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SINGLE PARTICLE RESONANCES IN CONTINUUM NUCLEAR STRUCTURE CALCULATIONS

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ABSTRACT

Accuracy and stability of single–particle resonance parameters under changes of a "resonance wavefunction" are examined in the context of a projection technique. Implications for their use in nuclear structure calculations are discussed.

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Several different discretization methods for the single particle continuum in nuclear structure calculations (notably when using the Random Phase Approximation (RPA) are currently used in the literature or are reportedly being implemented. They include projection methods in a number of variations[1–5], including the use of Weinberg "quasi–particles"[5], and the use of Gamow states[4]. Their common aim is to provide for a sound scheme allowing one to include the relevant features of the continuous single–particle spectrum, notably single–particle resonances with the corresponding escape widths, at reduced computational cost. The variety of adopted methods eventually reflects the fact that a unique or priviledged way of meeting such practical demands actually does not exist. This implies, on the other hand, that considerations of convenience are applicable and legitimate. The purpose of this note is to discuss in some detail the accuracy and stability of the simple and yet flexible and physically transparent projection method of ref. [1], with the expectation that this may contribute both to technical and conceptual unification.

The basic scheme behind the method as used in connection with an isolated single–particle resonance lies in writing the scattering solution $|\psi^+>$ of the single–particle hamiltonian H at energy E as

$$|\psi^+> = |u><u|\psi^+> + P|\psi^+> \qquad (1)$$

where $|u>$ is some normalized single–particle state and $P = 1-|u><u|$ projects onto the complementary subspace of the single–particle Hilbert space. Projection and formal manipulation of the Schrödinger equation $[E-H]|\psi^+> = 0$ then gives

$$P|\psi^+> = |\varphi^+> + G^+_{PP}(E)\, PH|u><u|\psi^+> \qquad (2)$$

$$\langle u|\psi^+\rangle = \frac{\langle u|H|\varphi^+\rangle}{E - \langle u|H|u\rangle - \langle u|HG^+_{PP}(E)H|u\rangle} \qquad (3)$$

where $G^+_{PP}(E) = (E+i\eta-H_{PP})^{-1}$ and $|\varphi^+\rangle$ is the scattering solution of the projected hamiltonian H_{PP} at energy E. As noted in ref. [1], this can easily be obtained by solving the inhomogeneous equation

$$[E-H]|\varphi^+\rangle = |u\rangle\alpha \qquad (4)$$

with α adjusted so that $\langle u|\varphi^+\rangle = 0$ and ψ satisfying appropriate asymptotic conditions. In this case $\alpha = -\langle u|H|\varphi^+\rangle$. Similarly, the more involved object $|\chi^+\rangle = G^+_{PP}(E)H|u\rangle$ appearing in eq. (2) can be obtained by integrating

$$[E-H]|\chi^+\rangle = |u\rangle\beta + H|u\rangle \qquad (5)$$

with β adjusted so that $\langle u|\chi^+\rangle = 0$ and enforcing appropriate asymptotic conditions. All the ingredients in eqs. (2) and (3) are therefore easily calculable numerically for any given single particle wavefunction $|u\rangle$. Furthermore, writing

$$\langle u|HG^+_{PP}(E)H|u\rangle = \langle u|H|\chi^+\rangle \equiv \Delta_u(E) - \frac{i}{2}\Gamma_u(E) \qquad (6)$$

the single–particle scattering matrix associated with H appears as

$$S(E) = S_\varphi(E)\,\frac{1 - i\pi K(E)}{1 + i\pi K(E)} \;; \quad K(E) = \frac{1}{2\pi}\,\frac{\Gamma_u(E)}{E - \langle u|H|u\rangle - \Delta_u(E)} \qquad (7)$$

where $S_\varphi(E)$ is the S–matrix associated with the projected hamiltonian H_{PP}. A crucial point is, therefore, to choose $|u\rangle$ so that the relevant resonant behavior of $S(E)$ is

essentially carried by the second factor on the right hand side of eq. (7), which contains the reduced reactance matrix $K(E)$. The main content of ref. [1] consists in showing that this can be achieved in a simple and stable way by taking for $|u\rangle$ the (normalized) internal part of the resonant wavefunction $|\psi^+\rangle_{E=E_0}$ itself. Stability, in this connection, refers to relative insensitivity both to the precise definition of resonance energy E_0 and cut–off radius to define the internal wavefunction, provided it lies outside the single–particle potential in H.

It should be stressed, however, that stability in this particular sense does not entail the stability e.g. of $\Gamma_u(E_0)$, in view of the energy dependence of $\Delta_u(E)$ and $\Gamma_u(E)$. It turns out, in fact, that both the values and the energy dependence of these quantitites are much more sensitive to the particular cut–off radius which is used, so that extra care is required to extract resonance parameters from the reduced reaction matrix K. This is shown in the column labelled as $\Gamma(E_0)$ of Table 1 for the $1d_{3/2}$ and the $1f_{7/2}$ proton resonances in the Woods–Saxon potential described in Table 2, which stands for a ^{16}O target. In this calculation, we used the smooth cut–off

$$\langle r|u\rangle = N \times \left[1 + e^{\frac{r-R_u}{A_u}}\right]^{-1} \langle r|\psi^+\rangle_{E=E_0} \qquad (8)$$

and chose E_0 as the value of E which minimizes the normalization factor N (i.e., for which the integrated internal probability density is largest).

The stability of deduced resonance parameters is considerably improved, however, by associating them with the pole and residue of the reduced reactance matrix. In this way, the resonance energy E_R is given by the solution of

$$E_R - \langle u|H|u\rangle - \Delta_u(E_R) = 0 \qquad (9a)$$

and the width Γ_R is given as

$$\Gamma_R = \frac{\Gamma_u(E_R)}{1 - \frac{d\Delta_u}{dE}(E_R)} \quad . \tag{9b}$$

For practical purposes, the energy dependence of $\Delta_u(E)$ and $\Gamma_u(E)$ is simple enough so that a linear approximation to it in the vicinity of $E = E_0$ is useful[6]. This allows one to approximate resonance parameters in terms of quantities evaluated numerically for $E=E_0$ as

$$E_R \cong \langle u|H|u\rangle + \frac{\Delta_u(E_0) + [\langle u|H|u\rangle - E_0]\frac{d\Delta_u}{dE}(E_0)}{1 - \frac{d\Delta_u}{dE}(E_0)} \tag{10a}$$

and

$$\Gamma_R \cong \frac{\Gamma_u(E_0) + (E_R - E_0)\frac{d\Gamma_u}{dE}(E_0)}{1 - \frac{d\Delta_u}{dE}(E_0)} \quad . \tag{10b}$$

The last two columns of table 1 show the values obtained in the case of proton resonances in ^{16}O for several choices of the cut–off parameters.

A last but important point refers to the use of these projection techniques in the framework of nuclear structure calculations[7,8]. An obvious and typical application consists in analysing the single–particle continuum in terms of a set of normalized resonance states such as $|u\rangle$ plus a nonresonant, background continuum. In this context one may have to deal, in particular, with more than one single–particle resonance in a given channel. In order to handle this situation one can (a) solve eq. (4) in the energy span of a second resonance and take the smoothly cut–off $|\varphi\rangle$ (in the sense of eq. (8)) to define the second normalized resonance state $|u_2\rangle$. The orthogonality of this to the first resonance state, $\langle u_2|u_1\rangle = 0$, is in this case taken care of by the condition $\langle u_1|\varphi\rangle = 0$ provided the second cut–off radius is sufficiently large. The twice–subtracted background continuum is then obtained by solving

$$[E - H]|\varphi^+\rangle = |u_1\rangle\alpha_1 + |u_2\rangle\alpha_2 \tag{11}$$

with α_1 and α_2 fixed so that $\langle u_1|\varphi\rangle = \langle u_2|\varphi\rangle = 0$. Alternatively, one can (b) choose $|u_1\rangle$ and $|u_2\rangle$ independently according to eq. (8) in the energy domains of the two resonances. In this case they will be linearly independent but in general non–orthogonal. If an orthogonal set of resonance states is sought one has just to construct

$$|\tilde{u}_i\rangle = \sum_j (g^{-1/2})^*_{ij}|u_j\rangle \quad \text{with} \quad g_{ij} = \langle u_i|u_j\rangle \quad .$$

Both strategies are of course immediately extended to more than two resonances per channel, while the first indicates further how the previous discussion concerning resonance parameters is generalized.

The non–resonant background continuum, together with the normalized resonance–states and the bound single–particle states allows for the setting up of a suitably partitioned single–particle basis in which to express the many–body dynamics. In particular, the coupling of the resonance states to the background continuum will give rise to energy–dependent shifts (Δ_{u_i}) and widths (Γ_{u_i}) which act in fact as (complex) one–body selfenergies of the resonance states. These can easily be accomodated in standard nuclear structure calculations provided the energy–dependence can be ignored for practical purposes. This then indicates that the most adequate choice of resonance wavefunctions $\langle r|u_i\rangle$ is that which minimizes energy–dependence effects. Even though we found that resonance parameters can be reliably extracted under less stringent conditions, it should be borne in mind that the nuclear structure calculation will involve the wavefunctions themselves, and not just those parameters. The numbers quoted in the third and fourth column of Table I indicate that the energy dependence of the uncorrected width resulting from the present partitioning of the single–particle basis is decreased by taking large enough cut–off radii while the shift energy dependence is essentially stable. The overall criterion appears in fact to be that the radial node structure of the resonance state wavefunctions should be preserved up to distances where the potential becomes negligible (or pure Coulomb, for charged particles).

REFERENCES

1. W.L. Wang and C.M. Shakin, *Phys. Lett.* **32B**, 421 (1970).
2. S. Yoshida and S. Adachi, *Nucl. Phys.* **A457**, 84 (1986).
3. F. Zardi and P.F. Bortignon, *Europhys. Lett.* **1**, 281 (1986).
4. T. Vertse, P. Curutchet, O. Civitarese, L.S. Ferreira and R.J. Liotta, *Phys. Rev.* **C37**, 876 (1988); P. Curutchet, T. Vertse and R.J. Liotta, *Phys. Rev.* **C39**, 1020 (1989).
5. M. Buballa, A. Gattone, R. de Haro, R. Jessenberger and S. Krewald, *Nucl. Phys.* **A517**, 61 (1990); See S. Weinberg, *Phys. Rev.* **B133**, 232 (1964).
6. G.W. Bund and J.S. Blair, *Nucl. Phys.* **A144**, 384 (1970).
7. M. Kawai, A.K. Kerman and K.W. McVoy, *Ann. Phys.* (N.Y.) **75**, 156 (1973).
8. A.F.R. de Toledo Piza, *Nucl. Phys.* **A184**, 303 (1972); *Rev. Bras. Fis.* **17**, 195 (1987); N. Teruya, H. Dias and A.F.R. de Toledo Piza, to be published.

	R_u (fm)	A_u(fm)	$\left.\frac{d\Gamma_u}{dE}\right\|_{E=E_0}$	$1-\left.\frac{d\Delta_u}{dE}\right\|_{E=E_0}$	$\Gamma_u(E_0)$ (MeV)	Γ_R (MeV)	E_R (MeV)
$(\pi_{1d_{3/2}})$ E_0=4.500 MeV	3.20	0.65	1.120	1.371	1.761	1.329	4.555
	7.00	0.65	0.289	0.806	0.931	1.135	4.445
	15.00	0.65	0.010	0.742	0.787	1.059	4.345
	7.00	2.00	0.206	0.784	0.884	1.106	4.417
	10.00	2.00	0.092	0.753	0.821	1.075	4.378
	15.00	2.00	0.020	0.743	0.791	1.061	4.349
	H.O.		0.813	1.129	1.418	1.280	4.534
$(\pi_{1f_{7/2}})$ E_0=10.610 MeV	3.20	0.65	1.375	1.207	5.193	4.899	11.134
	7.00	2.00	0.136	0.722	2.429	3.311	10.330
	10.00	2.00	0.049	0.709	2.310	3.231	10.221
	15.00	2.00	0.012	0.706	2.265	3.201	10.171
	H.O.		0.626	0.870	3.356	3.995	10.802

Table 1 – Single particle resonances in ^{16}O as a function of arbitrary cut–off radius parameters (R_u, A_u) in wave functions $\langle r|u\rangle$ of the eq. (8) (see text). In the table H.O. line corresponds the utilization of harmonic oscillator wavefunction.

$$U(r) = V_0 f(r) + \ell \cdot \sigma V_{\ell s} f'(r)/r$$
$$f(r) = 1/\{1+\exp[(r-R)/a]\}$$

$V_0 = -51.8$ MeV

$a = 0.65$ fm

$V_{\ell s} = 13$ MeV·fm

$R = 3.17$ fm

Table 2 – Parameters of the Woods–Saxon well (for protons in ^{16}O).