SEPARATION OF THE VARIABLES ILLUSTRATED
BY THE EXAMPLE OF THE THREE-BODY PROBLEM

N. F. Stepanov and B. I. Zhilinskii   UDC 539.192

Most quantum-mechanical problems can be solved only by means of approximation methods. Although the accuracy of a method chosen depends on the actual problem to which it is applied, it has nevertheless been attempted to estimate the accuracy of a method by taking accurately solved problems as an example [1-3]. The one-particle approximation [1] and the Born—Oppenheimer (BO) approximation [2, 3] have been discussed. These methods were used for solving problems in Cartesian coordinates. However, a characteristic feature of methods in which the variables are approximately separated is that their accuracy depends on the coordinate system chosen [4, 5]. Therefore, the error of the various methods can be decomposed into the true approximation error and a methodical error, the latter of which is related to the coordinate system chosen.

The true error is defined as follows. The Hamiltonian of the system is written down for various coordinate systems (strictly speaking, this should be done for all conceivable coordinate systems), and the problem is solved approximately for all these Hamiltonians. As was mentioned above, the result and, hence, also the error will depend on the coordinate system chosen. The minimum error is called the true error of the approximate separation of the variables. The additional error, which differs from zero unless the optimum coordinate system has been chosen, is the methodical error related to the coordinate system chosen. If the one-particle approximation or the BO approximation is applied to a problem which has been accurately solved by separation of the variables in some coordinate system, the true error of these two methods equals zero. Therefore, by taking such a problem as an example, the methodical error related to the coordinate system chosen can be conveniently discussed.

In the present study the problem of three arbitrary particles interacting by means of harmonic forces [6, 7] was taken as accurately solved problem.

The Hamiltonian of the system reads

$$H = \sum_{i=1}^{3} \left[\frac{1}{2m_i} P_i^2 + \frac{\mu_i \omega_i^2}{2} (r_j - r_k)^2 \right],$$ (1)

where r_i denotes the three-dimensional coordinate vector, P_i is the momentum operator conjugate to r_i, and $\mu_i^{-1} = m_j^{-1} + m_k^{-1}$. In the summation the indices i, j, k are permuted in cyclic fashion: $i \rightarrow j$.

We shall proceed as follows. After separating out the coordinates of the mass center we apply a linear transformation to the internal coordinates and find the best and worst values of the energy, the latter being derived by means of the BO method and the one-particle approximation method in the solution of the problem for various coordinate systems. The maximum methodical errors related to the linear transformation of the variables are thus determined.

The Hamiltonian for the system of the mass center reads

$$H = -\frac{1}{2\mu} \frac{\partial^2}{\partial \xi_1^2} - \frac{1}{2\mu} \frac{\partial^2}{\partial \xi_2^2} + a_1 \xi_1^2 + a_2 \xi_2^2 + a_{12} \xi_1 \xi_2,$$ (2)

$$\xi_1 = \frac{1}{d}\,(r_2 - r_1),$$

$$\xi_2 = d\left(r_3 - \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2}\right),$$

$$d^2 = \frac{m_3}{\mu}\left(\frac{m_1 + m_2}{m_1 + m_2 + m_3}\right); \quad \mu^2 = \frac{m_1 m_2 m_3}{m_1 + m_2 + m_3},$$

$$a_1 = \frac{d^2}{2(m_1 + m_2)^2}\,[\mu_3 \omega_3^2 (m_1 + m_2)^2 + \mu_2 \omega_2^2 m_2^2 + \mu_1 \omega_1^2 m_1^2],$$

$$a_2 = \frac{1}{2d^2}(\mu_1 \omega_1^2 + \mu_2 \omega_2^2), \quad a_{12} = \frac{1}{m_1 + m_2}(\mu_2 \omega_2^2 m_2 - \mu_1 \omega_1^2 m_1).$$

We change over to other coordinates using a linear transformation of the variables

$$\xi_1 = \lambda_1 \cos \varphi \eta_1 + \lambda_2 \sin \varphi \eta_2,$$

$$\xi_2 = -\lambda_1 \sin \varphi \eta_1 + \lambda_2 \cos \varphi \eta_2. \tag{3}$$

The Hamiltonian then becomes

$$H = -\frac{1}{2\mu\lambda_1^2}\frac{\partial}{\partial \eta_1^2} - \frac{1}{2\mu\lambda_2^2}\frac{\partial}{\partial \eta_2^2} + \lambda_1^2 b_1(\varphi)\eta_1^2 + \lambda_2^2 b_2(\varphi)\eta_2^2 + \lambda_1 \lambda_2 b_{12}(\varphi)\eta_1 \eta_2; \tag{4}$$

$$b_1(\varphi) = \frac{a_1 + a_2}{2} + \frac{a_1 - a_2}{2}\cos 2\varphi - \frac{a_{12}}{2}\sin 2\varphi,$$

$$b_2(\varphi) = \frac{a_1 + a_2}{2} - \frac{a_1 - a_2}{2}\cos 2\varphi + \frac{a_{12}}{2}\sin 2\varphi,$$

$$b_{12}(\varphi) = (a_1 - a_2)\sin 2\varphi + a_{12}\cos 2\varphi.$$

The accurate eigenvalue obviously remains unaltered by this transformation of the Hamiltonian, but if the eigenvalues for the operator (4) are determined by means of the one-particle approximation or the BO method, the eignevalues found turn out to depend on the angle and to be independent of the scale parameters λ_1, λ_2 of the transformation.

By using the BO type approximation, we get

$$\left\{-\frac{1}{2\mu\lambda_1^2}\frac{\partial^2}{\partial \eta_1^2} + \lambda_1^2 b_1(\varphi)\eta_1^2 + \lambda_2^2 b_2(\varphi)\eta_2^2 + \lambda_1 \lambda_2 b_{12}(\varphi)\eta_1 \eta_2\right\}\Psi_n(\eta_1, \eta_2) = E_{en}(\eta_2)\Psi_n(\eta_1, \eta_2), \tag{5}$$

$$\left\{-\frac{1}{2\mu\lambda_2^2}\frac{\partial^2}{\partial \eta_2^2} + \left[\lambda_2^2 b_2(\varphi) - \lambda_2^2\frac{b_{12}^2(\varphi)}{4b_1(\varphi)}\right]\eta_2^2 + 3(2n+1)\sqrt{\frac{b_1(\varphi)}{2\mu}}\right\}\chi_{nm}(\eta_2) = E_{nm}\chi_{nm}(\eta_2);$$

$$E_{\text{BO }nm}(\varphi) = \frac{3}{\sqrt{2\mu}}\left\{\sqrt{b_1(\varphi)}\,(2n+1) + \left[\frac{4a_1 a_2 - a_{12}^2}{4b_1(\varphi)}\right]^{1/2}(2m+1)\right\}. \tag{6}$$

Since the diagonal correction to the nuclear equation is left out of consideration in the BO approximation, it follows from a well-known theorem [8, 9] that the energy value yielded by the BO approximation always is a lower bound to the total energy.

Solution of the problem by means of the one-particle approximation leads to the equations

$$\left(-\frac{1}{2\mu\lambda_1^2}\frac{\partial^2}{\partial\eta_1^2}+\lambda_1^2 b_1(\varphi)\eta_1^2\right)\Psi_{1n}(\eta_1)=\epsilon_{1n}\Psi_{1n}(\eta_1),$$

$$\left(-\frac{1}{2\mu\lambda_2^2}\frac{\partial^2}{\partial\eta_2^2}+\lambda_2^2 b_2(\varphi)\eta_2^2\right)\Psi_{2m}(\eta_2)=\epsilon_{2m}\Psi_{2m}(\eta_2);\tag{7}$$

$$E_{\text{one-part}}(\varphi)=\epsilon_{1n}+\epsilon_{2m}=\frac{3}{\sqrt{2\mu}}[\sqrt{b_1(\varphi)}(2n+1)+\sqrt{b_2(\varphi)}(2m+1)].\tag{8}$$

Owing to the specific nature of the problem, the maximum of $E_{\text{BO}}(\varphi)$ and the minimum of $E_{\text{one-part}}(\varphi)$ must be identical to the accurate solution. The minimum of $E_{\text{BO}}(\varphi)$ and the maximum of $E_{\text{one-part}}(\varphi)$ are the worst values for the BO and the one-particle approximations, respectively:

$$E_{\text{acc}}=E_{\text{BO}}(\varphi)=E_{\text{one-part}}(\varphi)=\frac{3}{\sqrt{2\mu}}[\sqrt{b_1(\varphi_\tau)}(2n+1)+\sqrt{b_2(\varphi_\tau)}(2m+1),\tag{9}$$

$$\varphi_\tau=\arctg\frac{a_1-a_2\pm\sqrt{(a_2-a_1)^2+a_{12}^2}}{a_{12}}.\tag{10}$$

Equation (9) for the ground state can be transformed into the simple form

$$E_{\text{acc}}=\frac{3}{2}\left\{\omega_1^2+\omega_2^2+\omega_3^2+2\left[\frac{m_1+m_2+m_3}{m_1m_2m_3}(\mu_1\mu_2\omega_1^2\omega_2^2+\right.\right.$$
$$\left.\left.+\mu_2\mu_3\omega_2^2\omega_3^2+\mu_1\mu_3\omega_1^2\omega_3^2)\right]^{1/2}\right\}^{1/2},\tag{11}$$

$$E_{\text{BO worst}}=\frac{3}{\sqrt{2\mu}}\left(a_1a_2-\frac{1}{4}a_{12}^2\right)^{1/4}2\sqrt{(2n+1)(2m+1)},\tag{12}$$

$$E_{\text{one-part worst}}=\frac{3}{\sqrt{2\mu}}\sqrt{b_1(\varphi_\text{B})}\left[2n+1+\frac{(2m+1)^2}{2n+1}\right],\tag{13}$$

where φ_B satisfies the equation

$$b_1(\varphi_\text{B})(2m+1)^2=b_2(\varphi_\text{B})(2n+1)^2.\tag{14}$$

For the ground state we derive the following equations suited for estimating the maximum errors related to the linear transformations of the variables:

$$\frac{E_{\text{BO worst}}}{E_{\text{acc}}}=\frac{(\mu_1\mu_2\omega_1^2\omega_2^2+\mu_2\mu_3\omega_2^2\omega_3^2+\mu_1\mu_3\omega_1^2\omega_3^2)^{1/4}}{\left\{\frac{\mu}{2}(\omega_1^2+\omega_2^2+\omega_3^2)+(\mu_1\mu_2\omega_1^2\omega_2^2+\mu_2\mu_3\omega_2^2\omega_3^2+\mu_1\mu_3\omega_1^2\omega_3^2)^{1/2}\right\}^{1/2}},\tag{15}$$

$$\frac{E_{\text{one-part worst}}}{E_{\text{acc}}}=\frac{[2(\omega_1^2+\omega_2^2+\omega_3^2)]^{1/2}}{\left\{\omega_1^2+\omega_2^2+\omega_3^2+\frac{2}{\mu}(\mu_1\mu_2\omega_1^2\omega_2^2+\mu_2\mu_3\omega_2^2\omega_3^2+\mu_1\mu_3\omega_1^2\omega_3^2)^{1/2}\right\}^{1/2}}.\tag{16}$$

The one-particle and the BO approximations yield the same maximum absolute errors in the determination of E^2:

$$E_{\text{acc}}^2-E_{\text{BO worst}}^2=E_{\text{one-part worst}}^2-E_{\text{acc}}^2=\frac{9}{\mu}\left(\frac{b_1(\varphi_\tau)+b_2(\varphi_\tau)}{2}-\sqrt{b_1(\varphi_\tau)b_2(\varphi_\tau)}\right).\tag{17}$$

Consequently, the maximum error in the determination of E by means of the BO approximation will be slightly higher than that in the determination carried out with the one-particle approximation. This indicates that in the case considered the one-particle approximation is the more stable of the two upon a change of the variables.

Finally, we shall consider the dependence of the maximum absolute error on the parameters of the particles. We shall restrict ourselves to the special case

$$m_1 = m_2 = m; \quad \mu_1\omega_1^2 = \mu_2\omega_2^2 = \mu_3\omega_3^2 = 1.$$

Here

$$a_1 = \frac{3\sqrt{m_3}}{2\sqrt{2m+m_3}}, \quad d^2 = 2\sqrt{\frac{m_3}{2m+m_3}},$$

$$\sigma_2 = \frac{\sqrt{2m+m_3}}{2\sqrt{m_3}},$$

$$a_{12} = 0,$$

$$\frac{E_{BO\,worst}}{E_{acc}} = \frac{1}{2}\left[\left(\frac{3m_3}{2m+m_3}\right)^{1/4} + \left(\frac{2m+m_3}{3m_3}\right)^{1/4}\right]^{-1},$$

$$\frac{E_{one\text{-}part\,worst}}{E_{acc}} = \left[\sqrt{\frac{1}{2}\left(1 + \frac{2m+m_3}{3m_3}\right)^{-1}} + \sqrt{\frac{1}{2}\left(1 + \frac{3m_3}{2m+m_3}\right)^{-1}}\right]^{-1}$$

The results are unusual, since it is generally believed that the BO type approximation works well only in the case of two subsystems with markedly different masses. However, it should be borne in mind that, owing to the specific features of the problem considered here, the best (true) BO approximation will yield the accurate value. Therefore, the data reported only indicate the stability or instability of the approximation upon a change of the coordinate system, i.e., the maximum error related to the coordinate system chosen.

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