and

$$H_l(r,r') = O_l T_l \frac{r'^{\,l+1}}{r^{l-2}} + R_l S_l \frac{r'^{\,l+3}}{r^l}, \quad r' < r,$$

$$= O_l T_l \frac{r^{l+1}}{r'^{\,l-2}} + R_l S_l \frac{r^{l+3}}{r'^{\,l}}, \quad r' > r;$$

O_l, R_l, S_l, and T_l being defined by

$$O_l = 1/(2l+1)!!, \quad R_l = \tfrac{1}{2}O_{l+1},$$

$$S_l = (2l-1)!!, \quad T_l = \tfrac{1}{2}S_{l-1}.$$

Using the above expansions, one obtains from Eq. (A1) the expression

$$k^{2l+1}\cot\delta_l \approx -\frac{1}{a_l} + \tfrac{1}{2}r_l k^2, \quad \text{(A2)}$$

which is the very familiar form of the effective-range formula for local potentials. In Eq. (A2), a_l and r_l are defined by

$$a_l = \frac{\lambda D_l^2}{1+\lambda e_l}, \quad r_l = \frac{2}{\lambda D_l^2}\left[\lambda h_l - \frac{2(1+\lambda e_l)E_l}{D_l}\right].$$

For $l=0$, one obtains

$$a_0 = \frac{\left(\int_0^\infty r q_0(r)dr\right)^2}{(1/\lambda) + \int_0^\infty\int_0^\infty F_0(r,r')q_0(r)q_0(r')drdr'},$$

where now

$$F_0(r,r') = r', \quad r' < r;$$

$$= r, \quad r' > r.$$

Hence for repulsive potentials ($\lambda > 0$), a_0 is always positive, and for attractive potentials ($\lambda < 0$), a_0 is positive or negative according to whether

$$\int_0^\infty\int_0^\infty F_0(r,r')q_0(r)q_0(r')drdr' > -1/\lambda \quad \text{or} < -1/\lambda.$$

[1]H. Fiedeldey, Nucl. Phys. A96, 463 (1967).
[2]H. Fiedeldey, Nucl. Phys. A115, 97 (1968).
[3]R. Marriott, Proc. Phys. Soc. (London) 72, 121 (1958).
[4]D. Husain and S. Ali, Am. J. Phys. 38, 597 (1970); see also R. L. Cassola and R. D. Koshel, Proc. Phys. Soc. (London) 1, 224 (1968).
[5]R. A. Buckingham and H. S. Massey, Proc. Roy. Soc. (London) A179, 123 (1941).
[6]C. W. Gardiner, Low Energy Proton-Proton Scattering with a Separable Potential and Applications to Final State Interactions Involving Two Protons, Syracuse University, 1969 (to be published).

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Hard-Core Potential Representation by δ' in Variation and Hartree Calculations

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The δ' interaction has been used to represent the hard-core potential in variation and Hartree calculations. These calculations were compared with exact calculations for a two-body bound-state problem and a soluble three-body problem. The trial wave function in the variational problem with the δ' interaction is shown to approach rapidly its hard-core limit with increasing number of trial parameters. The δ' interaction is superior to current soft-core representations of the nucleon-nucleon potential in the Hartree calculations.

INTRODUCTION

It has been shown previously[1] that an interaction proportional to $\delta'(r-r_c)$ (the derivative of a Dirac δ function) yields a wave function vanishing for $r \le r_c$. It is attractive to think of using this interaction in many-body calculations.[2] To test the feasibility of this, we have performed variation calculations in a two-body bound-state problem and Hartree calculations for an exactly soluble three-body problem. We have found that the δ' interaction successfully produces "hard-core effects" in these problems. The trial wave function in the variational problem rapidly approaches its hard-core limit with increasing number of trial parameters. The accuracy in the Hartree calculations using δ' is very competitive with current soft-core forms used in the nucleon-nucleon potential.

TWO-BODY PROBLEM

Figure 1 shows the exact and approximate ground-state wave functions $u(r)=r\psi(r)$ for two particles of mass m_0 interacting via a harmonic-oscillator potential and a hard core of radius r_c. The Hamiltonian for relative motion is given as

$$\hat{H}=\frac{\hbar^2}{2m_0}(-\nabla_{\vec{r}}^2+\alpha^4r^2)+V_{\text{H.C.}}(r)\,, \tag{1}$$

where $V_{\text{H.C.}}$ is the interaction representing the hard core. The exact ground-state wave function was found by numerically integrating the Schrödinger equation $\hat{H}\psi=E\psi$ toward the origin, seeking the lowest value of E for which the solution vanishes at $r=r_c$. The variation calculations were performed using trial wave functions of the form

$$\psi_{T_N}(r)=u_{T_N}(r)/r=\sum_{n,m}^{N}a_{nm}r^n e^{-\beta_m r}\,, \tag{2}$$

where the parameters a_{nm} and β_m were varied so as to minimize the trial energy

$$E_{T_N}=\int\psi_{T_N}{}^*(r)\hat{H}\psi_{T_N}(r)d\vec{r}\bigg/\int\psi_{T_N}{}^*(r)\psi_{T_N}(r)d\vec{r}\,. \tag{3}$$

In evaluating E_{T_N}, the δ' form of $V_{\text{H.C.}}$ was used, i.e.,

$$V_{\text{H.C.}}=-2(\hbar^2/m_0)\delta'(r-r_c)\,. \tag{4}$$

The quantities m_0, α, and r_c were picked to correspond to values used in the three-body problem which will next be described.

THREE-BODY PROBLEM

For the three-body problem, we have considered two identical interacting particles in the harmonic-oscillator potential of a third particle. The Hamiltonian for this system is given as

$$\hat{H}=-\frac{\hbar^2}{2m_0}\nabla_{\vec{r}_1'}^2-\frac{\hbar^2}{2m_0}\nabla_{\vec{r}_2'}^2-\frac{\hbar^2}{2M}\nabla_{\vec{r}_3'}^2 +K((\vec{r}_1'-\vec{r}_3')^2+(\vec{r}_2'-\vec{r}_3')^2)+V(|\vec{r}_1'-\vec{r}_2'|)\,. \tag{5}$$

Written in terms of group-resonating coordinates,[3] the problem separates into that of the free three-particle center-of-mass motion and two particles interacting in a harmonic-oscillator field. The latter case is a well-known exactly soluble problem,[4]

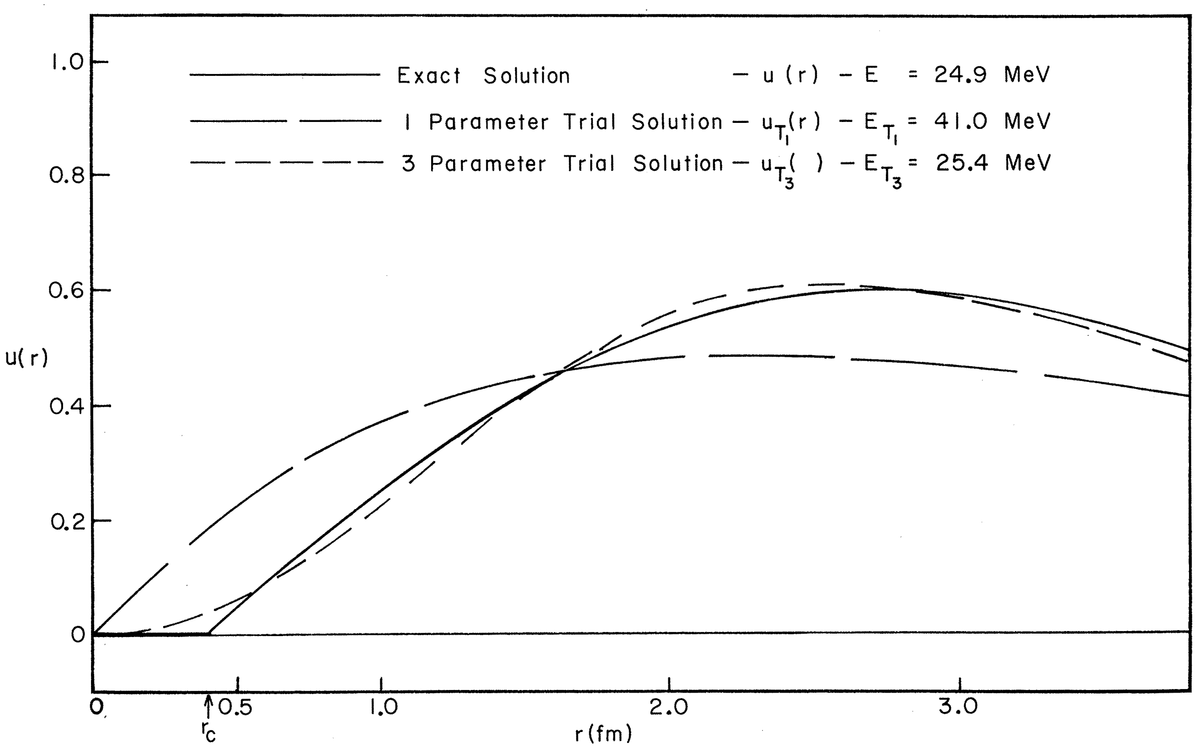

FIG. 1. Exact and trial ground-state wave functions for two particles interacting via a harmonic-oscillator plus hard-core potential. The hard core is simulated by $-2(\hbar^2/m_0)\delta'(r-r_c)$.

where the Hamiltonian separates for the center of mass and relative motion of the two interacting particles. The exact solution's wave function has the form

$$\psi(\vec{r}_1', \vec{r}_2', \vec{r}_3') = \Phi(\vec{R}_{\text{c.m.}}, \vec{R}, \vec{r}) = \sum a_{1mn}\eta_1(\vec{R}_{\text{c.m.}})\chi_m(\vec{R})\phi_n(\vec{r}) , \qquad (6)$$

where $\vec{R}_{\text{c.m.}}$, $\vec{R}$, and $\vec{r}$ represent the three-particle center of mass, two-particle center of mass, and two-particle relative motion, respectively. $\eta_1(\vec{R}_{\text{c.m.}})$ is a free-particle solution. The wave functions $\chi_m(\vec{R})$ and $\phi_n(\vec{r})$ satisfy the following equations

$$\frac{\hbar^2}{2\mu}(-\nabla_{\vec{R}}^2 + \alpha_R{}^4R^2)\chi_m(\vec{R}) = E_{R_m}\chi_m(\vec{R}) , \qquad (7)$$

$$\left[\frac{\hbar^2}{m_0}(-\nabla_{\vec{r}}^2 + \alpha_r{}^4r^2) + V(r)\right]\phi_n(\vec{r}) = E_{r_n}\phi_n(\vec{r}) , \qquad (8)$$

where $\mu = 2m_0M/(M+2m_0)$.

For the Hartree calculations

$$\chi_m(\vec{R})\phi_m(\vec{r}) = \psi_m(\vec{r}_1, \vec{r}_2) \simeq \psi_{H_m}(\vec{r}_1, \vec{r}_2) = f_m(\vec{r}_1)f_m(\vec{r}_2) , \qquad (9)$$

where for the analysis reported in this paper we have, for convenience, considered χ_m and ϕ_n to be in the same state of excitation ($m = n$). The particle coordinates $\vec{r}_1$ and $\vec{r}_2$ are defined by $\vec{r}_2 - \vec{r}_1 \equiv \vec{r}$ and $\frac{1}{2}(\vec{r}_2 + \vec{r}_1) \equiv [M/(M+2m_0)]^{1/2}\vec{R}$. The Hartree single-particle wave function $f_m(\vec{r}_1)$ satisfies the equation

$$\left[\frac{\hbar^2}{2m_0}(-\nabla_{\vec{r}}^2 + \alpha_H{}^4r_1{}^2) + V_{H_m}(\vec{r}_1) - \epsilon_{H_m}\right]f_m(\vec{r}_1) = 0 , \qquad (10)$$

where

$$V_{H_m}(\vec{r}_1) = \int f_m{}^*(\vec{r}_2)V(r)f_m(\vec{r}_2)d\vec{r}_2 . \qquad (11)$$

With this, the Hartree energy E_{H_m} of the three-particle system is given as

$$E_{H_m} = 2\epsilon_{H_m} - \int f_m{}^*(\vec{r}_1)V_{H_m}(\vec{r}_1)f_m(\vec{r}_1)d\vec{r}_1 . \qquad (12)$$

The quantity E_{H_m} is the Hartree approximation to the exact internal energy of the three-particle system $E_m = E_{r_m} + E_{R_m}$ (E_0, for example, is the ground-state energy). When the two-particle interaction $V(r)$ is the zero, E_{H_m} and E_m are identical.

It should be noted that Eq. (11), when $V(r)$ is the δ' form of $V_{\text{H.C.}}$ in Eq. (4), has the form[5]

$$V_{H_m}(r_1)_{\text{H.C.}} = 2\frac{\hbar^2}{m_0}\int\left[\frac{2}{r_c}|f_m(r_2)|^2 + \frac{d}{dr_2}|f_m(r_2)|^2\frac{r_c{}^2 + r_2{}^2 - r_1{}^2}{2r_cr_2}\right] \times \delta(|\vec{r}_1 - \vec{r}_2| - r_c)d\vec{r}_2 , \qquad (13)$$

which reduces to

$$V_{H_m}(r_1)_{\text{H.C.}} = \frac{1}{r_1}\frac{\hbar^2}{m_0}\left\{\int_{r_c^-}^{r_c^+}\frac{|U_m(r_2)|^2}{r_2}dr_2 + r_c \times\left[\frac{|U_m(r_c^+)|^2}{r_c^+} - \frac{(r_c - r_1)|U_m(r_c^-)|^2}{(r_c^-)^2}\right]\right\} , \qquad (14)$$

where $r_c^+ = r_c + r_1$, $r_c^- = |r_c - r_1|$, and $U_m(r_2) = 2\sqrt{\pi}\, r_2 f_m(r_2)$.

Exact and approximate results for the three-body problem are presented in Figs. 2 and 3, where energy spectra are shown for several forms of the two-particle interaction $V(r)$. The values of E_m and E_{H_m} were obtained by numerically integrating Eqs. (8) and (10),[5] respectively. The value of E_{H_0} was also estimated ($E_{H_0}{}^{(1)}$) by minimizing the expectation value of the Hamiltonian in Eq. (5) using a single-parameter Gaussian form for the Hartree wave functions $f_m(\vec{r}_1)$. The "zero" column represents $V(r) = 0$, where $E_m^0 \equiv E_m = E_{H_m}$.

Figure 2 shows the exact and approximate spectra obtained when $V(r)$ is simply a repulsive core. Results for the hard-core interaction of Eq. (4) are compared with those for two representative soft-core forms, a repulsive square well and a

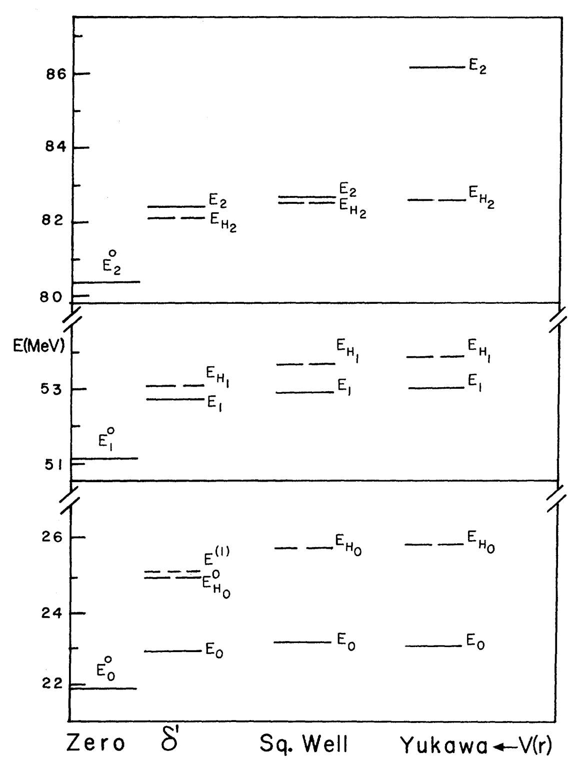

FIG. 2. Exact and Hartree spectra with various repulsive (soft-core) potentials for the two-particle interaction $V(r)$.

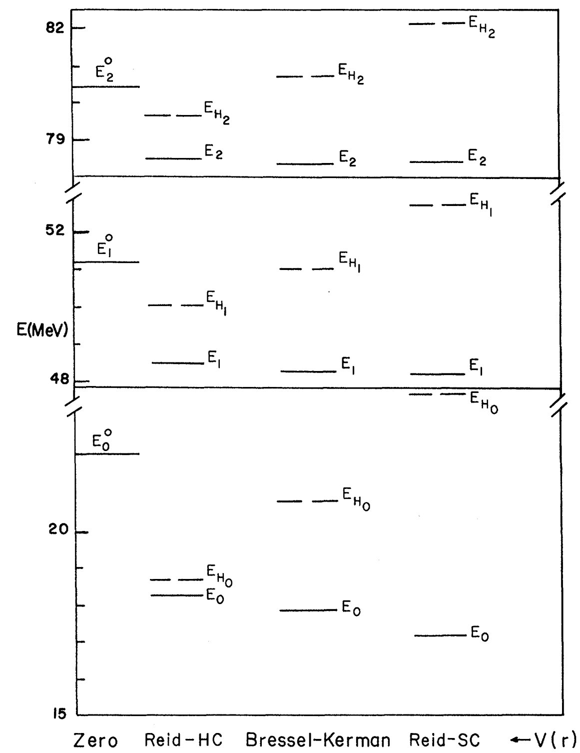

FIG. 3. Exact and Hartree spectra with various nucleon-nucleon potential models for the two-particle interaction $V(r)$. The hard-core part of Reid-HC is simulated by $-2(\hbar^2/m_0)\,\delta'(r-r_c)$.

repulsive Yukawa potential. (The parameters of the square well and Yukawa potentials were picked to be those which produce the soft-core parts of the nucleon-nucleon potentials discussed below.)

Figure 3 shows the exact and approximate spectra obtained when $V(r)$ is one of three current phenomenological models of the nucleon-nucleon potential. The first is the Reid hard-core potential[6] (REID-HC), where we have used $V_{\text{H.C.}}$ of Eq. (4) to represent the hard core and set the attractive part equal to a constant[7] for $r \leq r_c$. The other two are the Bressel-Kerman potential[8] (square-well repulsive core) and the Reid soft-core potential[6] (REID-SC, Yukawa repulsive core). In these calculations, $\alpha_H(=0.42 f_m^{-1})$ and $M(=16 m_0)$ were adjusted to correspond to the situation of two nucleons outside a light nucleus core. Other choices of α_H and M gave qualitatively the same findings.

DISCUSSION

The results presented here demonstrate that the δ' interaction, which has been shown to be equivalent to the usual hard core in *exact* calculations,[1] it also successful in *variational* calculations where it is desirable or necessary to extend the trial function into the hard-core region. Applications to Hartree-Fock theory of light nuclei[9] and low-energy nucleon-nucleus scattering[10] are in progress.

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[1]R. E. Schenter, R. L. Cassola, and H. S. Zwibel, Am. J. Phys. 37, 1242 (1969).

[2]Several papers in the past have discussed the use of the Dirac δ function and its derivatives sometimes combined with derivative operators to be used in many-body calculations. See for example, K. Huang and C. N. Yang, Phys. Rev. 105, 767 (1957); H. Fesbach, Ann. Phys. (N.Y.) 5, 357 (1958); R. Lipperheide, *ibid.* 17, 114 (1962); E. L. Loman and M. McMillan, *ibid.* 23, 439 (1963); M. Luban, Phys. Rev. 138, A1028, A1033 (1965).

[3]J. A. Wheeler, Phys. Rev. 52, 1083 (1937).

[4]I. Talmi, Helv. Phys. Acta 25, 185 (1952); M. Bauer and M. Moshinsky, Nucl. Phys. 4, 615 (1957); M. Moshinsky, Rev. Mex. Fis. 6, 185 (1957).

[5]For the work reported in this letter only s-wave solutions were considered.

[6]R. V. Reid, Ann. Phys. (N.Y.) 50, 411 (1968).

[7]This is necessary because Hamiltonians using $V_{\text{H.C.}}$ for a hard core possesses some solutions which are nonzero within the hard core. By setting the attractive potential equal to a constant $V_c\,(m_0/\hbar^2\,|V_c| \leq \pi/2r_c)$ within the hard core, we ensure that these solutions belong to large eigenvalues which do not affect the lower-energy hard-core solutions. See Ref. 1 and Luban (Ref. 2) for discussion of this point.

[8]C. N. Bressel, A. K. Kerman, and B. Rouben, Nucl. Phys. A124, 624 (1969).

[9]R. C. Braley, W. F. Ford, and R. E. Schenter, to be published.

[10]R. E. Schenter and R. L. Cassola, Bull. Am. Phys. Soc. 14, 529 (1969); R. E. Schenter and R. L. Cassola, to be published.