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Coupled-channel continuum eigenchannel basis

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The goal of this Letter is to calculate bound, resonant and scattering states in the coupled-channel formalism without relying on the boundary conditions at large distances. The coupled-channel solution is expanded in eigenchannel bases i.e. in eigenfunctions of diagonal Hamiltonians. Each eigenchannel basis may include discrete and discretized continuum (real or complex energy) single particle states. The coupled-channel solutions are computed through diagonalization in these bases. The method is applied to a few two-channel problems. The exact bound spectrum of the Poeschl–Teller potential is well described by using a basis of real energy continuum states. For deuteron described by Reid potential, the experimental energy and the S and D contents of the wave function are reproduced in the asymptotic limit of the cutoff energy. For the Noro–Taylor potential resonant state energy is well reproduced by using the complex energy Berggren basis. It is found that the expansion of the coupled-channel wave function in these eigenchannel bases requires less computational efforts than the use of any other basis. The solutions are stable and converge as the cutoff energy increases.

1. Introduction

Considerable amount of effort is devoted all around the world to studying the properties of unstable nuclei [1]. Because of this, new theoretical approaches, which takes into account the continuum explicitly, is called for revealing their properties. The coupled-channel method is a very powerful formalism for studying the structure of both strongly-bound nuclei [2,3] and loosely-bound nuclei [4]. Here we propose a way to calculate the coupled-channel solutions in which all bound and continuum (resonant and non-resonant continuum) states are treated on the equal footing.

Complex eigenenergies, i.e. Gamow [5] or Siegert [6] states were calculated using the Green's function approach in momentum space in Refs. [7,8] for coupled channel problems. Gamow states for realistic deformed potentials were calculated first in Ref. [9] by solving the logarithmic derivative of the coupled equations with outgoing boundary condition. In Refs. [10] and [11] the coupled-channel Schrödinger equation with outgoing wave boundary condition was used to study the proton decay states in a rare-earth nucleus.

The complex scaling method has been successfully combined with the coupled-equation formalism to calculate resonances [12–15]. The extension of the Gamow Shell Model [16,17] to reaction problems in the framework of coupled-channel formalism was recently implemented in Ref. [18], where the low-lying states of ^{7}Li were calculated. The result of the direct integration of coupled equations was compared with that of the Berggren [19] expansion for the calculation of bound states of dipolar molecules in Ref. [20]. A full complex energy representation was used in Ref. [21] for the calculation of the Isobaric Analog State by coupled Lane equations. The present Letter extends the use of the continuum bases to the inelastic processes in coupled-equation systems and to the calculation of scattering states.

The method presented in this Letter allows the calculation of bound, resonances and scattering states in coupled systems on the same footing. All these states may be found by a single diagonalization simultaneously. Each channel wave function is expanded in an optimized basis set defined by the eigensolution of the corresponding uncoupled Schrödinger equation, that is the meaning of eigenchannel bases. Since this method prescinds from explicit boundary conditions, it might be useful for dealing with Coulomb breakup problems that appear, for instance, in electron-impact ionization [22] or in breakup reactions important in astrophysics [23,24] or in studying the three-body Coulomb breakup reaction of ^{11}Li [25].

In Section 2 we develop the method in which the coupled Schrödinger equations are expanded in the continuum bases of uncoupled channels. The first application of the method is done in

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Section 3. It solves the problem of the exactly solvable two-channel Poeschl–Teller potential. This works as a test case. It shows the reliability of the method and it shows the relative importance of the continuum for the deep and for the loosely bound states. In Section 4, the method is applied to the bound and scattering states of the deuteron. The last application in Section 5 is devoted to the simultaneous calculation of bound and resonant states. The outline for the next applications and some remarks are given in the last Section 6.

2. Formalism

Let us denote by H the Hamiltonian which describes a collision between two nuclei being in bound states (a, A). We split H into two parts: (1) the Hamiltonian H'_α that is left when the two initial fragments are far away from each other and (2) $V = \sum_{i\in a, j\in A} V_{ij}$ which includes the projectile (a)–target (A) interaction. Changing in H'_α to relative coordinates in each fragments and then changing to the relative coordinates between the fragments [26], we end up with $H'_\alpha = H_\alpha + T$ (we have set the centroid kinetic energy to zero), where $T = -\frac{\hbar^2}{2\mu}\nabla_r^2$ is the relative kinetic energy, μ is the projectile–target reduced mass, and $H_\alpha = H_a + H_A$, where H_a and H_A are the intrinsic Hamiltonians of the projectile and target, respectively. Then, the total Hamiltonian reads $H = H_\alpha + T + V$. The residual interaction $V = V_\mathrm{d} + V_\mathrm{od}$ is split into a diagonal part V_d and an off-diagonal one V_od [27]. The eigenfunction $\psi_{J^\pi M}$ of H is expanded into different channels using the channel basis functions $\Phi_\alpha^{J^\pi M}$ defined as

$$\Phi_\alpha^{J^\pi M}(\hat{r}, a, A) = \big[\mathcal{Y}^j_{lJ_a}(\hat{r}, a)\phi_{J_A}(A)\big]_{J^\pi M} \tag{1}$$

where $\alpha = \{(lJ_a)j, J_A\}$, $\mathcal{Y}^{jm}_{lJ_a}(\hat{r}, a) = [Y_l(\hat{r})\phi_{J_a}(a)]_{jm}$, $H_a\phi_{J_aM_a} = \varepsilon_a\phi_{J_aM_a}$, $H_A\phi_{J_AM_A} = \varepsilon_A\phi_{J_AM_A}$, $H_\alpha\phi_\alpha = \varepsilon_\alpha\phi_\alpha$, and $\varepsilon_\alpha = \varepsilon_a + \varepsilon_A$.

Then,

$$\psi_{J^\pi M}(\mathbf{r}, a, A) = \sum_{\alpha'} \frac{u_{\alpha'}^{J^\pi M}(r)}{r}\Phi_{\alpha'}^{J^\pi M}(\hat{r}, a, A) \tag{2}$$

Substituting the channel expansion (2) into the Schrödinger equation $H\psi_{J^\pi M}(\mathbf{r}, a, A) = E\psi_{J^\pi M}(\mathbf{r}, a, A)$ and projecting into a certain channel Φ_α we get (omitting the index $J^\pi M$)

$$(\varepsilon_\alpha + h_\alpha - E)u_\alpha(r) + \sum_{\alpha'\neq\alpha} V_{\alpha\alpha'}(r)u_{\alpha'}(r) = 0 \tag{3}$$

where we have separated the diagonal matrix elements $V_{\alpha\alpha}$ and we have defined the single particle channel Hamiltonians,

$$h_\alpha = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu}\frac{l_\alpha(l_\alpha+1)}{r^2} + V_{\alpha\alpha} \tag{4}$$

with $V_{\alpha\alpha'} = \langle\Phi_\alpha|V|\Phi_{\alpha'}\rangle_{\hat{r}aA}$, where the suffix indexes mean integration over the angular coordinate $\hat{r}$ of the relative motion and the internal coordinates of the projectile a and target A nuclei, respectively. Notice that the structures of Eqs. (3) and (4) are the same as that of Eq. (25) of Ref. [27].

Although, in principle any complete set of states will allow the computation of the interaction matrix elements, in practice, a judicious choice of the basis states will minimize the number of matrix elements to be calculated and reduce the computation time needed. Here we use the diagonal part V_d of the residual interaction $V = V_\mathrm{d} + V_\mathrm{od}$ to generate the basis. Notice that the basis does not correspond to the one generated without residual interaction $V = 0$.

In the next step, we expand the wave functions $u_\alpha(r)$ in each channel in the basis generated by its own channel Hamiltonian h_α

$$h_\alpha u^{(0)}_{\alpha,n}(r) = \varepsilon^{(0)}_{\alpha,n}u^{(0)}_{\alpha,n}(r) \tag{5}$$

$$u_{\alpha'}(r) = \sum_{n'} c_{\alpha',n'}u^{(0)}_{\alpha',n'}(r) \tag{6}$$

where the summation includes integration over the continuum part of the spectrum of h_α.

Replacing the expansion of $u_\alpha(r)$ (Eq. (6)) in Eq. (3) and projecting over $u^{(0)}_{\alpha,n}(r)$ we get

$$\sum_{\alpha'=1}^{N}\sum_{n'=1}^{M_{\alpha'}}\big[\big(\varepsilon_\alpha + \varepsilon^{(0)}_{\alpha,n} - E\big)\delta_{\alpha\alpha'}\delta_{nn'} + (1-\delta_{\alpha\alpha'})V_{\alpha n,\alpha'n'}\big]c_{\alpha',n'} = 0 \tag{7}$$

where N denotes the number of channels and M_α is the number of single particle basis states for the channel α.

The coupled equations problem in Eq. (7) can be transformed to an eigenvalue problem with a sparse symmetric matrix of dimension $M = M_1 + \cdots + M_N$ by defining the index $i = \{\alpha, n\}$ of the following order $i = \{(\alpha_1, 1), (\alpha_1, 2), \ldots, (\alpha_1, M_1), (\alpha_2, 1), \ldots, (\alpha_2, M_2), \ldots, (\alpha_N, 1), \ldots, (\alpha_N, M_N)\}$. The matrix is diagonal in each channel block α of dimension M_α. The diagonal elements in each channel block α are given by $\varepsilon_\alpha + \varepsilon^{(0)}_{\alpha,n} - E$, with $n = \{1, 2, \ldots, M_\alpha\}$. The matrix elements between different channels contain only the interaction $V_{ii'}$ given by

$$V_{\alpha n,\alpha'n'} = \int dr\, u^{(0)}_{\alpha,n}(r)V_{\alpha\alpha'}(r)u^{(0)}_{\alpha',n'}(r)$$

Using the basis generated by the diagonal part of the channel interaction one can save the calculation of $M_\mathrm{saved} = \sum_{\alpha=1}^{N}\frac{M_\alpha(M_\alpha+1)}{2}$ interaction matrix elements. The number of these matrix elements increases rapidly as the number of open channels N and the dimension of the basis M_α increase.

There are two advantages of using a basis expansion method instead of using the asymptotic boundary conditions. The matrix diagonalization does not diverge even if the coupling terms are large. This might happen in the direct numerical integration [3] of the coupled equations. The matrix diagonalization does not face any instability of the numerical integration of the coupled equations. The disadvantage of using a basis expansion is that one has to deal with the completeness problem of the basis. A difficulty of using the basis expansion is that one needs an efficient and accurate method to solve the single particle Schrödinger equation, that is, to find real and complex poles as well as the real and complex energy scattering states. The real and complex energy scattering states were calculated by using a piecewise perturbation method [28]. The code implements the so called Ixaru's method [29]. The real and complex energy poles were also calculated by using a modified version of the program [28]. This version has a higher precision than the GAMOW code [30], which however is more flexible.

3. Application to the Poeschl–Teller potential: bound state calculation using bases composed of bound states and real energy continuum

In this section we compare the exact solution of the two-channel Poeschl–Teller potential with the numerical solution using the same eigenchannel bases for both channels. The bases are composed of bound and real energy scattering states.

Let us consider the Schrödinger equations with two channels and with $\hbar = 2\mu = 1$, $l_1 = l_2 = 0$, $\varepsilon_1 = \varepsilon_2 = 0$ and $V_{\alpha\alpha'}(r)$ given by Ixaru [31]

$$V_{\alpha\alpha'}(r) = \begin{pmatrix} V_\mathrm{d}(r) & V_\mathrm{od}(r) \\ V_\mathrm{od}(r) & V_\mathrm{d}(r) \end{pmatrix} \tag{8}$$