 0$ and $l = 1$ partial waves. Intuitively a halo involves a nuclear core and one or two neutrons far outside the core, implying the major role of single particle properties. In the literature are mentioned so-called "pre-halo states" as deuteron bound state (binding energy 2.25 MeV) and the hypertriton (consisting from a proton, a neutron and a lambda particle with a separation energy 0.13 MeV). It is interesting to remark that in some cases the nuclear potential can leave a single neutron marginally unbound; however for two neutrons the additional attractive contribution from *n-n* interaction can be sufficient to bind two neutrons to the nucleus. These are two-neutron halos which can be treated as a three-body problem; this can be reduced to the problem of two resonant-interacting particles in a potential well, a case that has been considered long time ago by Migdal [10], [11]. The halo phenomenon is not specific only to nuclear systems. In the literature [9] there are mentioned marginally bound atomic and molecular systems. These states have been estimated to be quite extended spatially and represent atomic or molecular halo states. The potential which can bind such states decreases faster than $1/r$; there are dipole fields r^{-2} or even attractive forces of shorter range as exemplified in molecular physics by the van der Waals forces between noble gas molecules.

One has to remark here that the problem of *s*-wave halo states has been until now in no way related to the problem of the *s*-wave neutron virtual states [12]. The virtual states are negative energy neutron *s*-wave states but with a non-zero decay width. This phenomenon can be explained within S-matrix theory but not in the R-matrix theory because of using specific boundary conditions at channel radius. Recently the role of virtual states in producing two-neutron halo nuclei has been considered [13]. The description of a system of two interacting neutrons in the presence of a core was done in the Schrödinger picture by using hyperspherical coordinates. The main point was to characterize both the neutron-core and neutron-neutron interactions only by their scattering lengths. The conclusion was that the most favorable case to observe a two-neutron halo is the existence of a large negative neutron-core scattering length (it corresponds to a virtual state in the neutron-core system). This conclusion is consistent with the existence of a well-developed halo in ^{11}Li and the appearance of the $2s$ virtual state around mass number 10.

The concept of coulombian (and centrifugal) threshold states appears as a natural extension of that of the single channel (particle) resonances. According to initial description [14], they have three specific properties: a) are energetically related to the coulombian - centrifugal threshold of the two-particle decay of a nucleus, b) they are a pair of threshold particles in a definite state of relative motion, and c) they have an anomalous large radius. In the external region $(r > a)$, (a - channel radius), the relative motion is described by the out scattering wave function $\varphi_i^{(+)}(r) \sim \exp[i(k_i r - l\pi/2)]$ with i - channel index, k_i - wave number, l - orbital angular momentum. The width of the "threshold resonance" $\Gamma_i = \gamma_i^{\,2} \,|\, k_i a \,|\, / \,|\, \varphi_i^{(+)}(a) \,|^2$ is large if the reduced width $\gamma_i^{\,2}$ is large; it corresponds to a large probability to find threshold pair at channel radius a. It is proved that the probability to find the threshold pair i in the outer region $[a, \infty)$ is

$$W_i = \frac{\gamma_i^{\,2} a}{\Gamma} \sqrt{\frac{2m_i}{E_r - Q_i}}$$

where m_i and Q_i are reduced mass and coulombian threshold and E_r - the threshold state energy. If the resonance is near the threshold ($E_r \to Q_i$) then W_i becomes very large and this corresponds to "explosion" of the level from usual radius to the $r \approx \hbar / \sqrt{2m_i \,|\, E_r - Q_i \,|}$. This picture does not depend apparently on the interior of nucleus, the main parameter is here the reduced width $\gamma_i^{\,2}$ which is a measure of the single particle character of the level. The threshold states are quasi-stationary states (a) located near coulombian threshold and (b) having a large reduced width (order of Wigner unit). If there is an additional attractive interaction in the peripheral region then the "effective" width becomes even larger

$$\gamma_i^{\,2}{}_{eff} = \gamma_i^{\,2} \,|\, \varphi_{i\,free}(a) / \varphi_i^{(+)}(a) \,|^2 >> \gamma_i^{\,2}$$

We have also to mention here the interplay of the core states with the peripheral threshold states, (doorway aspects), [6].

The kinematical threshold states are of interest in rapid proton capture reactions (*rp* - processes occurring in nuclear astrophysics), e.g. [15]. Of special interest are threshold states in light medium nuclei $A \cong 20 - 30$, whose knowledge is vital in study of thermonuclear reaction rates for some burning stellar cycles, e.g. [16]. The kinematical threshold states are proton (or other charged particle) resonant states occurring just above threshold. They penetrate coulombian and centrifugal barrier having an extended tail.

The exact knowledge of their properties is important in calculus of astrophysical S-factor and of reaction rates; the last one depends on the resonant widths in an exponential manner. The wave function tail, extended outside the nuclear radius, has to be taken into account in defining their spectroscopic properties, via a renormalization factor. We will study this factor when presenting methods to describe the spatial extension of their wave functions, out of channel radius.

The fission phenomena are explained in terms of the double well potential, e.g. [7]. The fission can be described in the R-matrix theory in two complementary ways. A first attempt assumes the two classes of R-matrix states (corresponding to first and second minimum of the fission double well potential). The alternative description considers as inner configuration space only the states of the first minimum, by defining the channel radius for η - deformation parameter, between the two wells, $\eta = \eta_A$. Now the second potential minimum is located in external part of the configuration space and it will influence the behaviour of the logarithmic derivative. The vibrational levels in the second potential well are present as poles in the logarithmic derivative dependent on η - deformation parameter; this method was named "extended logarithmic derivative". In the region of v vibrational resonance of energy ε_v, the logarithmic derivative is [7], [17]

$$L = S + iP = S_b + \frac{4k_A{}^2\gamma_v{}^2(\eta_A)(\varepsilon_v - \varepsilon)}{(\varepsilon_v - \varepsilon)^2 + W_v{}^2} + i\,\frac{4k_A{}^2\gamma_v{}^2(\eta_A)W_v}{(\varepsilon_v - \varepsilon)^2 + W_v{}^2}$$

where S_b is a smoothly varying (background) term, W_v is half-width for decay of the resonant state v through the outer barrier and $\gamma_v{}^2(\eta_A)$ is the reduced width of the vibrational state v of the secondary well defined at the "wave number"

$$k_A = \sqrt{2B(\varepsilon - V_A)/\hbar}$$

with B - an inertial parameter and V_A potential magnitude at η_A.

The electron scattering in presence of Rydberg states can be also described by a modified interaction outside the channel radius. The Rydberg states (large principal quantum number n) are located at large radial distances $\sim n^2$. For the hydrogenoid atoms the core is formed from the completed electron shells; the channel radius can be identified with the radius of the core. Outside the core the effective interaction can support Rydberg (bound) states. The effect of the core on Rydberg states was taken into account, in a first approximation, by the Quantum Defect, e.g. [18]. Extension of this concept to scattering has resulted into the Multichannel Quantum Defect Theory, e.g. [19]. The logarithmic derivative, in this case, in zero energy limit $|k| \to 0$, for negative coulombian parameter $\eta = Z_1 Z_2 / \hbar v < 0$ (coulomb attraction) is proportional to [20], [21]

$$L \approx \begin{cases} i, & E > E_{thr} \\ (-1)^l ctgi\pi\eta, & E < E_{thr} \end{cases}$$

which means an oscillatory behaviour below the threshold. It is related to the energies of Rydberg states as

$$(-1)^l ctgi\pi\eta = (-1)^{l+1} ctg\pi\,\frac{Z_1 Z_2}{\hbar}\sqrt{\frac{m}{2(E_n - E)}}$$

$$E_{thr} - E_n = \frac{m}{n^2}\frac{Z_1{}^2 Z_2{}^2}{2}$$

The main problem of Multichannel Quantum Defect Theory is the evaluation of the collision matrix below threshold (where L_n - oscillatory) in terms of collision matrix calculated at energies above threshold (where L_n - monotone energy dependent).

In the following we will look for the description of the spatial extended state in terms of logarithmic derivative, irrespective of the specific form of the peripheral interaction. The logarithmic derivative L, together with R-matrix describing the internal part of the configuration space, result into scattering or collision matrix U which describes dynamics of the scattering process

$$U = P^{1/2}[1-RL]^{-1}[1-RL^{*}]P^{-1/2}\ , \qquad P = \operatorname{Im} L$$

(In this definition the coulombian and hard-sphere phase shift diagonal matrix are disregarded; this does not modify the main U-matrix property, as unitarity).

The asymptotic behaviour of the bound states is

$$u(r) \to e^{-\chi r} \quad \text{(for } r \to \infty\text{)} \quad \text{where} \quad \chi = \sqrt{2m\,|E\,|}\,/\,\hbar$$

If a denote channel radius, then the normalizing conditions for large and small wave numbers χ, are

$$\int_0^{\infty} u^2 dr = 1 = \int_0^{a} u^2 dr\,, \qquad (\chi >> 0) \quad \text{and}$$

$$\int_0^{a} u^2 dr < 1\,, \quad \text{(for } \chi \to 0\text{, state near zero energy)}$$

One can define the spatial extension of a bound state by the parameter [22]

$$\beta(E) = \frac{\int_0^{a} u^2 dr}{\int_0^{a} u^2 dr + [u(a)/\,f(a)]^2 \int_a^{\infty} f^2 dr}\,, \qquad f(r) \approx e^{-\chi r}$$

In R-matrix single channel theory one proves that, [4],

$$\beta(E) = \frac{1}{1+\gamma^2 dS/dE}$$

where $S(E) = \operatorname{Re} L$ is the shift function, which is monotone increasing with energy, and γ^2 is the corresponding reduced width. The spatial extension, out of channel radius, of a bound state near zero-energy (β - decreases) does increase with the reduced width, with the positive derivative of the shift function dS/dE and attains its largest value just near threshold (zero energy). In order to extend this definition to the positive energy one has to introduce firstly the scattering states $\chi_k(r)$ subject to orthonormality conditions, e.g. [21]

$$\int_0^{\infty} \chi_k(r)\chi^{*}_{k'}(r)dr = \delta(k-k')$$

$$\int_0^{\infty} u_m(r)u_n(r)dr = \delta_{mn}$$

$$\int_0^{\infty} u_m(r)\chi^{*}_k(r)dr = 0$$

For the quasi-stationary state ψ_k embedded in the continuum one knows that its amplitude $\int_0^a |\psi_k|^2\, dr$ decreases in time by decaying via the scattering states, (see e.g. [21] p. 298,299)

$$\psi_k(r > a) = \chi_k^{(-)} - U\chi_k^{(+)}$$

$$\psi_k(r \le a) = A(k)\chi_k^{(0)}(r)\ , \qquad \int_0^a \chi_k^{(0)}(r)^2 dr = 1$$

$$U(E) = \left(E_0 - E + i\frac{\Gamma}{2} \right)\left(E_0 - E - i\frac{\Gamma}{2} \right)^{-1}$$

$$\int_0^a \psi_k^2(r)dr = A^2(k) \sim \frac{\Gamma}{2}\left[\left(E_0 - E\right)^2 + \frac{\Gamma^2}{4} \right]^{-1}$$

The last formula was a starting point for definition of the norm of a quasi-stationary state, [4] (see also [21])

$$\int_0^a \psi_k{}^2(r)dr + a\psi_k{}^2(a)dL / d\rho^2 , \qquad (\rho = ka)$$

This norm can be used in definition of the wave function spatial extension factor

$$\beta(E) = \frac{\int_0^a \psi_k{}^2(r)dr}{\int_0^a \psi_k{}^2(r)dr + a\psi_k{}^2(a)\frac{dL}{d\rho^2}} \to \frac{1}{1+\gamma^2 \frac{dL}{dE}}$$

which is a generalization of the bound state case. For positive energies

$$|\beta| = \frac{1}{1+\gamma^2 \left| \frac{dL}{dE} \right|}$$

with $L = S^{(+)} + iP$ for $E > 0$ and $L = S^{(-)}$ for $E < 0$. For a given energy $|\beta|$ attains its minimum (largest spatial extension of the state) for a reduced width equal to Wigner unit $\gamma_W{}^2 = \hbar / ma^2$. The R-matrix interpretation of the β-factor is that of the "compression factor". It renormalizes both the resonance position and width $E_r \to \beta \cdot E_r$, $\Gamma_r \to \beta \cdot \Gamma_r$ so the resonance is shifted to the threshold and its width is decreased. There are other two interpretations of the β-factor namely "enhancement factor" ($1/\beta$ is the probability to find the level near threshold) and as ratio of the reduced R-matrix element $(\Re)$ to R-matrix element itself (R), [6]

$$\beta = \Re \cdot R^{-1}$$

One can prove within this framework the doorway aspects of the threshold states as well as the quasi-molecular aspects of the heavy ion threshold states, [6], [23]. A multichannel-multilevel reaction model for the threshold states was developed [24].

It is worth to remark that the "compression factor" β of the R-matrix theory does play an essential role also in kinematical threshold states. These states appear just above kinematical threshold (zero energy) as resonances or even below threshold (negative energy resonances). The negative energy resonances can influence the positive energy cross-section, via their tail extended above threshold. The low-energy cross-sections, deconvoluted with penetration factors, define the astrophysical factor $S(E)$, which is essential in evaluation of thermonuclear reaction rates, e.g. [15]

$$\sigma(E) = S(E)e^{-2\pi\eta} / E$$

where η - coulombian parameter and σ - cross section (for example, for capture reactions). One has to remark that the R-matrix width is normalized in terms of the compression factor, e.g. [25], [22], [4]

$$\Gamma \to \Gamma / \left[1 + \sum_c \gamma_c{}^2 \left(dS_c / dE \right) \right]$$

The logarithmic derivative in the double well potential is necessary in studying phenomena like fission. It can be derived from Schrödinger equation

$$-\frac{\hbar^2}{2B}\frac{d^2}{d\eta^2}\psi(\eta)-[V(\eta)-E]\psi(\eta)=0$$

where B is the inertial parameter and $V(\eta)$ is the potential, function on η deformation parameter. The logarithmic derivative is defined by

$$L=S+iP=\left[\frac{1}{O(\eta)}\frac{dO(\eta)}{d\eta}\right]_{\eta=\eta_A}$$

where $O(\eta)$ is the outgoing solution of Schrödinger equation. It is subject of a Ricatti equation

$$\frac{dL(\eta)}{d\eta}=\frac{2B}{\hbar^2}[V(\eta)-E]-L^2(\eta)$$

which was studied numerically for double well potentials composed of the segments of the form $V_i+a_i\left(\frac{1}{\eta}-\frac{1}{\eta_i}\right)^2$ in the work [17]. The vibrational states in second minimum of double well decay as single channel resonances. One has to mention that in a quite different framework (Shell Model Approach to Nuclear Reactions, [26]) one obtains a dispersive behaviour of the penetration factor

$$P=P_0\left[\frac{f_0+E-\zeta}{|E-\xi|}\right]^2$$

where P_0 is R-matrix penetration factor and there is a resonance at complex energy $\xi=\zeta-\frac{i}{2}\Gamma$.

The Rydberg atomic states are located outside of inner electronic core. The effect of the electronic core on these states is taken into account via a phenomenological parameter "quantum defect". If the electronic core is not inert, resulting in many reaction channels one obtains the Multichannel Quantum Defect Theory (MQDT), e.g. [19]. This theory describes in a remarkable way the two types of resonances of the electron-atom scattering, namely multielectronic resonances and the Rydberg states. The multielectronic resonances originate in excitation of electronic cloud; the Rydberg states are single particle resonances originating in attractive coulombian forces from channels. Until now MQDT was considered as a theory specific to structure and collisions in the systems electron-atom and electron-ion; this is because of the central role in this theory of the coulombian functions. Lane [27] has related this theory to R-matrix; in the same spirit we proved [28] that Rydberg single channel states originate in jump across threshold of the logarithmic derivative. The collision matrix form [28] of MQDT

$$U_{ab}^{<}=U_{ab}^{>}-U_{an}^{>}\frac{1}{-(U_{nn}^{\delta})^{*}+U_{nn}^{>}}U_{nb}^{>}$$

does connect elements of the collision matrix below (<) threshold to elements of the same matrix above (>) threshold; a,b-open channels and n-opening channel. The jump of the logarithmic derivative across n-channel threshold $\Delta L_n=L_>-L_<$ does enter into "defect" collision matrix element U_{nn}^{δ}

$$(U_{nn}^{\delta})^{*}=e^{-2i\delta}=e^{-2i\phi}\frac{(\Delta L_n)^{*}}{\Delta L_n}$$

where ϕ is coulombian hard-sphere phase shift. In this work no hypothesis with respect to peripheral interaction was used; this makes the theory more general. If applied to attractive coulombian interaction, one obtains the "classical" results of MQDT $\Delta\sigma=\pi|\eta|$. For zero peripheric interaction one obtains for phase shift the result $\Delta\sigma=\pi/4$, identical to work [18]. The dipolar potential $-a_2/r^2$, also of interest in neutron-halo physics [29], results into phase shift $\Delta\sigma = \alpha \ln|\eta| - \arg\Gamma(1 - i\alpha)$ where imaginary α is related to strength of dipolar field $2a_2 = \alpha^2 + \frac{1}{4}$.

The nuclear Rydberg state of the di-neutron could be approached also in the inverse sense, [29]; one assumes the existence of a dineutron-halo, and one asks what effective interactions could bind the two neutrons into the dineutron, $\psi_{2n} \approx e^{-Kr}/r$, $\varepsilon_{2n} = 2(\hbar^2 K^2 / 2m_n)$, ($r$ - relative coordinate in dineutron). To fulfill this condition, one needs the effective interaction $U_{eff} \approx -\lambda / R^2$, ($R$ - dineutron-core relative distance). For interaction strong enough ($\lambda > 1/4$), [20], to produce dineutrons, the following inequality between dineutron energy ε_{2n} and its angular momentum l in potential well

$$\varepsilon_{2n} > const[1/4 + l(l+1)]^2$$

must be satisfied. The dineutronic-halo looks like a Rydberg nuclear state in an attractive "dipolar" potential ($-\gamma / r^2$).

The dipolar attractive potential is a usual one in atomic quantum defect studies, e.g. [18]; it is specific to peripheral region, extending from core to infinity. The exact formula for energy levels provides an infinity of levels accumulating at zero energy

$$E_n = E_0 \exp\left[-2\pi n / \sqrt{\gamma - 1/4}\right], \quad (n = 1,2,\cdots),$$

$$E_0 = (\hbar^2 / ma^2)\exp\left[-\pi / \sqrt{\gamma - 1/4}\right]\exp\left[2\pi\mu / \sqrt{\gamma - 1/4}\right]C_\gamma$$

$$C_\gamma = \exp\left[2\pi\Theta_\gamma / \sqrt{\gamma - 1/4}\right]$$

the constant C_γ is apparently not strongly dependent on potential strength, due to O_γ -phase in asymptotic form of wave function,

$$u(r) \sim r^{1/2} \cos\left[\sqrt{\gamma - 1/4}\ln r + \Theta_\gamma\right]$$

This study could be extended to a dipolar attractive and coulombian repulsive potential and also to Kratzer-Fuess potential; both cases allow analytical solutions.

The dipolar attractive potential in the exact formula could reproduce the numerical results of dineutronic halo state for ^{11}Li nucleus with halo radius $a = 6.5\,fm$ and s-wave state energy of $E_0 = 0.4MeV$. The parameters reproducing different partial waves ($l = 0,1,2,3,4$) levels are $(\Theta_\gamma + \mu) \cong -1/2$ and $\gamma \cong 1$.

Another remarkable result, that the R_n-matrix element corresponding to defect collision matrix element U_{nn}^{δ} is given by $R_n^{-1} = S_n^{(-)}$, which is just condition for a bound state, [4]. By extension to multichannel case this condition becomes $\Re_n^{-1} = L_n^{(-)}$, where $\Re_n$ is the reduced R-matrix taking into account the coupling to other competing open reaction channels. The phase shift $\Delta\sigma$ is related in a simple way to penetration factor P and to jump ΔS of the real part of logarithmic derivative, $\tan\Delta\sigma = P / \Delta S$. One has to remark that this formalism could be extended to single channel resonances of positive energies (as e.g. the cases of threshold states and fission vibrational states). In this case $L_<$ is evaluated at positive energies corresponding to presence of single channel resonance and $L_>$ is evaluated also at positive energies but having a monotone energy behaviour (no resonance). In this case the phase shift $\Delta\sigma$ becomes a complex function. If the single-channel state occurs at positive energies (threshold states, vibrational states in fission phenomenon) then the previous result becomes

$$e^{-2i\delta} = e^{-2i\phi} \frac{L_>^* - L_<}{L_> - L_<}$$

The real part of the phase shift $\Delta\sigma = \mathrm{Re}\,\delta$ is given by

$$2\Delta\sigma = \arctan\frac{P_> + P_<}{\Delta S} + \arctan\frac{\Delta P}{\Delta S}$$

which, obviously, reduces to $2\Delta\delta = 2\arctan(P_> / \Delta S)$ corresponding to a state below threshold ($P_< = 0$). The imaginary part of the phase-shift is positive

$$e^{2\mu} = \sqrt{1+(P_> + P_<)^2/(\Delta S)^2} \,/\, \sqrt{1+(\Delta P)^2/(\Delta S)^2}$$

which reduces to unity for a state below threshold ($P_< = 0$, $\Delta P = P_> - P_< = P_>$).

In this work we discussed the essential role of the logarithmic derivative in describing some types of extended nuclear or atomic states. The only hypothesis is that peripheral interaction (involved in extended states) is a non-polarizing one. The logarithmic derivative, corresponding to external part of configuration space is the inverse of the R-matrix (in this part of space). The R-matrix for inner configuration space and logarithmic derivative for external configuration space are combined together in collision matrix, describing the process as a whole. The problem of description for virtual and neutron halo states in terms of channel logarithmic derivative is subject of forthcoming research.

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