

# Scattering and Nuclear Structure with Oscillator Basis

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## Abstract

We demonstrate that the harmonic oscillator basis can be generated by the Lanczos algorithm. We use this remarkable feature to formulate a formalism in quantum scattering theory utilizing an expansion of scattering wave functions in infinite series of oscillator functions. The continuum spectrum solutions of the Schrödinger equation are found by means of Lanczos iterations. This formalism provides a possibility to extend a nuclear shell model, in particular, an *ab initio* no-core shell model, on a scattering domain.

**Keywords:** *Non-relativistic quantum scattering theory; nuclear structure; oscillator basis*

An impressive progress in *ab initio* description of nuclear structure has been achieved during the last decade. In addition, research projects aimed at an *ab initio* description of nuclear reactions have advanced. First should be mentioned a combined no-core shell model/resonating group method (NCSM/RGM) approach developed by Navrátil, Quaglioni *et al.* [1]. Various reactions with light nuclei were successfully calculated by means of the NCSM/RGM method. Unfortunately, the RGM approach involves some model assumptions regarding the reaction mechanism which limit the predictive power usually associated with *ab initio* methods. The first attempt to calculate nucleon-nucleus scattering based on quantum Monte Carlo calculations was performed in Ref. [2]. The Gamow shell model [3] provides a possibility to calculate widths of nuclear resonant states. A Lorentz Integral Transform method [4] makes it possible to calculate observables in photonuclear and electroweak reactions within various *ab initio* approaches. This method was successfully used in calculations of cross sections of various photodisintegration, electrodisintegration and electroweak reactions on light nuclei within the hyperspherical harmonics approach [5]. A generalized Lanczos technique was suggested in Ref. [6] for calculations of nuclear response for any multipole operator and general electroweak response functions and electromagnetic responses in particular within theoretical approaches utilizing Slater determinants built on harmonic oscillator basis functions.

A harmonic oscillator provides a natural basis for many-body nuclear structure studies. It is widely used in various shell model applications, in particular, in *ab initio* NCSM [7, 8]. A diagonalization of the shell model Hamiltonian matrix in the many-body oscillator basis is conventionally performed using the Lanczos algorithm.

We demonstrate below that the complete infinite harmonic oscillator basis can be generated by the Lanczos algorithm. The Lanczos technique of generating the oscillator basis can be naturally reformulated as a formalism of non-relativistic quantum scattering theory where scattering wave functions are expanded in infinite series of oscillator functions. We note that this scattering theory formalism is formally equivalent to the  $J$ -matrix formalism with oscillator basis [9–12]. An advantage of our formalism is that it utilizes the Lanczos iterations and oscillator basis, the basic tools of various conventional approaches to nuclear structure. Therefore this scattering formalism can be naturally integrated into modern *ab initio* methods for nuclear structure studies

generalizing them to the scattering domain. As a result, one can hope to obtain a unified *ab initio* theory of nuclear structure and reactions.

We start the discussion of the proposed formalism from the case of a two-body scattering problem. Within the quantum scattering theory, one compares the asymptotics of the wave functions  $\Psi_E$  fitting the Schrödinger equation with the Hamiltonian  $H$  describing the relative motion in the system of interest,

$$H\Psi_E = E\Psi_E, \quad (1)$$

with the asymptotics of the wave function  $\Psi_E^0$  of the reference Hamiltonian  $H^0$ ,

$$H^0\Psi_E^0 = E\Psi_E^0. \quad (2)$$

We discuss here the case of  $H^0$  being a free Hamiltonian, i. e., it includes the operator of kinetic energy of relative motion of colliding particles  $T$  only,

$$H^0 = T. \quad (3)$$

We are studying the states of a given angular momentum  $J$  and denote by  $\phi_i$  the oscillator state with  $i$  excitation quanta, i. e. the state with  $i$  oscillator excitations as compared with the lowest oscillator state with the particular value of  $J$ . The kinetic energy operator is known to have a tridiagonal matrix in the basis of states  $\phi_i$ , i. e., matrix elements  $T_{ij} = \langle \phi_i | T | \phi_j \rangle$  differ from zero only if  $i = j$  or  $i = j \pm 2$ . Therefore applying the operator  $T$  to the state  $\phi_i$ , we obtain

$$T\phi_i = T_{i,i-2}\phi_{i-2} + T_{ii}\phi_i + T_{i,i+2}\phi_{i+2}. \quad (4)$$

We note that the Lanczos algorithm with kinetic energy operator  $T$  generates the oscillator basis of states with any given angular momentum.  $\phi_0$  is the lowest oscillator state with the angular momentum  $J$ . Let us use  $\phi_0$  as a pivot vector in the Lanczos procedure. By applying  $T$  to  $\phi_0$ , we get

$$T\phi_0 = T_{00}\phi_0 + T_{02}\phi_2. \quad (5)$$

Orthogonalizing  $T\phi_0$  to  $\phi_0$  and normalizing the resulting function, we obtain  $\phi_2$  as the first Lanczos vector. The second Lanczos vector is obtained by applying  $T$  to  $\phi_2$ ,

$$T\phi_2 = T_{20}\phi_0 + T_{22}\phi_2 + T_{24}\phi_4, \quad (6)$$

by orthogonalizing the result to  $\phi_0$  and  $\phi_2$  and normalization. Clearly,  $\phi_4$  appears to be the second Lanczos vector. In the same manner we obtain  $\phi_6$  as the third Lanczos vector, etc. Thus the oscillator basis appears to be a Lanczos basis generated by the kinetic energy operator with  $\phi_0$  as a pivot vector.

We can construct the oscillator basis by Lanczos procedure not only from below, i. e. starting from the lowest oscillator state, but also from above starting from oscillator states with arbitrary large oscillator quanta. Suppose we have oscillator functions  $\phi_N$  and  $\phi_{N+2}$ . Applying  $T$  to  $\phi_N$ , orthogonalizing the result to  $\phi_N$  and  $\phi_{N+2}$  and normalizing, we obtain  $\phi_{N-2}$  as the next Lanczos basis state. At the next step we obtain  $\phi_{N-4}$ , etc.

Expanding the wave function  $\Psi_E$  in series of oscillator functions,

$$\Psi_E = \sum_{n=0}^{\infty} a_{2n}(E) \phi_{2n}, \quad (7)$$

we reduce the free Schrödinger equation (2) to an infinite set of three-term recurrent relations (TRR)

$$T_{N,N-2} a_{N-2}(E) + (T_{NN} - E) a_N(E) + T_{N,N+2} a_{N+2}(E) = 0. \quad (8)$$

For positive energies  $E$ , these TRR have two linearly-independent solutions,  $S_N(E)$  and  $C_N(E)$ , which analytical expressions are well-known [9, 11, 12]. Only  $S_N(E)$  fits the physical TRR boundary condition,

$$T_{00} S_0(E) + (T_{02} - E) S_2(E) = 0, \quad (9)$$

while  $C_N(E)$  does not,

$$T_{00} C_0(E) + (T_{02} - E) C_2(E) \neq 0. \quad (10)$$

The solution  $S_N(E) \equiv S_{2n}(E)$  is related to the physical solution  $\Psi_E^0$  of the free Schrödinger equation (2) with sine-like asymptotics:

$$\sum_{n=0}^{\infty} S_{2n}(E) \phi_{2n} = \Psi_E^0 = \sqrt{\frac{2}{\pi}} kr j_l(kr) \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} \sin\left(kr - \frac{\pi l}{2}\right), \quad (11)$$

where  $k = \sqrt{2mE}/\hbar$  is the momentum,  $m$  is the reduced mass, and  $l$  is the orbital angular momentum. The solution  $C_N(E) \equiv C_{2n}(E)$  defines the function

$$\Psi_E^C = \sum_{n=0}^{\infty} C_{2n}(E) \phi_{2n} \quad (12)$$

which is regular at the origin and asymptotically coincides with the irregular solution

$$\Psi_E^{0irreg} = -\sqrt{\frac{2}{\pi}} kr n_l(kr) \quad (13)$$

of the free Schrödinger equation (2):

$$\Psi_E^C \xrightarrow{r \rightarrow \infty} \Psi_E^{0irreg} \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} \cos\left(kr - \frac{\pi l}{2}\right). \quad (14)$$

An arbitrary solution of the TRR (8) is a linear combination of the solutions  $S_N(E)$  and  $C_N(E)$ . Properly normalized solutions can be expressed as

$$a_N(E) = \cos \delta S_N(E) + \sin \delta C_N(E), \quad N = 0, 2, 4, \dots \quad (15)$$

The respective wave function defined through Eq. (7) behaves asymptotically as

$$\Psi_E \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} \sin\left(kr - \frac{\pi l}{2} + \delta\right), \quad (16)$$

where  $\delta$  is a scattering phase shift.

Instead of the TRR solutions  $S_N(E)$  and  $C_N(E)$ , one can use another pair of linearly independent solutions,  $C_N^+(E)$  and  $C_N^-(E)$ :

$$C_N^\pm(E) = C_N(E) \pm i S_N(E). \quad (17)$$

With the help of  $C_N^+(E)$  and  $C_N^-(E)$  we can define wave functions  $\Psi_E^+$  and  $\Psi_E^-$ ,

$$\Psi_E^\pm = \sum_{N=0}^{\infty} C_N^\pm(E) \phi_N, \quad (18)$$

with asymptotic behavior

$$\Psi_E^\pm \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} (\mp i)^l e^{\pm ikr}. \quad (19)$$

The functions  $\Psi_E^\pm$  are of a particular importance in the case of negative energies  $E$  when  $k = i\sqrt{2m|E|}/\hbar$  since they decrease asymptotically as bound state wave functions.

We suppose that the Hamiltonian  $H$  can be accurately enough approximated by

$$H = T + V^{N_{\max}}, \quad (20)$$

where  $T$  is a kinetic energy operator and  $V^{N_{\max}}$  is a potential energy in the  $P$  space spanned by oscillator states with excitation quanta  $N \leq N_{\max}$ , i. e. an infinite potential energy matrix in the oscillator basis is well-approximated by a truncated finite matrix which involves only oscillator states with excitation quanta  $N \leq N_{\max}$ :

$$V^{N_{\max}} = \sum_{n,m=0}^{N_{\max}/2} |\phi_{2n}\rangle \langle \phi_{2n}| V |\phi_{2m}\rangle \langle \phi_{2m}|. \quad (21)$$

The kinetic energy operator  $T$  is not truncated in Eq. (20). We note that in conventional shell model applications not only the potential energy  $V$  but the kinetic energy operator  $T$  is also truncated to the  $P$  space. Therefore the suggested approach can be used to extend the nuclear shell model Hamiltonian which is expected to improve the results obtained in conventional nuclear structure calculations. Note also that the potential energy matrix elements  $\langle \phi_N | V | \phi_M \rangle$  decrease with  $N$  and  $M$  when excitation quanta  $N$  and  $M$  are large enough. On the other hand, the diagonal  $T_{NN}$  and off-diagonal  $T_{N,N\pm 2}$  kinetic energy matrix elements increase linearly with  $N$  for large excitation quanta  $N$ . This different behavior of  $T$  and  $V$  matrix elements with excitation quanta justifies the approximation (20).

We use  $H$  to produce the Lanczos basis from above. When applied to the oscillator states  $\phi_N$  and  $\phi_{N+2}$  with large enough quanta  $N$  and  $N+2$ ,  $N > N_{\max}$ ,  $H$  has the same effect as the pure kinetic energy operator  $T$ . Therefore we reproduce with  $H$  the oscillator basis states  $\phi_{N-2}$ ,  $\phi_{N-4}$ , ...,  $\phi_{N_{\max}+2}$  in the  $Q$  space and the highest oscillator state in the  $P$  space  $\phi_{N_{\max}}$ . The matrix elements of  $H$  in our Lanczos basis in the  $Q$  space and the only off-diagonal matrix element  $H_{N_{\max}, N_{\max}+2}$  relating the  $P$  and  $Q$  spaces are equivalent to the kinetic energy matrix elements in the oscillator basis:

$$H_{NN} = T_{NN}, \quad (22)$$

$$H_{N,N-2} = H_{N-2,N} = T_{N,N-2}, \quad (23)$$

$$H_{N,N-m} = H_{N-m,N} = 0, \quad (24)$$

where  $N > N_{\max}$  and  $m > 2$ .

Starting from  $\phi_{N_{\max}}$ , the potential energy enters the Lanczos procedure. The Lanczos procedure mixes the oscillator states in the  $P$  space. The obtained matrix elements in the Lanczos basis  $H_{NN}$  and  $H_{N,N-2} = H_{N-2,N}$  with  $N \leq N_{\max}$  differ from  $T_{NN}$  and  $T_{N,N+2}$  respectively, all matrix elements  $H_{N,N-m} = H_{N-m,N}$  with any  $N$  and  $m > 2$  vanish. As a result, for the set of coefficients  $a_N(E)$  of the expansion (7) of the wave function  $\Psi_E$  in the Lanczos basis, we obtain a TRR

$$H_{N,N-2} a_{N-2}(E) + (H_{NN} - E) a_N(E) + H_{N,N+2} a_{N+2}(E) = 0. \quad (25)$$

This TRR should be supplemented by the boundary condition at  $N = 0$ :

$$H_{00} a_0(E) + (H_{02} - E) a_2(E) = 0. \quad (26)$$

The TRR (25) is infinite, i. e.  $N$  can take any even positive value.

To find the solutions of TRR (25), we assign any non-zero value to  $a_0(E)$  and obtain  $a_2(E)$  using the boundary condition (26), with known  $a_0(E)$  and  $a_2(E)$  we calculate  $a_4(E)$  using TRR (25), next we calculate  $a_6(E)$  by means of TRR (25), etc.

In the case of scattering states ( $E > 0$ ), the expansion coefficients  $a_N(E)$  with  $N \geq N_{\max}$  should be proportional to the r.h.s. of Eq. (15). Knowing the values of two expansion coefficients in the  $Q$  space, say,  $a_N(E)$  and  $a_M(E)$  with  $M \neq N$ ,  $M \geq N_{\max}$ ,  $N \geq N_{\max}$ , we obtain the scattering phase shift as

$$\tan \delta = -\frac{a_M(E) S_N(E) - a_N(E) S_M(E)}{a_M(E) C_N(E) - a_N(E) C_M(E)}. \quad (27)$$

Expression (27) can be easily derived from Eq. (15).

In the case of bound states ( $E < 0$ ), the coefficients  $a_N(E)$  in the  $Q$  space are linear combinations of  $C_N^+(E)$  and  $C_N^-(E)$ . The solution  $C_N^-(E)$  exponentially increases with  $N$  while  $C_N^+(E)$  exponentially decreases with  $N$  in the limit of  $N \rightarrow \infty$ . We need to find numerically a negative energy  $E$  which provides the decreasing behavior of  $a_N(E)$  with  $N$ . This is the bound state energy associated with the  $S$ -matrix pole which improves the pure variational calculation in the finite oscillator basis.

We use the neutron-nucleus elastic scattering as an example to demonstrate how this Lanczos formalism can be used for a description of nuclear reactions. In this case, we construct a conventional shell model Hamiltonian  $H^{A+1}$  of the  $(A+1)$ -body system which includes all oscillator states with excitation quanta  $N \leq N_{\max}^{A+1}$ . The Hamiltonian  $H^{A+1}$  acts in the  $P$  space and describes the relative kinetic energy of all  $A+1$  particles and interactions between them.

We need to define also a channel Hamiltonian

$$h^{ch} = T^{n-A} + H^A \quad (28)$$

describing scattering of the neutron on the  $A$ -body nucleus. The Hamiltonian  $h^{ch}$  includes a kinetic energy operator of the relative  $n-A$  motion  $T^{n-A}$  and a truncated Hamiltonian of the  $A$ -body subsystem

$$H^A = T^A + V^A. \quad (29)$$

The operator  $T^A$  describes the relative kinetic energy of  $A$  particles and interaction  $V^A$  between them. The operator  $H^A$  is defined in the  $A$ -body relative motion oscillator states with excitation quanta  $N \leq N_{\max}^A$ . The wave function  $\Psi^A$  describes the internal motion of the  $A$ -body subsystem in the ground state,

$$H^A \Psi^A = E^A \Psi^A. \quad (30)$$

The  $A$ -body nucleus is supposed to be bound, and hence  $E^A < 0$ .

We need the channel Hamiltonian to extend the action of the  $(A+1)$ -body Hamiltonian  $H^{A+1}$  on the subspace of the  $(A+1)$ -body  $Q$  space associated with the motion in our channel. We note that the channel Hamiltonian  $h^{ch}$  acts not only in the  $Q$  space but has also some terms acting in the  $P$  space already included in  $H^{A+1}$ . Therefore we cannot add  $h^{ch}$  to  $H^{A+1}$ , we should first project out  $P$ -space terms in  $h^{ch}$  to avoid double counting. However we should preserve the terms of  $h^{ch}$  providing a coupling between the  $P$  and  $Q$  spaces. Therefore we define the projected channel Hamiltonian as

$$H^{ch} = P h^{ch} Q + Q h^{ch} P + Q h^{ch} Q, \quad (31)$$

where  $P$  is a projector on the  $P$  space,  $Q$  is a projector on the  $Q$  space and

$$Q + P = 1. \quad (32)$$

Now we can define the Hamiltonian describing our system as

$$H = H^{A+1} + H^{ch}. \quad (33)$$

We construct the Lanczos basis from above starting from channel states  $\phi_N \Psi^A$  and  $\phi_{N+2} \Psi^A$ . Here  $\phi_N$  and  $\phi_{N+2}$  are oscillator functions of relative  $n-A$  motion

with  $N$  and  $N + 2$  quanta respectively. It is supposed that  $N > N_{\max}^{A+1}$  where  $N_{\max}^{A+1} = N_{\max}^{A+1} + N_{\text{tot}}^{A+1} - N_{\text{tot}}^A$  and  $N_{\text{tot}}^A$  and  $N_{\text{tot}}^{A+1}$  are the *total* oscillator quanta in the lowest configuration of the  $A$ -body and  $(A + 1)$ -body systems respectively. Clearly our states belong to the  $Q$  space, and applying the Hamiltonian  $H$  to them is equivalent to the application of the channel Hamiltonian  $H^{ch}$  to them. Applying  $H^{ch}$  to  $\phi_N \Psi^A$  we obtain successively Lanczos states  $\phi_{N-2} \Psi^A$ ,  $\phi_{N-4} \Psi^A$ , ...,  $\phi_{N_{\max}^{A+1}} \Psi^A$ . The respective TRR is

$$T_{N,N-2}^{n-A} a_{N-2}(E) + (T_{NN}^{n-A} - E^{A+1} + E^A) a_N(E) + T_{N,N+2}^{n-A} a_{N+2}(E) = 0, \quad N > N_{\max}^{A+1}. \quad (34)$$

Here  $E^{A+1}$  is the total energy of the  $(A + 1)$ -body system, and

$$E^{n-A} = E^{A+1} - E^A \quad (35)$$

is a kinetic energy of the relative  $n-A$  motion.

Up to this point all Lanczos states  $\phi_{N-2} \Psi^A$ ,  $\phi_{N-4} \Psi^A$ , ...,  $\phi_{N_{\max}^{A+1}} \Psi^A$  were obtained analytically. Starting from the Lanczos vector  $\phi_{N_{\max}^{A+1}} \Psi^A$ , the complete  $(A + 1)$ -particle  $P$ -space Hamiltonian  $H^{A+1}$  is involved in the Lanczos procedure. All the remaining Lanczos iterations look like the conventional Lanczos procedure used in standard shell model codes with a specific pivot vector  $\phi_{N_{\max}^{A+1}} \Psi^A$ . Note however that the Hamiltonian (33) involves an additional term  $H^{ch}$  [see Eq. (31)] and the pivot vector  $\phi_{N_{\max}^{A+1}} \Psi^A$  generally includes a few terms with excitation quanta  $N > N_{\max}^{A+1}$  when the  $A$ -body wave function  $\Psi^A$  is a mixture of  $A$ -body components  $\Psi_M^A$  with excitation oscillator quanta  $M = 0, 2, 4, \dots, N_{\max}^A$ :

$$\Psi^A = \alpha_0 \Psi_0^A + \alpha_2 \Psi_2^A + \alpha_4 \Psi_4^A + \dots + \alpha_{N_{\max}^A} \Psi_{N_{\max}^A}^A. \quad (36)$$

By means of the Lanczos algorithm we obtain TRR

$$H_{N,N-2}^{A+1} a_{N-2}(E) + (H_{NN}^{A+1} - E^{A+1}) a_N(E) + H_{N,N+2}^{A+1} a_{N+2}(E) = 0, \quad N \leq N_{\max}^{A+1}, \quad (37)$$

where

$$H_{N_{\max}^{A+1}, N_{\max}^{A+1}+2}^{A+1} = T_{N_{\max}^{A+1}, N_{\max}^{A+1}+2}^{n-A}. \quad (38)$$

The Lanczos iterations will mix all many-body states in the  $(A + 1)$ -body system. Generally the number of Lanczos iterations can be as large as the dimensionality of the  $(A + 1)$ -body  $P$  space.  $N$  in the TRR (37) does not have a meaning of oscillator quanta, it is used only to distinguish various Lanczos basis states and can take negative values. After some reasonable number of Lanczos iterations we should stop and solve the combined set of TRR (34) and (37) for bound or scattering states by the methods discussed above.

The proposed approach can be extended to describe the scattering of charged particles. The Coulomb interaction between all protons should be, of course, included in  $H^{A+1}$ . The problem is how to account for the long-range Coulomb interaction between two colliding clusters  $V^{Coulomb}$  in the channel Hamiltonian  $H^{ch}$ . This can be done by two different ways.

One of the respective techniques has been suggested in Ref. [13] and was widely used in various applications within Resonating Group Method by Kiev group (see, e. g., Ref. [14]). In this case, we explicitly include the Coulomb interaction between two colliding clusters  $V^{Coulomb}$  in the channel Hamiltonian  $H^{ch}$ . At large excitation quanta, the operator  $T^{n-A} + V^{Coulomb}$  can be accurately approximated by a tridiagonal matrix [13]. Therefore at large excitation quanta we can still use TRR (34) with

matrix elements  $T_{NN}^{n-A}$  corrected by the Coulomb interaction. However the Coulomb interaction starts mixing  $P$  and  $Q$  space states at larger values of excitation quanta than the strong nucleon-nucleon interaction. Therefore Lanczos iterations will involve the  $P$  space states at larger values of excitation quanta than in the case of neutron-nucleus scattering. This is equivalent to adding a few additional vectors from the  $Q$  space to a huge number of basis states in the  $P$  space in the conventional diagonalization of the shell model Hamiltonian by means of Lanczos iterations.

Another method for calculating of Coulomb-distorted scattering phase shifts was suggested in Ref. [12] and further verified in Ref. [15]. The idea of this method is that we can cut the Coulomb interaction at some distance  $r_b$  from the origin and to use the above technique to calculate the scattering phase shifts in this system which does not have a long-range interaction any more. The Coulomb-distorted scattering phase shifts should be recalculated from the obtained phase shifts by means of a simple analytical formula (see Refs. [12, 15] for details). If the cutoff distance  $r_b$  coincides with the classical turning point of the highest single-particle oscillator state involved in the  $P$  space, the matrix elements of the Hamiltonian  $H^{A+1}$ , the most complicated part of the total Hamiltonian (33), are unaffected (or only very slightly affected) by the Coulomb potential cutoff due to the fast decrease of oscillator functions beyond the classical turning point. The Coulomb interaction can be omitted in the  $Q$ -space part of the channel Hamiltonian  $H^{ch}$ ; however it may be needed to account for the Coulomb interaction in calculation of some of the  $H^{ch}$  matrix elements coupling the  $P$  and  $Q$  spaces.

We hope that the suggested Lanczos approach will be efficient in the *ab initio* description of various nuclear reactions with light nuclei and for improving results for bound state energies obtained in shell model calculations.

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