Towards microscopic optical potentials in deformed nuclei

A Idini, J Rotureau, J Boström, J Ljungberg, B G Carlsson
Division of Mathematical Physics, Physics dept., LTH, Lund University, S-22100 Lund, Sweden
E-mail: andrea.idini@matfys.lth.se

Abstract. A microscopic and consistent description of both nuclear structure and reactions is instrumental to extend the predictivity of models calculating scattering observables. In particular, this is crucial in the case of exotic nuclei not yet discovered.

In this manuscript, we will present the plan of the Lund effort for a symmetry breaking description of bound and scattering observables using a generator coordinate method model based on an effective Hamiltonian constrained with a (Skyrme) functional. Following this, we will illustrate the steps to construct an optical potential for deformed nuclei from microscopic wavefunctions obtained with projected generator coordinate method from Hartree-Fock-Bogoliubov basis.

1. Introduction
It has been proven very difficult to study nuclear reactions using state-of-the-art nuclear structure information in a consistent framework for many nuclei of interest, cf. [1, 2] and refs. therein for context regarding the importance of a consistent description of nuclear structure and reactions. Despite efforts and progress in later years in developing optical potentials from first principles using Green’s function based methods [3–6] or multi-scattering [7–9] approaches, it is especially difficult to develop microscopic potentials for deformed nuclei. The description of deformed nuclei imposes an additional complexity to the calculation and formalism.

The following is a short summary concerning the construction of a model of atomic nuclei that relies on an effective Hamiltonian and generator coordinate method, introducing of the steps to derive optical potentials for deformed nuclei from microscopic symmetry breaking formalism.

2. Method
Models of quantum many-body systems try to provide a microscopic description of a system composed of many particles affected by a general Hamiltonian $\hat{H}$ with the best degree of approximation. It is convenient to notice that a general Hamiltonian in tensor form, can be decomposed in a sum of a product of lower-rank tensors (cf. e.g. [10]). Without loss of generality, it is possible to assume these lower rank tensors to be expressed in a multipole expansion, resulting in a general Hamiltonian to be expressed and expanded as product of multipoles in order to exploit the natural degrees of freedom of nuclei. Following this principle, we developed a formalism and code to provide multi-reference solutions of Hamiltonians expressed in separable multipoles using generator coordinate method (GCM) with symmetry restoration.
At the present moment, we focus our attention on a simple Hamiltonian that captures the physical properties of nuclei with the least amount of terms. It was shown using particle–vibration coupling that it is possible to achieve a satisfactory agreement with spectroscopic properties of nuclei using an Hamiltonian composed of separable multipole terms and seniority pairing, with the low–lying quadrupole being the most important contribution [11,12].

**Figure 1.** A schematic representation of the method expressed in [13], cf. the main text.

Therefore, the effective Hamiltonian that was used in [13] (and also in the calculation of superheavy isotopes [14]) is postulated to be,

$$\hat{H} = \hat{H}_0 + \hat{H}_Q + \hat{H}_P,$$

that is, $H$ includes a spherical mean field $H_0 = \sum_i \epsilon_i a_i^\dagger a_i + E_0$, and two separable terms for the pairing and the quadrupole-quadrupole interaction. The pairing is chosen to be seniority pairing between time reversal states $H_P = -G \sum_{ijkl} P_{ij} P_{kl} a_i^\dagger a_j a_k a_l$, the constant strength $G$ is calculated according to the uniform spectra method [15]. The $H_Q$ term is defined as $-\frac{1}{4} \chi \sum_{ijkl} \sum_{\mu} [Q_{ij}^{2\mu} Q_{kl}^{2\mu\ast} - Q_{ij}^{2\mu} Q_{kl}^{2\mu\ast}] a_i^\dagger a_j a_k a_l$, with $Q_{ij}$ the modified quadrupole operator with a radial profile that is obtained from the derivative of a parametrised Wood-Saxon [16]. The real parameter $\chi$ is fitted to reproduce axially constrained calculations of a parametrization of Skyrme functional, e.g. SLy4, generating the Sly4-H effective Hamiltonian. More information can be found in [13], with comparison of different Skyrme functionals in [17]. This effective Hamiltonian with few terms is chosen because it explicitly breaks particle number and rotational symmetries. In this way, we can describe the many–body properties as comprehensively as possible in a large scale calculation, projecting angular momentum $I$ and particle number.

The many-body basis that is used to solve the effective Hamiltonian in Eq. (1) consists of HFB vacuua $|\Phi\rangle$ with a variation over a set of generator coordinates, which are the familiar $\beta$ and $\gamma$ for deformation and triaxiality, pairing strengths for protons and neutrons $g_{p,n}$, and cranking frequencies $\omega$. Therefore, a set of HFB vacua for different coordinates $\{|\Phi(\beta,\gamma,g_{p,n},\omega)\rangle\} \equiv \{|\Phi(i)\rangle\}$ is obtained. This choice accounts for the most important collective degrees of freedom of collective vibrations, rotations and pairing vibrations.

The GCM solution can be written as,

$$|\Psi^A_J(a)\rangle = \sum_{iK} h^{A,a}_{JMK}(i) P^N P^Z P^J_{MK} |\Phi(i)\rangle,$$  

where the state $a$ of total number of nucleons $A$ is obtained summing over the basis states $|\phi(i)\rangle$, considering the coefficients of the solutions of the Hill–Wheeler equation $h_i$, and restoring the symmetry with projection operators $P^N$, $P^Z$, and $P^J_{MK}$ projecting to good number of neutrons $N$, protons $Z$ and good angular momentum $J$. 

The Green’s function can, in principle, be constructed with several many-body methods from densities and eigenstates (cf. [4, 5, 18]). It is defined from the eigenstates of $H$,

$$G(\alpha, \beta, E, \eta) = \langle \Psi_0^A | a_\alpha | E - (H - E_0^A) + i\eta \rangle \beta | \Psi_0^A \rangle + \langle \Psi_0^A | a_\beta \rangle \alpha | E + (H - E_0^A) - i\eta \rangle | \Psi_0^A \rangle,$$

with $E_0^A$ as the energy of the ground state $\Psi_0^A$ for system of $A$ particles. In the case under consideration, the reference state is an even–even state $A$.

After the insertion of the identity resolution

$$\sum | \Psi_{J+1}(k) \rangle \langle \Psi_{J+1}(k) |$$

the matrix elements of the creation and annihilation operators define the components of the numerator of the Green’s function and are called the spectroscopic amplitudes $S^J$. Together with the energy of the states, $S^J$ are the elements needed to construct the Green’s functions (3). From the Green’s functions the optical potential can be derived inverting the Dyson equation

$$\Sigma = G_0^{-1} - G^1,$$

with $G_0$ the unperturbed Green’s function propagator corresponding to $H_0$ [1]. $\Sigma$ can then be transformed in momentum space and used to solve the Schrödinger equation in the continuum as in [4].

The familiar basis associated to the creation operator $a^\dagger$ can be either a spherical Hartree Fock or harmonic oscillator basis. The spectroscopic amplitudes between GCM states are obtained following (2) considering the overlap between even and odd states,

$$S^J(k, \alpha) = \sum_{aK} h_{00}^A(i)(h_{J+1,k}^A(a))^\ast \langle \Phi^{A+1}(a) | a_\alpha P^N P^Z P^0_{00} | \Phi(i) \rangle.$$

Therefore, in the Bogoliubov quasiparticle basis $\beta$ the calculation of $S^J(k, \alpha)$ is then composed of two contributions: $\langle \Phi^A(z) | P^N P^Z P^0_{00} | \Phi(i) \rangle$ and $\langle \Phi^A(z) | \beta_\alpha \beta_\beta P^N P^Z P^0_{00} | \Phi(i) \rangle$, cf. [19].

3. Conclusions

The provided definition of $S^J$ in the Bogoliubov basis for GCM states can be used to calculate them, hence defining Green’s functions, optical potentials, and calculate reaction observables consistently. An important seminal example of use of GCM in a small–scale calculation of $S^J$ can be found in [20]. The first results of the calculation of the $S^J$ for $^{24}$Mg are in [19], using these results we plan to progress to the construction of optical potentials as described here.

Acknowledgments

We were supported by Swedish Research Council 2020-03721, Crafoord foundation, Knut & Alice Wallenberg foundation (KAW 2015.0021), and Lunarc computing facility.

[1] Johnson C W, Launey K D and others 2020 J. Phys. G 47 123001
[2] Hebborn C et al. 2022 arXiv preprint arXiv:2210.07293
[3] Idini A, Barbieri C and Navrátil P 2018 J. Phys.: Conf. Ser. 981 012005
[4] Idini A, Barbieri C and Navrátil P 2019 Phys. Rev. Lett. 123(9) 092501
[5] Rotureau J, Danielewicz P, Hagen G, Nunes F M and Papenbrock T 2017 Phys. Rev. C 95(2) 024315
[6] Rotureau J, Danielewicz P, Hagen G, Jansen G R and Nunes F 2018 Phys. Rev. C 99 044625
[7] Holt J D, Menéndez J and Schwenk A 2013 J. Phys. G 40 075105
[8] Vorabbi M et al. 2021 Phys. Rev. C 103 024604
[9] Burrows M et al. 2020 Phys. Rev. C 102 034606
[10] Tichai A, Schütschi R, Scuseria G E and Duguet T 2019 Phys. Rev. C 99(3) 034320
[11] Idini A, Barranco F and Vigezzi E 2012 Phys. Rev. C 85 014331
[12] Idini A, Potel G, Barranco F, Vigezzi E and Broglio R A 2015 Phys. Rev. C 92(3) 031304
[13] Ljungberg J, Carlsson B G, Rotureau J, Idini A and Ragnarsson J 2022 Phys. Rev. C 106(1) 014314
[14] Sämark-Roth A et al. 2021 Phys. Rev. Lett. 126(3) 032503
[15] Ragnarsson I and Gösta Nilsson S 2005 Shapes and Shells in Nuclear Structure
[16] Kumar K and Sørensen B 1970 Nuclear Physics A 146 1–14 ISSN 0375-9474
[17] Ljungberg J et al. 2022 in this volume (Preprint arXiv 2212.07673 [nucl-th])
[18] Salvioni G et al. 2020 J. Phys. G 47 085107
[19] Boström J et al. 2022 in this volume
[20] Häkansson H B, Berggren T and Bengtsson R 1978 Nucl. Phys. A 306 406–428