The Two Center Oscillator Potential with Finite Depth*

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It is suggested to diagonalize the Hamilton operator of a two- or more center shell model in terms of oscillator functions concentrated around the individual centers. The method is applied to the case of a two center oscillator with finite depth.

I. Introduction

In the theory of nuclear fission and heavy ion scattering the shell effects to the potential energy surface are calculated with the aid of two center shell models [1–3]. Only for a restricted class of single particle potentials with two and more centers analytical eigensolutions can be obtained, e. g. for the symmetric two-center oscillator with infinite depth [1, 4].

Already when one includes the l^2- and $\boldsymbol{l}\cdot\boldsymbol{s}$-terms in the symmetric two-center oscillator, the single particle Hamilton operator has to be numerically diagonalized in order to obtain the eigensolutions. Depending on the basis functions used in the diagonalization procedure we distinguish between three different methods. As basis functions the following three sets can be used: a) the solutions of a deformed harmonic oscillator potential around the common center of mass [5], b) the solutions of the asymmetric two center oscillator [2], and c) the solutions of harmonic oscillator potentials around the individual centers [4, 6]. Whereas the sets of functions in a) and b) form an orthogonal set this is not the case with the oscillator functions around different centers in c). Therefore, in applying the third method the basis set has first to be orthogonalized. This disadvantage is compensated by the advantage that the matrix elements of the various single particle Hamilton operators can be analytically calculated [7]. Also the basis wave functions have the right asymptotic behaviour for large center distances which is convenient for scattering problems.

The purpose of this paper is to describe the third method in Sect. II by which not only two but also more center problems can be treated numerically quite easily. The method will be applied to the two center oscillator with infinite and finite depth in Section III.

II. The Method

2.1 General Case

Let us state the problem: In general a single particle Hamilton operator H is given in which the potential has minima around the centers at $\boldsymbol{R}_i$:

$$H = p^2/2\,M + V(\boldsymbol{r}, \boldsymbol{p}, \boldsymbol{s}, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_N) \qquad (1)$$

where $\boldsymbol{s}$ denotes the spin vector of the nucleon. Examples for V are the two-center oscillator potentials shown in Fig. 1 or the three-center oscillators investigated by Bergmann and Scheefer [4]. For large separations of the centers, i. e. $|\boldsymbol{R}_i - \boldsymbol{R}_j| \to \infty$, the potential approaches the sum of single-particle potentials around the individual centers.

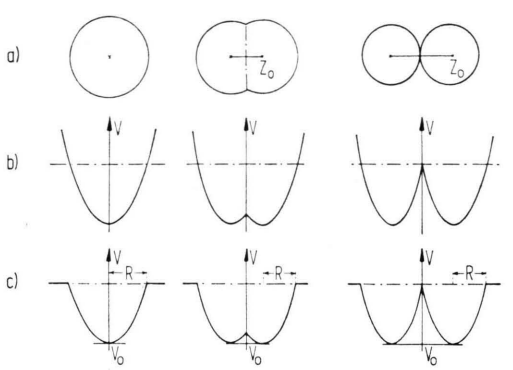

Fig. 1. Shapes of the nuclear system and the potential for various distances. a) Equipotential surfaces. b) Two-center oscillator potential with infinite depth. c) Two-center oscillator potential with finite depth.

To find the bound states of

$$H\,\psi'_n = E_n\,\psi'_n \qquad (2)$$

we suggest a diagonalization of the Hamiltonian with a very simple set of basic functions, namely with oscillator wave functions.

$$\psi'_{\lambda i}(\boldsymbol{r}) = \varphi_{n_x}[(x - R_{ix})/a_{ix}] \cdot \varphi_{n_y}[(y - R_{iy})/a_{iy}] \cdot \varphi_{n_z}[(z - R_{iz})/a_{iz}] \qquad (3)$$

where $\lambda = (n_x, n_y, n_z)$ and $i = 1, \ldots, N$.

The solutions of the one-dimensional harmonic oscillator are given by [8]:

$$\varphi_n(x) = \frac{1}{\sqrt{\pi^{1/2}\, 2^n\, n!}} \exp\{-x^2/2\}\, H_n(x)\,. \tag{4}$$

The oscillator lengths $a_{ix} = \sqrt{\hbar/M\,\omega_{ix}}$, a_{iy} and a_{iz} are arbitrary and can be optimally adapted to the potential V in the vicinity of the centers. The basis set in Eq. (3) is overcomplete, i. e.

$$\psi_{\lambda i} \to \psi_{\lambda j} \quad \text{for} \quad |\boldsymbol{R}_i - \boldsymbol{R}_j| \to 0$$

and nonorthogonal with respect to different centers.

$$\langle \mu\, j \,|\, \lambda\, i\rangle \neq 0 \quad \text{for} \quad i \neq j\,. \tag{5}$$

The eigenenergies of Eq. (2) are the solutions of the eigenvalue equation:

$$\| \langle \mu\, j \,|\, H \,|\, \lambda\, i\rangle - E \langle \mu\, j \,|\, \lambda\, i\rangle \| = 0\,. \tag{6}$$

For solving Eq. (6) we propose a two-step procedure. First the basis functions (3) are orthonormalized:

$$|\, m\rangle = \sum_{\lambda, i} A_{m,\lambda i}\, |\, \lambda\, i\rangle \tag{7}$$

with $$\langle m \,|\, n\rangle = \delta_{mn}\,.$$

Then we apply an usual diagonalization procedure to solve the transformed eigenvalue equation:

$$\| \sum_{\mu j} \sum_{\lambda i} A_{m,\mu j}\, A_{n,\lambda i}\, \langle \mu\, j \,|\, H \,|\, \lambda\, i\rangle - E\, \delta_{mn} \| = 0\,. \tag{8}$$

2.2 *Symmetrical Two-Center Potentials with Rotational Symmetry*

To illustrate the method we consider the special case, where the two-center potential is rotationally symmetric around the z-axis and additionally symmetric with respect to the origin at $z = 0$. The potential centers are at $z = \pm z_0$. Examples of such potentials [1] will be discussed in the next sections.

Because of the rotational symmetry the oscillator wave functions (3) have the following ϱ- and φ-dependence in terms of Laguerre polynomials [1]:

$$G_{n\varrho,m}(\varrho, \varphi) = \frac{(-1)^{\frac{m+|m|}{2}}}{a_\varrho} \frac{e^{im\varphi}}{\sqrt{2\pi}}\, g_{n_\varrho, |m|}(\varrho/a_\varrho)$$

with $$g_{\alpha\beta}(x) = \sqrt{\frac{2\,\alpha!}{(\alpha+\beta)!}}\, x^\beta\, L_\alpha^{\,\beta}(x^2) \cdot \exp\{-x^2/2\}$$

and $$a_\varrho = \sqrt{\hbar/M\,\omega_\varrho};\; n_\varrho = 0, 1, 2, \ldots, \quad m = 0, \pm 1, \pm 2, \ldots \tag{9}$$

Since the potential is also symmetric with respect to $z = 0$, the eigenfunctions have good parity. Therefore, we construct normalized functions with parity $P = \pm 1$ by superposing two corresponding oscillator wave functions (3) [9].

$$f_{n,\mathrm{p}}(z) = \frac{1}{\sqrt{2\, a_z\, M_{n,\mathrm{p}}}} [\varphi_n((z - z_0)/a_z) + P(-1)^n \cdot \varphi_n((z + z_0)/a_z)] \tag{10}$$

with $$a_z = \sqrt{\hbar/M\,\omega_z}\,.$$

The normalization constant can be obtained from the overlap integrals ($x_0 = z_0/a_z$):

$$\int_{-\infty}^{\infty} f_{m,\mathrm{p}}\, f_{n,\mathrm{p}}\, \mathrm{d}z = \frac{1}{\sqrt{M_{m\mathrm{p}}\, M_{n\mathrm{p}}}} \{\delta_{mn} + P(-1)^m\, I_{mn}(x_0)\} \tag{11}$$

where I_{mn} is given by [9] (see Appendix A):

$$I_{mn} = \int_{-\infty}^{\infty} \varphi_m(x + x_0)\, \varphi_n(x - x_0)\, \mathrm{d}x \tag{12}$$

$$= (-1)^n \sqrt{m!\, n!\, 2^{m+n}}\, e^{-x_0^2} \sum_{t=0}^{\mathrm{Min}(m,n)} \frac{(-1)^t\, 2^{-t}\, x_0^{\,m+n-2t}}{t!\,(m-t)!\,(n-t)!}$$

In the special case $m = n$ it results:

$$M_{n,\mathrm{p}} = 1 + P(-1)^n\, e^{-x_0^2} \sum_{s=0}^{n} \binom{n}{s} \frac{1}{s!}\, (-2\, x_0^2)^s\,. \tag{13}$$

Asymptotically the functions (10) approach the solutions of the one dimensional two-center oscillator. For $z_0 \to 0$ all functions with a factor $P \cdot (-)^n = -1$ would vanish if no normalization constant is multiplied. Including the normalization these functions approach a linear combination of two neighbouring oscillator functions of the class $P \cdot (-)^n = 1$.

For $z_0 \to 0$:

$$P(-1)^n = 1\,, \quad f_{n,\mathrm{p}} = \varphi_n(z/a_z)/\sqrt{a_z}\,, \tag{14}$$

$$P(-1)^n = -1\,, \; f_{n,\mathrm{p}} = -\sqrt{\frac{2\, a_z}{2n+1}}\, \frac{\mathrm{d}}{\mathrm{d}z}\, \varphi_n(z/a_z) = \frac{1}{\sqrt{(2n+1)\, a_z}} [\sqrt{n+1}\, \varphi_{n+1}(z/a_z) - \sqrt{n}\, \varphi_{n-1}(z/a_z)]\,.$$

Since the wave functions (9) are already orthogonal, we have only to orthonormalize the z-dependent functions (10). For that we use the Schmidt procedure in which the orthonormalized functions F_k are constructed as follows [10]:

$$F_k(z) = \sum_{n=0}^{k} a_{kn}\, f_n(z) = \frac{1}{\sqrt{N_k}} \left(f_k - \sum_{i=0}^{k-1} F_i \int_{-\infty}^{+\infty} F_i\, f_k\, \mathrm{d}z\right) \tag{15}$$

with the coefficients:

$$a_{kn} = \frac{1}{\sqrt{N_k}} \left[\delta_{kn} - (1-\delta_{kn}) \sum_{i=n}^{k-1} a_{in} \int_{-\infty}^{+\infty} F_i f_k \, dz\right] \quad (15\,a)$$

and

$$N_k = 1 - \sum_{i=0}^{k-1} \left(\int_{-\infty}^{+\infty} F_i f_k \, dz\right)^2 . \quad (15\,b)$$

All the formulas are separately valid for $P = \pm 1$. The integrals can be written as sums over the overlap integral given in Equation (11).

Because of the overcompleteness of the set of functions f_n for $z_0 \to 0$, care must be taken in the range of small values of z_0. Two ways are possible: a) Instead of using the functions (10) one diagonalizes the two-center Hamiltonian with one-center oscillator wave functions concentrated at $z = 0$: $F_n = \varphi_n$. b) When we apply the formulas (15) for $z_0 \to 0$, the normalization constant N_k, Eq. (15 b), approaches zero in all cases where the wave function f_k becomes linearly dependent on the functions f_i, resp. F_i, with $i < k$ [see Eq. (15 b)]. This means, no function F_k can be constructed which is orthogonal to the F_i with $i < k$. Then the function f_k is superfluous in the basis set (15) and may be disregarded. In practical calculations one gives a lower limit $\varepsilon \ll 1$ for N_k. If the normalization constant N_k results smaller than this limit ($N_k < \varepsilon$), the coefficients a_{kn} are set zero, respectively $F_k = 0$.

Finally we end with an orthonormal basis set which is suitable to diagonalize symmetric two-center Hamiltonians:

$$\psi_{k,P,n_\varrho,m} = F_{k,P}(z) \cdot G_{n_\varrho,m}(\varrho, \varphi) . \quad (16)$$

III. Application to Symmetric Two-Center Hamilton Operators

In the following we apply the formalism of the preceding section to symmetric two-center Hamilton operators with oscillator potentials of infinite and finite depth.

3.1 Two-Center Oscillator Potential with Infinite Depth [1]

The Hamiltonian operator has the following form in the simplest version, where one disregards $\boldsymbol{l}\boldsymbol{s}$- and l^2-terms [1].

$$H = -\frac{\hbar^2}{2M} \Delta + \frac{M}{2} \left[\omega_\varrho^2 \varrho^2 + \omega_z^2 (|z| - z_0)^2\right] . \quad (17)$$

Since the eigensolutions of H can be analytically found, the example is suitable to test the method of the previous section. The eigensolutions are given according to Ref. [1] as:

$$\psi = G_{n_\varrho,m}(\varrho, \varphi) \cdot v_{n_z,P}(z) \quad (18)$$

with $(x = z/a_z)$:

$$v_{n_z,P} = N_{n_z}[\theta(x) + P\,\theta(-x)] \exp\{-\tfrac{1}{2}(|x| - x_0)^2\} \cdot U[-\tfrac{1}{2} n_z, \tfrac{1}{2}, (|x| - x_0)^2] .$$

Here we denote the normalization constant by N_{n_z}, the step function by θ, the parity by $P = \pm 1$, and Kummer's confluent hypergeometric function by U. The eigenvalues can be written:

$$E = \hbar\omega_\varrho (2n_\varrho + |m| + 1) + \hbar\omega_z (n_z + \tfrac{1}{2}) . \quad (19)$$

The noninteger values n_z are functions of x_0 and solve the equations:

$$P = -1: U(-\tfrac{1}{2} n_z, \tfrac{1}{2}, x_0^2) = 0 , \quad (20)$$

$$P = 1: \quad \frac{d}{dx_0} \exp\{-\tfrac{1}{2} x_0^2\} U(-\tfrac{1}{2} n_z, \tfrac{1}{2}, x_0^2) = 0 .$$

After this review of the analytical solution, we solve the eigenvalue problem with the diagonalization procedure. The Hamilton operator separates into (ϱ, φ)- and z-dependent parts. Since the (ϱ, φ)-dependence is already solved by the functions $G_{n_\varrho,m}$, we need only to diagonalize the z-dependent part of (17). For that we calculate the energy matrix h_{ki} with the orthonormalized functions F_k of Equation (15).

$$h_{ki} = \int_{-\infty}^{+\infty} F_k(z)\, h(z)\, F_i(z) \, dz \quad (21)$$

with

$$h(a_z x) = \frac{\hbar\omega_z}{2} \left(-\frac{d^2}{dx^2} + (|x| - x_0)^2\right) .$$

In terms of the oscillator functions φ_n we obtain:

$$h_{ki} = \frac{\hbar\omega_z}{2} \sum_{m,n} \frac{a_{km}\, a_{in}}{\sqrt{M_{mp}\, M_{np}}} \cdot U_{mn} \quad (22)$$

with the matrix (see Appendix A):

$$\begin{aligned} U_{mn}(x_0) &= \int_{-\infty}^{+\infty} [\varphi_m(x - x_0) + P(-1)^m \varphi_m(x + x_0)] \\ &\quad \cdot [2n + 1 + 2x_0(x - |x|)]\, \varphi_n(x - x_0)\, dx \\ &= (2n+1)[\delta_{mn} + P(-1)^m I_{mn}] \quad (22\,a) \\ &\quad - \frac{4x_0(-1)^{m+n} e^{-x_0^2}}{\sqrt{2^{n+m}\, n!\, m!\, \pi}} \left(\sum_s \binom{m}{s} \binom{n}{s} \right. \\ &\quad \cdot 2^s\, s!\, H_{n+m-2s-2}(x_0) \\ &\quad + (-1)^m P \sum_{s,t} \binom{m}{s} \binom{n}{t} 2^{s+t-1} \left(\frac{s+t}{2}\right)! \\ &\quad \left. \cdot H_{m-s}(-x_0) H_{n-t}(x_0) \right) . \end{aligned}$$

The functions I_{mn} are defined in Equation (12). The Hermite polynomials satisfy the recurrence formula [8]:

$$\text{with} \qquad H_{n+1} = 2\,x\,H_n - 2\,n\,H_{n-1}$$

$$H_0 = 1 \quad \text{and} \quad H_{-1} \equiv e^{x_0^2}\,\frac{\sqrt{\pi}}{2}\,[1 - \operatorname{erf}(x_0)]\,. \qquad (23)$$

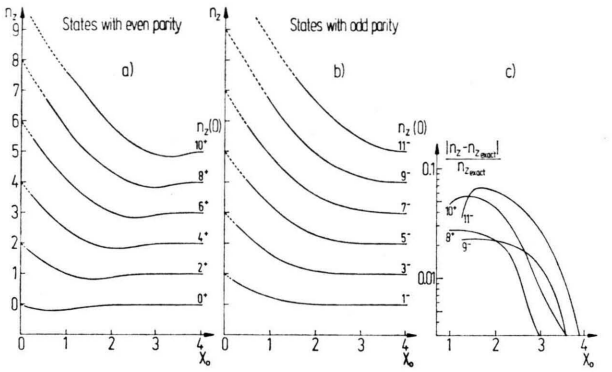

Fig. 2. In Figs. a) and b) the dependence of n_z on the separation x_0 is shown for the six lowest states of even and odd parity in the oscillator potential with infinite depth. The full drawn curves are obtained by diagonalizing the lowest basis states according to the method proposed in this paper. The dashed part of the curves is calculated by taking higher basis states in the diagonalization procedure into account. In Fig. c the deviations of the numerical values n_z from the exact values obtained by Eq. (20) are plotted for the two highest states shown in Figs. a and b.

Figure 2 shows an example for the diagonalization of the energy matrix (21). We have used the six lowest oscillator functions φ_n from which an even or odd set of basis functions (10) can be constructed. For small values of $x_0 < 1$ the orthogonalization procedure fails in the higher states because of the overcompleteness of the basis. In Fig. 2 c the numerical errors in the highest niveaus are drawn which are surprisingly small for such a small number of basis functions. The lower levels have much smaller errors. We conclude that already small basis sets are sufficient to reproduce the correct eigenvalues. I.e., the basis functions constructed as described, approximate the exact solutions very well.

3.2 Two-Center Oscillator Potential with Finite Depth

The oscillator potential of the previous section rises in the outside region, which is unrealistic for nuclear problems. A more realistic shell model potential which allows also for continuum states is the cut-off two-center potential [11] shown in Figure 1 c. The Hamilton operator is given by (without l^2- and $\boldsymbol{l}\boldsymbol{s}$-terms):

$$H = -\frac{\hbar^2}{2\,M}\,\Delta + (V - V_0)\,\theta\left(1 - \frac{V}{V_0}\right) \qquad (24)$$

with

$$V = \tfrac{1}{2}\,M[\omega_\varrho^2\,\varrho^2 + \omega_z^2\,(|z| - z_0)^2]\,. \qquad (25)$$

The potential depth V_0 does not strongly depend on the nuclear number A and can be assumed as a constant in first approximation. If we restrict our discussion to symmetric fission with spherical fragments, the frequencies are equal: $\omega_\varrho = \omega_z = \omega$. Then the potential surface $V - V_0 = 0$ is formed by two spheres with radii $R = \sqrt{2\,V_0/M\,\omega^2}$ around the centers at $z = \pm z_0$. To fix the frequency ω as function of z_0, we suppose that the volume enclosed by the potential surface $V - V_0 = 0$ is conserved during the fission process because nuclear matter is nearly incompressible. It results

$$\omega(z_0) = (1/R)\sqrt{2\,V_0/M} \qquad (26)$$

where R solves the equation for $z_0 \leqq R$:

$$(R + z_0)^2\,(2\,R - z_0) = 2\,R^3 \quad (z_0 = 0)\,. \qquad (26\,\text{a})$$

Only in the limitting cases $z_0 = 0$ and $z_0 \to \infty$ the eigenfunctions can be found analytically as shown in Appendix B where the harmonic oscillator with finite potential depth is solved. In the following we apply the diagonalization method of Sect 2.2 to obtain the bound states of the Hamilton operator (24), using the wave functions given in Eq. (16), we get:

$$H_{\lambda\lambda'} = \langle k\,P\,n_\varrho\,m\,|\,T + V - V_0\,|\,k'\,P\,n_\varrho'\,m\rangle - \langle k\,P\,n_\varrho\,m\,|\,(V - V_0)\,\theta(V/V_0 - 1)\,|\,k'\,P\,n_\varrho'\,m\rangle\,.$$

The Hamiltonian is divided into the Hamiltonian of the usual two center oscillator described in the previous section and into the rest potential acting in the region where $V > V_0$. With the result of Eq. (22) we obtain:

$$H_{\lambda\lambda'} = \delta_{n_\varrho n'_\varrho}\,[(\hbar\,\omega(2\,n_\varrho + |m| + 1) - V_0)\,\delta_{kk'} + h_{kk'}] - W^{m,P}_{kk',n_\varrho n_\varrho'} \qquad (27)$$

where

$$W = \frac{\hbar\omega}{2} \sum_{n_1 n_2} \frac{a_{kn_1} a_{k'n_2}}{\sqrt{M_{n_1 p} M_{n_2 p}}} \int_{x=0}^{\infty} \int_{y=0}^{\infty} \theta[y^2 + (x-x_0)^2 - r_0^2] \cdot [y^2 + (x-x_0)^2 - r_0^2]\; G_{n_e m}(y)\, G_{n_e' m}(y)\, y\, dy$$
$$\cdot [\varphi_{n_1}(x-x_0) + P(-1)^{n_1} \varphi_{n_1}(x+x_0)]\, [\varphi_{n_2}(x-x_0) + P(-1)^{n_2} \varphi_{n_2}(x+x_0)]\, dx \quad (28)$$

with $r_0 = R/a$, $x_0 = z_0/a$ and $a = \sqrt{\hbar/M\omega}$.

The integral has been solved analytically. Because of the finite Hermite and Laguerre polynomials it can be rewritten as a finite sum over integrals of the type

$$K_{m,n}(\alpha) = \int_{x=0}^{\infty} \int_{y=0}^{\infty} \theta[y^2 + (x-x_0)^2 - r_0^2]\; x^m\, e^{-(x+\alpha)^2}\, y^{2n+1}\, e^{-y^2}\, dx\, dy \quad (29)$$

with the special values of $\alpha = 0, \pm x_0$. The last integral K_{mn} is calculated in the Appendix A.

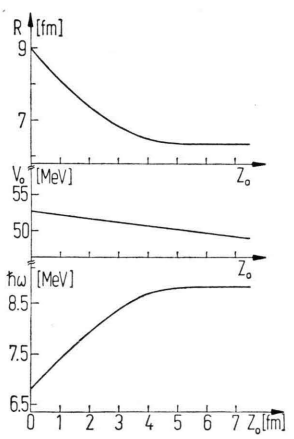

Fig. 3. The radius R, the potential depth V_0 and the frequency $\hbar\omega$ as functions of the two-center distance z_0 for the nuclear system with $A = 210$.

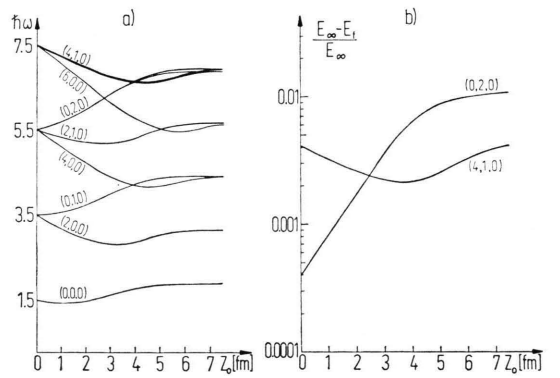

Fig. 4. a) Levels of the oscillator potential with finite and infinite depth are drawn as functions of z_0. The numbers in parentheses give the quantum number n_z, n_ϱ and $|m|$ for $z_0 = 0$. Only for the highest levels (4, 1, 0) and (0, 2, 0), differences can be recognized between the eigenenergies of the potential with finite and infinite depths. b) The energy differences are enlarged for these two levels. $E\infty$ denotes the energy in the infinite deep potential and E_f the energy in the potential with finite depth.

As an example we have calculated the levels of the finite two-center oscillator for the symmetric fission of a nucleus with $A = 210$. The used values of R, $\hbar\omega$ and V_0 are drawn in Fig. 3 as functions of the two-center distance z_0. Examples for the levels of the cut-off two-center oscillator are given in Fig. 4 a, in which the different curves are denoted by the quantum numbers n_z, n_ϱ, m for $z_0 = 0$. Only the energies of the highest bound levels differ notably from the levels of the infinite high two-center oscillator. This is shown in Fig. 4 b, where the energies of the highest levels are related to the corresponding levels of the infinite high two-center oscillator.

IV. Summary

In this paper we have calculated the bound states of the two-center oscillator with finite depth by a diagonalization procedure which uses one-center oscillator functions as basis states. The basis states are concentrated around the individual centers. The application of those basis states is adventageous because the matrix elements of the Hamiltonian can be found analytically. The method is not restricted to the problem of calculating bound states in two-center potentials, but may straigthforwardly extended to problems as the triple fission [14] and to cluster calculations [15] where three- and more-center potentials have to be introduced.

Appendix A:
Integrals with Oscillator Wave Functions [12]

In the following we consider integrals in which oscillator wave functions are involved [7, 12].

1. $$I_{mn} = \int_{-\infty}^{\infty} \varphi_m(x+x_0)\,\varphi_n(x-x_0)\,\mathrm{d}x$$

with the aid of

$$H_m(x+x_0) = \sum_{k=0}^{m} \binom{m}{k} (2x_0)^{m-k} H_k(x) \tag{A.1}$$

it follows

$$\varphi_m(x+x_0)\,\varphi_n(x-x_0) = e^{-x_0^2}(-1)^n \sqrt{m!\,n!\,2^{m+n}} \sum_{k=0}^{m}\sum_{l=0}^{n} \frac{(-1)^k x_0^{m+n-l-k}\,\varphi_k(x)\,\varphi_l(x)}{\sqrt{k!\,l!\,2^{l+k}}\,(m-k)!\,(n-l)!}\,.$$

Therefore, because of the orthonormalization of the functions φ_n we get:

$$I_{mn} = (-1)^n \sqrt{m!\,n!\,2^{m+n}}\, e^{-x_0^2} \sum_{t=0}^{\mathrm{Min}(m,n)} \frac{(-1)^t x_0^{m+n-2t}\,2^{-t}}{t!\,(m-t)!\,(n-t)!}\,, \tag{A.2}$$

2. $$L_{mn} = \int_{-\infty}^{\infty} [\varphi_m(x-x_0) + P(-1)^m\,\varphi_m(x+x_0)]\,(|x|-x)\,\varphi_n(x-x_0)\,\mathrm{d}x\,.$$

We have:

$$L_{mn} = 2(-1)^{m+n}\left[\int_0^{\infty} x\,\varphi_m(x+x_0)\,\varphi_n(x+x_0)\,\mathrm{d}x + (-1)^m P \int_0^{\infty} x\,\varphi_m(x-x_0)\,\varphi_n(x+x_0)\,\mathrm{d}x\right]. \tag{A.3}$$

With the relation $$H_m(x)H_n(x) = \sum_{s=0} 2^s s! \binom{m}{s}\binom{n}{s} H_{m+n-2s}(x)$$

the first integral in Eq. (A.3) becomes:

$$\int_{x_0}^{\infty} (x-x_0)\,\varphi_m(x)\,\varphi_n(x)\,\mathrm{d}x = \frac{1}{\sqrt{\pi\,2^{m+n}\,m!\,n!}} \sum_{s=0} 2^s s! \binom{m}{s}\binom{n}{s}(-1)^{m+n-2s} \int_{x_0}^{\infty} (x-x_0)\,\frac{\mathrm{d}^{m+n-2s}}{\mathrm{d}x^{m+n-2s}}\,e^{-x^2}\,\mathrm{d}x$$

$$= \frac{e^{-x_0^2}}{\sqrt{\pi\,2^{m+n}\,m!\,n!}} \sum_{s=0} 2^s s! \binom{m}{s}\binom{n}{s} H_{m+n-2s-2}(x_0) \tag{A.4}$$

with the definition

$$H_{-1} = e^{x_0^2}\frac{\sqrt{\pi}}{2}\,[1-\mathrm{erf}(x_0)] \quad \text{and} \quad H_{-2} = \tfrac{1}{2} - x_0 H_{-1}(x_0)\,.$$

The second integral in Eq. (A.3) is solved applying Eq. (A.1):

$$\int_0^{\infty} x\,\varphi_m(x-x_0)\,\varphi_n(x+x_0)\,\mathrm{d}x = \frac{e^{-x_0^2}}{\sqrt{\pi\,2^{m+n}\,m!\,n!}} \sum_{s,t=0} \binom{m}{s}\binom{n}{t} H_{m-s}(-x_0)\,H_{n-t}(x_0)\,2^{s+t} \int_0^{\infty} x^{s+t+1}\,e^{-x^2}\,\mathrm{d}x$$

$$= \frac{e^{-x_0^2}}{\sqrt{\pi\,2^{m+n}\,m!\,n!}} \sum_{s,t=0} \binom{m}{s}\binom{n}{t} H_{m-s}(-x_0)\,H_{n-t}(x_0)\,2^{s+t-1}\left(\frac{s+t}{2}\right)!\,. \tag{A.5}$$

So we obtain according to (A.4) and (A.5):

$$L_{mn} = \frac{2(-1)^{m+n}\,e^{-x_0^2}}{\sqrt{\pi\,2^{m+n}\,m!\,n!}}\left\{\sum_{s=0} 2^s s! \binom{m}{s}\binom{n}{s} H_{m+n-2s-2}(x_0)\right.$$

$$\left. + P(-1)^m \sum_{s,t=0} \binom{m}{s}\binom{n}{t} H_{m-s}(-x_0)\,H_{n-t}(x_0)\,2^{s+t-1}\left(\frac{s+t}{2}\right)!\right\}, \tag{A.6}$$

3. $$K_{mn}(\alpha) = \int_{x=0}^{\infty}\int_{y=0}^{\infty} \theta[y^2+(x-x_0)^2-r_0^2]\,x^m\,e^{-(x+\alpha)^2}\,y^{2n+1}\,e^{-y^2}\,\mathrm{d}x\,\mathrm{d}y\,. \tag{A.7}$$

We transform:

$$K_{mn}(\alpha) = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\beta^n}\left\{\int_{x=0}^{\infty}\int_{y=0}^{\infty} \theta[y^2+(x-x_0)^2-r_0^2]\,x^m\,e^{-(x+\alpha)^2}\,y\,e^{-\beta y^2}\,\mathrm{d}x\,\mathrm{d}y\right\}_{\beta=1}$$

$$= \frac{n!}{2}\int_{x=0}^{\infty} x^m\,e^{-(x+\alpha)^2}\,\mathrm{d}x + \frac{(-1)^n}{2}\frac{\mathrm{d}^n}{\mathrm{d}\beta^n}\left\{\frac{1}{\beta}\int_{(x_0-r_0)\,\Theta(x_0-r_0)}^{x_0+r_0} x^m\,e^{-(x+\alpha)^2}\,(e^{-\beta[r_0^2-(x-x_0)^2]}-1)\,\mathrm{d}x\right\}_{\beta=1}.$$

Thus we have reduced the expression (A.7) to elementary integrals.

Appendix B: Harmonic Oscillator with Finite Depth

The Schrödinger equation of the spherical harmonic oscillator with finite depth V_0 and radius $R = \sqrt{2 V_0/M\omega^2}$ is given by [13]:

$$\left[-\frac{\hbar^2}{2M}\Delta + \theta\left(1-\frac{r}{R}\right)\left\{\frac{M}{2}\omega^2 r^2 - V_0\right\}\right]\psi = E\psi\,. \tag{B.1}$$

The eigenenergies E are discrete for $E<0$ and continuous for $E>0$. The solutions of the problem can be factorized as:

$$\psi = \varphi(r)\, Y_{lm}\,.$$

The radial function φ has the form for $r<R$:

$$\varphi(r) = A\left(\frac{r}{a}\right)^l e^{-\frac{1}{2}(r/a)^2}\, {}_1F_1\left(-n, l+3/2, \left(\frac{r}{a}\right)^2\right) \tag{B.2}$$

With $a = \sqrt{\hbar/M\omega}$ and with the number n defined as function of the energy

$$E = \hbar\omega(2n + l + 3/2) - V_0\,. \tag{B.3}$$

For $r>R$ it results:

$$\varphi(r) = \beta\,[j_l(kr) - \operatorname{tg}\delta_l\, \eta_l(kr)] \tag{B.4}$$

with

$$k = \sqrt{2ME/\hbar^2}\,.$$

The phase shift δ_l is real for the continuum states ($E>0$) and $\delta_l \to -i\infty$, respectively $\operatorname{tg}\delta_l = -i$, for the discrete states:

$$E<0:\ \varphi(r) = B\, h_l^{(1)}(i|k|r)\,. \tag{B.5}$$

The steady continuation of the wave functions and their derivatives at $r=R$ leads to the condition:

$$kR\frac{j_{l-1}(kR) - \operatorname{tg}\delta_l\,\eta_{l-1}(kR)}{j_l(kR) - \operatorname{tg}\delta_l\,\eta_l(kR)} = (2l+1)\,\frac{{}_1F_1[-n, l+1/2, (R/a)^2]}{{}_1F_1[-n, l+3/2, (R/a)^2]} - (R/a)^2\,. \tag{B.6}$$

In the case of $E>0$ the last equation determines the phase shift δ_l as function of E. For $E<0$ we have $\operatorname{tg}\delta_l = -i$ and

$$kR = i(R/a)^2\sqrt{1 - (4n+2l+3)/(R/a)^2}\,. \tag{B.7}$$

Then Eq. (B.6) represents the eigenvalue equation for the discrete values n as functions of the ratio $(R/a)^2$ and angular momentum l. In the limit $R/a \to \infty$ we obtain the integer quantum numbers $n = 0, 1, 2\ldots$ of the harmonic oscillator. In nuclear problems one uses $\hbar\omega = 41\ \mathrm{MeV/A^{1/3}}$ and $V_0 = 50$ MeV which corresponds to a ratio of $(R/a)^2 = 2.44\cdot A^{1/3}$. For such large ratios an asymptotic expansion of the eigenvalues can be derived:

$$n - N = -\frac{(R/a)^{4N+2l+1}\, e^{-(R/a)^2}}{4(N+l+1/2)!\,N!}\cdot\left[1 + \left(\frac{7}{2} - (N-1)(2N+2l-1)\right)\left(\frac{a}{R}\right)^2 \ldots\right] \tag{B.8}$$

with $N = 0, 1, 2, \ldots$.

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