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VARIATIONAL ANALYSIS WITH HARMONIC-OSCILLATOR STATES FOR SQUARE POTENTIALS

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ABSTRACT: In this paper we discuss a variational analysis, for the square-well potential problem with a repulsive soft core, using harmonic-oscillator trial wave functions. We show that the core has a relatively small effect on the approximation except when its radius compares with that of the well. The dependence of the approximation on the number of quanta and the frequency of the oscillator is also discussed.

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I. INTRODUCTION

The two-body nuclear interactions proposed recently[1] have a common feature: the presence of repulsive soft cores. In a number of calculations these potentials are taken as the input in a variational analysis of the ground state of light nuclei with some trial function. Naturally, this function is chosen in such a way that a minimum of penetration into the core occurs. In the extreme case of a hard core no penetration at all is allowed. Frequently, the trial function does not show such properties, in which case simulation of it can be attained by introducing short-range correlation factors of the Jastrow[2] type.

The harmonic-oscillator functions do penetrate in the core so it is reasonable to analyze the validity of using a finite linear combination of uncorrelated harmonic-oscillator states in a variational analysis of a hamiltonian with repulsive-core interaction (the variational parameters here being the frequency of the oscillator and the coefficients in the linear combination).

With this objective in mind we consider the problem of a pseudo-deuteron, i.e., a deuteron interacting through square potentials, and calculate the ground-state energy using oscillator functions of up to 20 quanta. Drastic variations of the potential parameters are made only for the height of the core.

The mathematical treatment of the problem is presented in the next section while comparison with the exact results is made in section III. Nevertheless, we anticipate here the main information contained in the numerical results: the presence of a repulsive core does not affect the validity of the approximation very much, unless the range of the well approaches the radius of the core.

II. GROUND STATE OF THE PSEUDO-DEUTERON

The hamiltonian we have to deal with, in relative coordinates, is given by

$$H = \frac{1}{2\mu} p^2 + V(r) , \qquad \mu = \text{reduced mass} \qquad (2.1)$$

which will be put in a convenient dimensionless form. In order to do this we divide (2.1) by some energy, which arbitrarily will be chosen to be the electron mass mc^2 (= 0.511 MeV), and express r and p in units of $\sqrt{\hbar/\mu\omega}$

and $\sqrt{\hbar\mu\omega}$, respectively. In this way the hamiltonian (2.1) becomes

$$H' \equiv \frac{H}{mc^2} = \frac{1}{2}\epsilon p'^2 + V(r'\sqrt{\gamma/\epsilon}) \qquad (2.2)$$

with

$$\epsilon \equiv \frac{\hbar\omega}{mc^2} \qquad (2.3)$$

and

$$\gamma \equiv \frac{\hbar}{\mu mc^2} . \qquad (2.4)$$

The prime indicates that the corresponding variables are dimensionless.

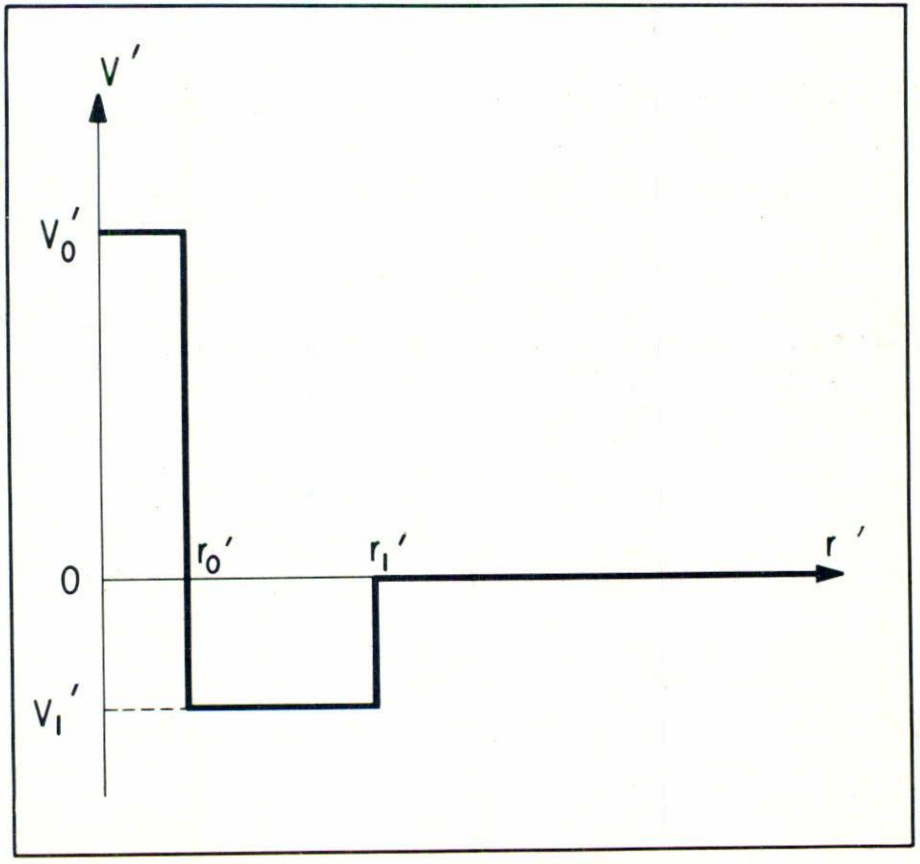

Fig. 1. The pseudo-deuteron

The potential in (2.2) is defined by

$$V'(r') = \begin{cases} V_0' & 0 \leq r' \leq r_0' \\ -V_1' & r_0' < r' \leq r_1' \\ 0 & r_1' < r' \end{cases} \qquad (2.5)$$

a. The Exact Solution

The hamiltonian (2.2) now defines an eigenvalue problem whose exact solution is given, for $l = 0$, by

$$u(r') = \begin{cases} A \sinh(k_0' r') & 0 \leq r' \leq r_0', \quad k_0'^2 = \frac{2\mu}{\hbar^2}[V_0 + |E|]\frac{\gamma}{\epsilon} \\ B \sin(k_1' r') + D \cos(k_1' r') & r_0' \leq r' \leq r_1', \quad k_1'^2 = \frac{2\mu}{\hbar^2}[V_1 - |E|]\frac{\gamma}{\epsilon} \\ F \exp(-k' r') & r_1' \leq r', \quad k'^2 = \frac{2\mu}{\hbar^2}|E|\frac{\gamma}{\epsilon} \end{cases} \qquad (2.6)$$

The boundary conditions on the solution lead to the energy spectrum from which we can obtain the exact ground-state energy, which comes out from the "lowest" solution of the transcendental equation

$$\begin{aligned} & k' k_0' \coth(k_0' r_0') [\cot(k_1' r_1') - \cot(k_1' r_0')] \\ & - k_0' k_1' \coth(k_0' r_0') [\cot(k_1' r_1') \cot(k_1' r_0') + 1] \\ & + k_1'^2 [\cot(k_1' r_0') - \cot(k_1' r_1')] \\ & - k' k_1' [\cot(k_1' r_1') \cot(k_1' r_0') + 1] = 0, \end{aligned} \qquad (2.7)$$

which was solved numerically.

b. The Variational Analysis

Now we assume that the solution (2.6) is unknown and proceed to determine it through a variational analysis of the hamiltonian (2.2) with harmonic-oscillator functions.

As we shall be concerned only with oscillators of angular momentum $l = 0$ the following short hand notation will be used

$$|n00> \equiv |n> \equiv R_{n0}(r') \tag{2.8}$$

and the proposed expansion of the trial function has the form

$$\Psi(r') = \sum_{n=0}^{\frac{1}{2}N} a_n |n>, \quad N \text{ even}, \tag{2.9}$$

where N is the maximum number of quanta. The definition of $R_{n0}(r')$ used here is given in reference 3.

As it is well known, the variational principle, with the normalization condition (assuming the a's real)

$$\sum_n a_n^2 = 1 \tag{2.10}$$

leads to the secular equation

$$\det |<n'|H'|n> - E' \delta_{n'n}| = 0, \quad 0 \leqslant n', n \leqslant \frac{1}{2} N. \tag{2.11}$$

Thus, the only problem left is to calculate the matrix elements of H' with respect to harmonic-oscillator states. Part of this program has already been done[4]:

$$<n'|p'^2|n> = (2n + \tfrac{3}{2})\delta_{n'n} + \sqrt{n(n+\tfrac{1}{2})}\,\delta_{n'n-1} + \sqrt{(n+1)(n+\tfrac{3}{2})}\,\delta_{n'n+1} \tag{2.12}$$

On the other hand, by introducing the B-coefficients defined and tabulated in Ref. 3, the matrix elements of V' can be put in terms of Talmi integrals

in the following way

$$\langle n' | V' | n \rangle = \sum_{p=0}^{n'+n} B(n'0, n0, p)\, I_p \,, \tag{2.13}$$

where

$$I_p \equiv \frac{2}{\Gamma\left(p + \frac{3}{2}\right)} \int_0^\infty r'^{2p+2} V'(r')\, e^{-r'^2}\, dr' \,. \tag{2.14}$$

Through a direct calculation we get for I_0 the value

$$I_0 = \frac{2}{\sqrt{\pi}} \left[(V_0' + V_1')\, \gamma\left(\frac{3}{2}, r_0'^2\right) - V_1'\, \gamma\left(\frac{3}{2}, r_1'^2\right) \right] \tag{2.15}$$

where $\gamma(a, x)$ is an incomplete gamma function, as defined in Ref. 5.

For other values of p the following recursion relation holds

$$I_p = I_{p-1} - \frac{(2p+1)!!}{\sqrt{\pi}\, 2^{p-1}} \left[(V_0' + V_1')\, r_0'^{2p+1} e^{-r_0'^2} - V_1'\, r_1'^{2p+1} e^{-r_1'^2} \right] \qquad p \geq 1 \tag{2.16}$$

With the help of eqs. (2.12), (2.13), (2.15) and (2.16) we determine the matrix elements of the hamiltonian (2.2).

In the next section we discuss the results obtained after diagonalizing H' with different number of quanta, and changing the frequency of the oscillator and the potential parameters.

III. RESULTS AND CONCLUSIONS

In all cases we discuss here, V_1 was taken as 80 MeV and the value of the oscillator parameter ϵ was chosen to be that which gives the best energy as compared with the exact solution, in the 20-quanta approximation. This value of ϵ was rather insensitive to the height of the core as shall be discussed below.

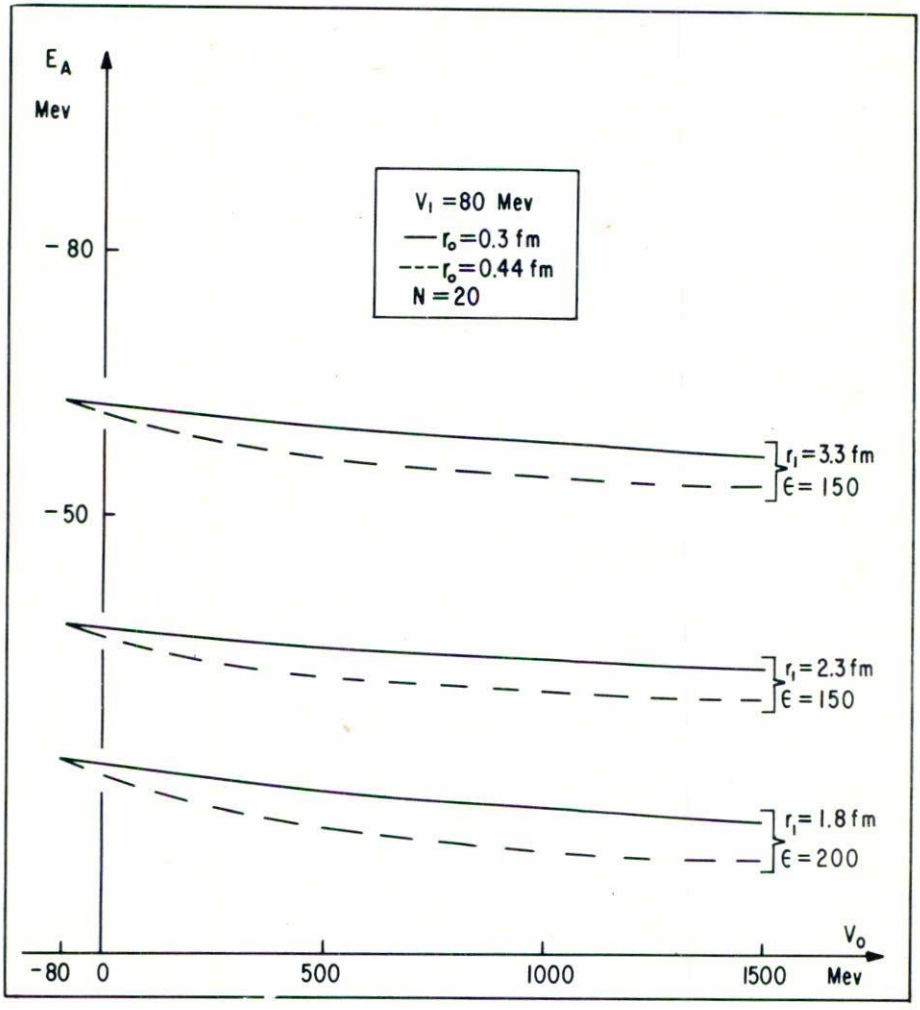

Fig. 2. Variation of the approximate ground-state energy (E_A) with the height V_0 of the core. The number of quanta N is equal to 20.

In Fig. 2 we see the dependence of the ground-state energy on the height of the core. Two values of the core radius and three well ranges are considered, as shown in the figure. One notices that the energy is practically independent of the core height, which varies from -80 (no core) up to 1500 MeV. For instance, in the case of $r_1 = 1.8$ fm and $r_0 = 0.3$ fm the energy decreases at most about 30% of the value at -80 MeV in the whole range of variation of V_0. Now, if we increase the core radius, then the dependence on V_0 will be more notorius.

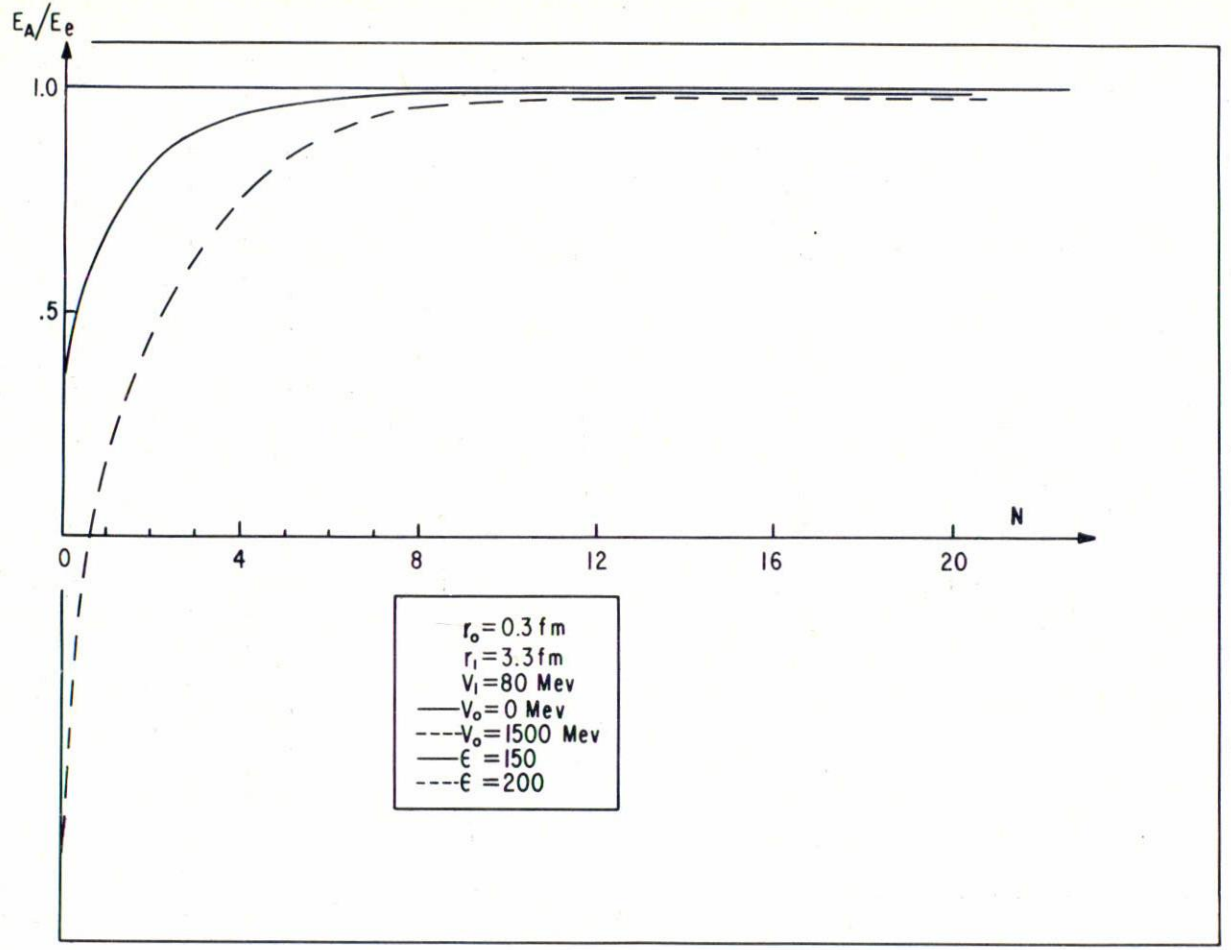

Fig. 3. Convergence of the approximate ground-state energy (E_A) as function of the number of quanta N. E_e is the exact energy.

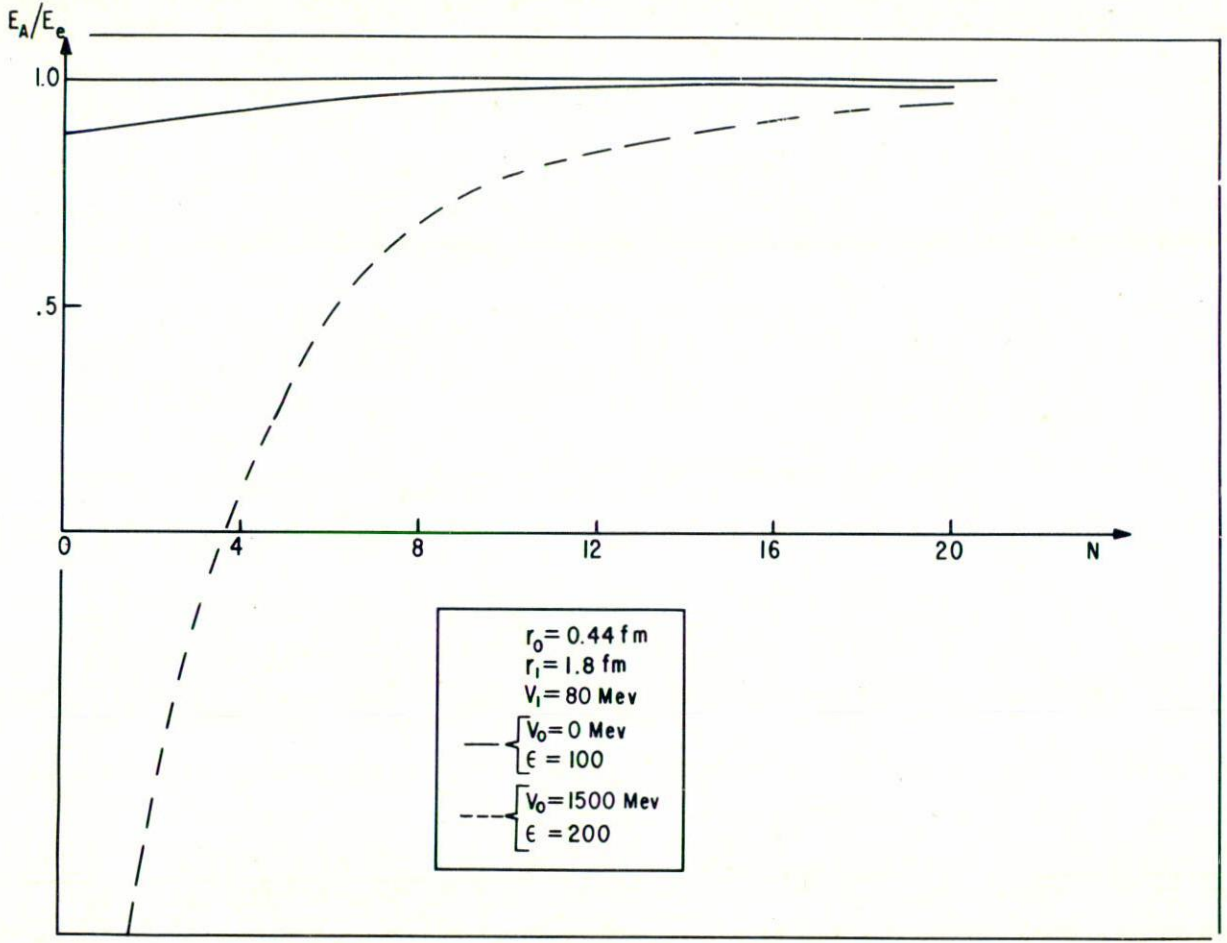

Fig. 4. Convergence of the approximate ground-state energy (E_A) as function of the number of quanta N. E_e is the exact energy.

We proceed now to compare the approximate and exact solutions when in the former we vary the number of quanta or the parameter ϵ.

In Fig. 3 we plot the ratio of the approximate to the exact binding energies as a function of the number of quanta. As before, we choose the ϵ that gives the best approximation at 20 quanta. The r_0 is fixed at 0.3 fm and r_1 at 3.3 fm. Two curves are shown, one for $V_0 = 0$ and the other (dashed) for $V_0 = 1500$ MeV. The approximation is of course poorer for the latter than for the former, but, from 8 quanta on, there is almost no difference.

In Fig. 4 we do the same for $r_0 = 0.44$ fm and $r_1 = 1.8$ fm. Because the radius of the core is now larger than before as compared with the range of the well, the binding energy for $V_0 = 1500$ MeV approaches much more slowly its exact value as we increase the number of quanta N.

We shall now discuss the role of ϵ in the analysis. First we consider the case when the range of the well is large compared to that of the core, specifically in Figs. 5 and 6, $r_0 = 0.44$ fm, $r_1 = 3.3$ fm, and $V_1 = 80$ MeV. In Fig. 5 we take $V_0 = 0$ and graph the ratio of the approximate to the exact binding energies as function of ϵ. Two curves are drawn corresponding to the values $N = 0$ and $N = 20$. For $N = 0$ the ϵ that gives the optimum value for the energy is well defined. For $N = 20$ there is a wide range of ϵ's that give almost the same value of the binding energy which is very close to the exact value. This should be expected because when $N \to \infty$ the variational approach should give the exact binding energy independently of the frequency of the oscillator.

In Fig. 6 we make a corresponding analysis for $V_0 = 1500$ MeV and the results are similar. We note though, that for 0 quantum the optimum energy is farther away from the exact value when $V_0 = 1500$ MeV than in the case for $V_0 = 0$, and, furthermore, the region for optimum approximation when $N = 20$ is narrower in Fig. 6 than in Fig. 5. Both results are expected from physical considerations.

It is interesting to discuss also the validity of the variational procedure where the range r_0 of the core is closer to the value of the range r_1 of the well. In Fig. 7 we consider the case $r_0 = 0.44$ fm, $r_1 = 1.8$ fm, $V_1 = 80$ MeV as before, but we take a core of 1500 MeV. We show the approximate, binding energy as a function of ϵ for $N = 0, 8$ and 20. For $N = 0$ we see that we almost get no binding even in the best case. For $N = 8$ we get 77% of the binding energy for a definite value of ϵ. Only for 20 quanta we approach to 96% of the exact value within a relatively narrow range of the ϵ's. Similar results to those discussed above were obtained with a deeper well ($V_1 = 270$ MeV).

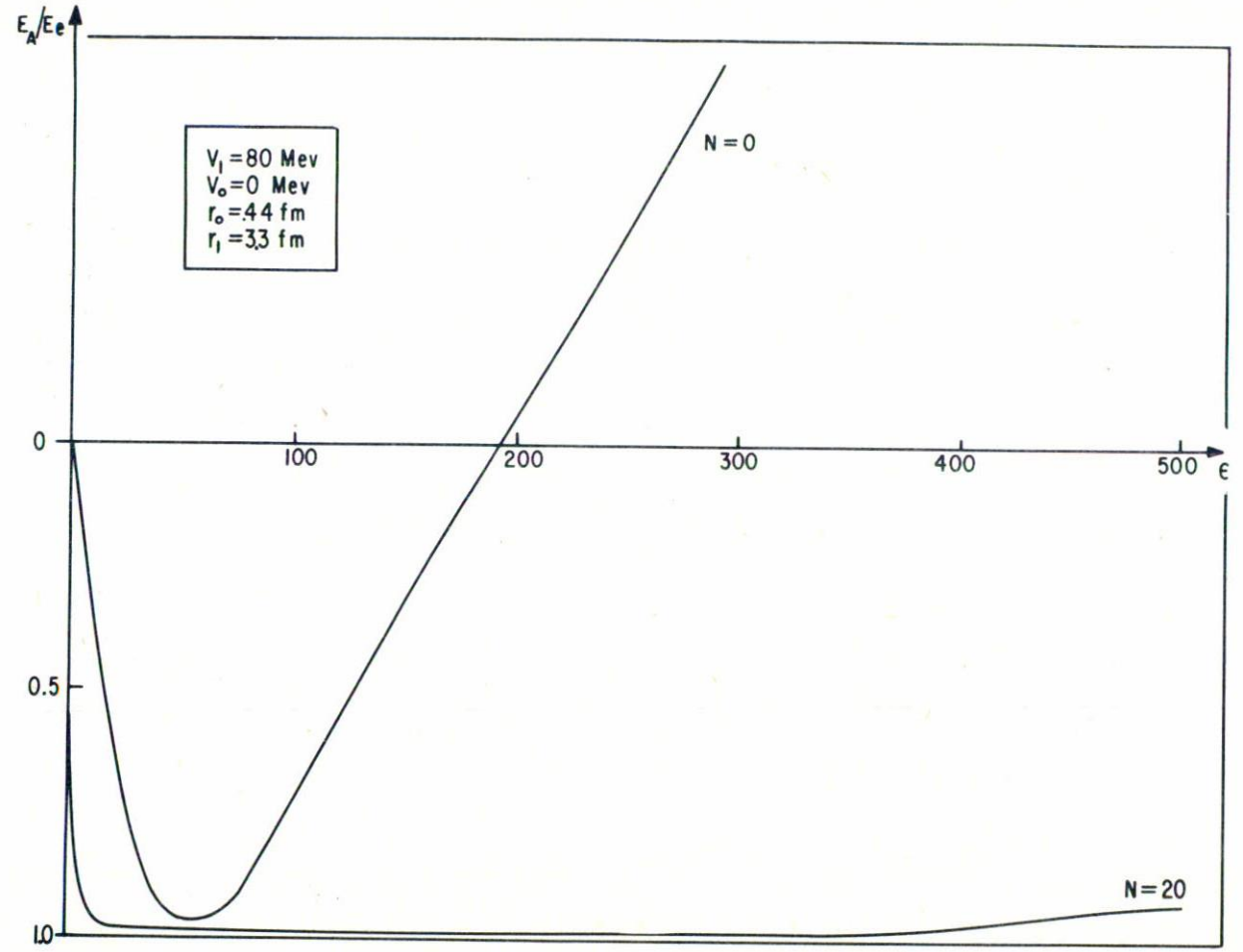

Fig. 5. The approximate ground-state energy (E_A) as function of the oscillator parameter ϵ compared with the exact energy (E_e).

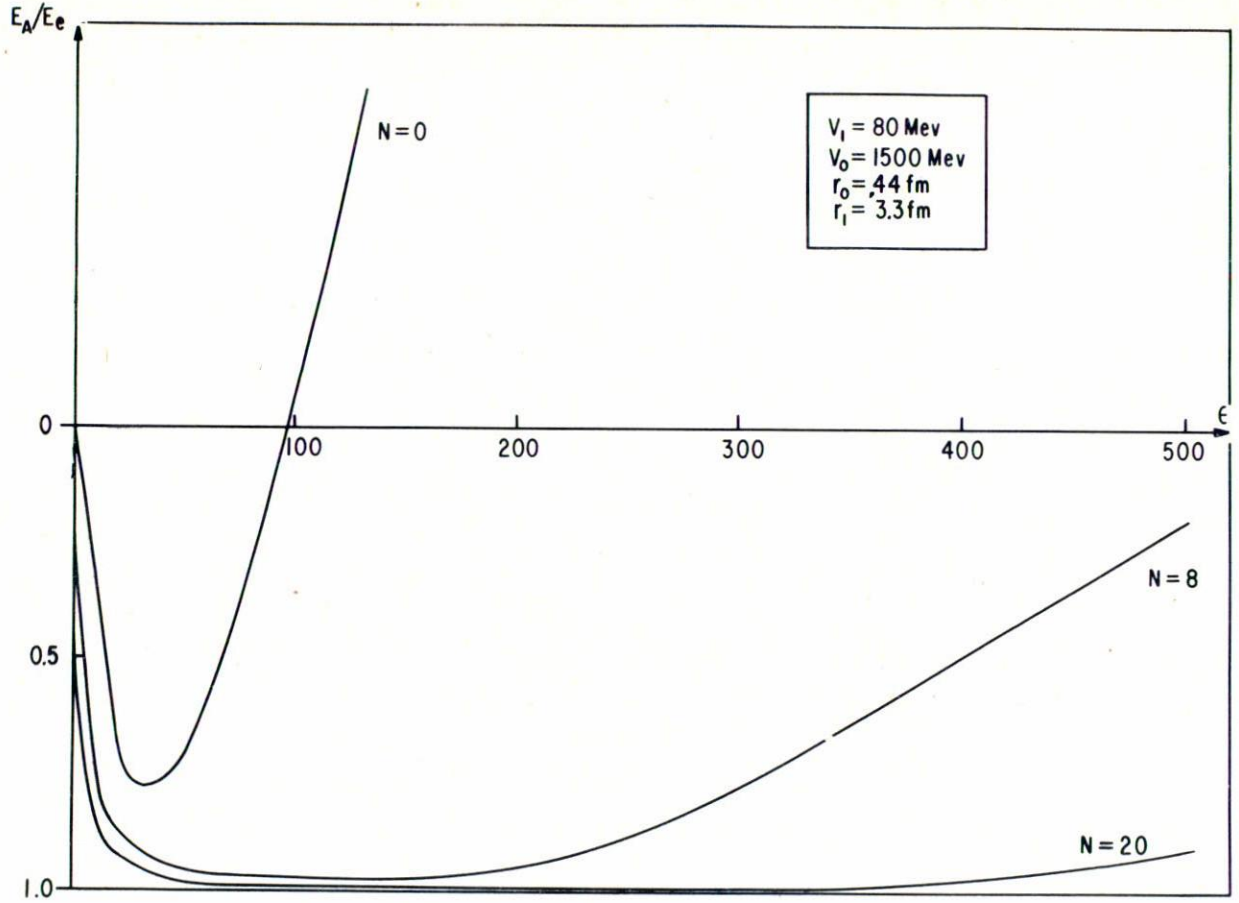

Fig. 6. The approximate ground-state energy (E_A) as function of the oscillator parameter ϵ compared with the exact energy (E_e).

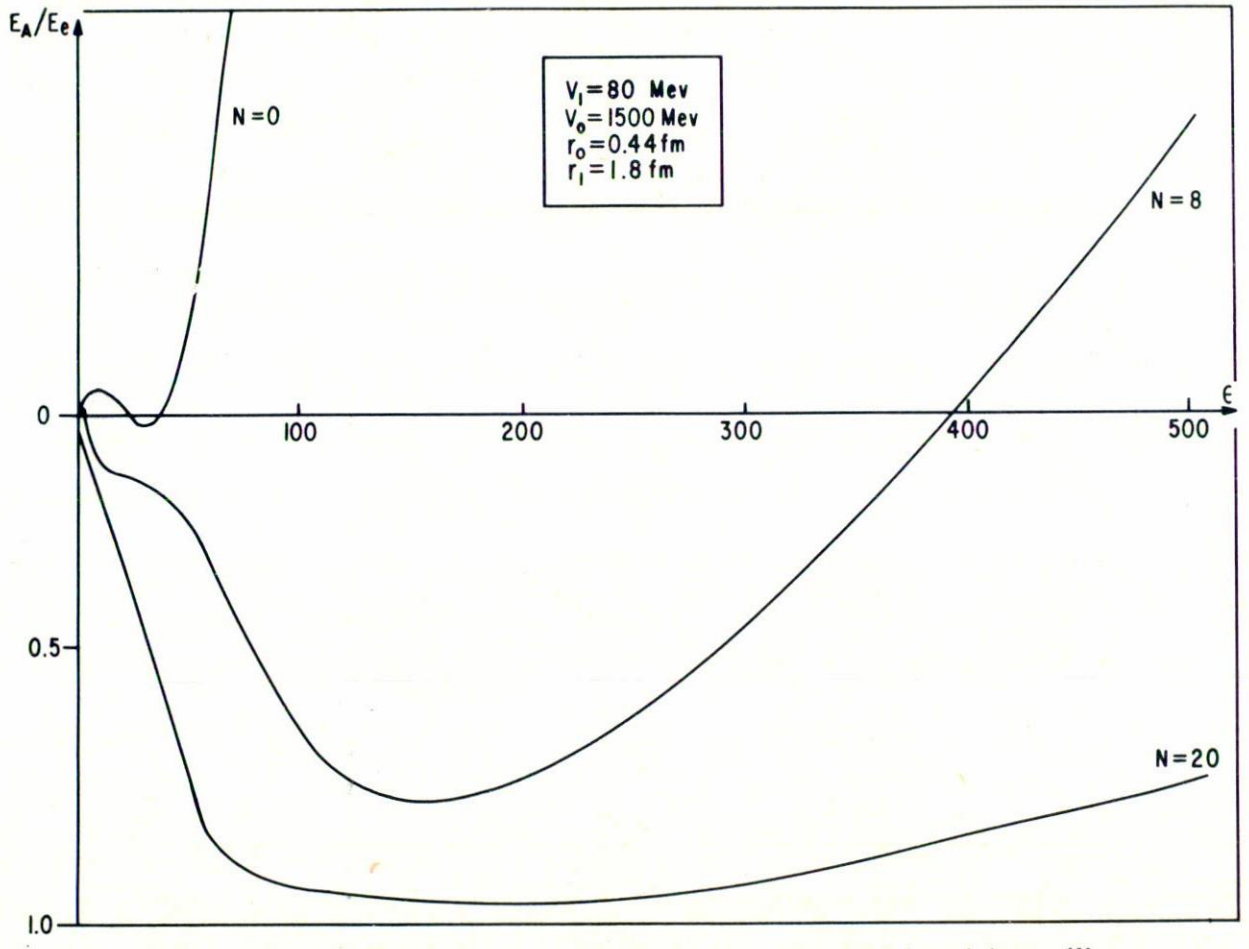

Fig. 7. The approximate ground-state energy (E_A) as function of the oscillator parameter ϵ compared with the exact energy (E_e).

In conclusion, the validity of the approximations in which we used uncorrelated harmonic-oscillator states is not affected by the presence of a repulsive core in the problem, unless the range of the well starts to approach the radius of the repulsive core. Also, when we increase the number of quanta, we approach the exact binding energy better and better over a wider range of frequencies of the harmonic-oscillator trial wave functions.

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RESUMEN

Se discute un análisis variacional utilizando, como función de ensayo, una combinación lineal de funciones de oscilador armónico para el problema de un pozo cuadrado, de profundidad fija, con un carozo repulsivo blando, cuya altura varía desde -80 hasta 1500 MeV.

Los cálculos numéricos fueron realizados hasta 20 cuantos en la aproximación. Se muestra que el carozo tiene un efecto relativamente pequeño en la aproximación, excepto cuando su radio es comparable al del pozo.

Se discuten, también, los resultados de la aproximación, comparados con el exacto, cuando se varían la frecuencia del oscilador y el número máximo de cuantos.