

Exact solvable three-dimensional models of many-body systems

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a uniform force F is present,

$$[H, T] = [H_0 - Fx, T] = FaT. \quad (5)$$

Hence, (2) becomes

$$\frac{d}{dt} \langle T \rangle = \frac{iFa}{\hbar} \langle T \rangle. \quad (6)$$

The solutions of this are of the form

$$\langle T \rangle = T_0 \exp[ik(t)a], \quad (7)$$

where T_0 is time independent and where $k(t)$ satisfies (1). This completes that part of the proof that does not address itself to the fact that a state with a single sharp value of k remains a state with a single sharp value of k .

So far, $k(t)$ need be only a certain kind of weighted average of the wavenumbers actually present in the state under consideration. To tighten up on the proof, we note that the expectation value $\langle T \rangle$ is simply the weighted average of the quantity $\exp(ika)$ for the different Bloch waves present in the state under consideration. The quantity $\exp(ika)$ may be viewed as a vector in the complex plane, whose endpoint is on the complex unit circle. The weighted average of two or more such vectors belonging to different reduced values of k and hence having different endpoints on the circle necessarily falls *inside* that circle. Hence we must have $|T_0| \leq 1$;

the limiting value $T_0 = 1$ occurs *if and only if* that state is a single Bloch wave or a linear superposition of Bloch waves belonging to the same *reduced* k . In this case, $k(t)$ is the reduced k , and we have shown that a state with a single sharp value of k remains indeed a state with a single sharp value of k .

This result holds independent of any interband transitions: Because such transitions take place between states that have the same expectation value of the translation operator, a consideration of the time evolution of the latter makes it unnecessary to consider interband transitions at all.

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¹See, for example, W. V. Houston, *Phys. Rev.* **57**, 184 (1940).

²For an in-depth survey, see G.H. Wannier, *Am. J. Phys.* **34**, 145 (1962).

³For example in C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1979), 5th ed., p. 212.

Exact solvable three-dimensional models of many-body systems

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This paper presents new realistic models of many-body systems. They provide a good insight into the dynamics of such systems as many-electron atoms, diatomic molecules, and various van der Waals complexes. These models can be used as excellent illustrations of the important topics of atomic and molecular physics.

I. INTRODUCTION

Exact solvable models of many-body systems are of great importance in the comprehension of the dynamics of motions of real systems. They are also useful from the theoretical point of view as they allow us to test various approximate methods.

The models set forth so far have been simplified too much to reflect even the principal features of the real systems. Most of them were based on the assumption of one-dimensional motions of particles interacting via Dirac delta function potentials. The models of such a kind were proposed for a two-electron atom,¹⁻⁶ a diatomic molecule,⁷⁻⁹ a collinear three-body system,¹⁰ and a system of N particles with equal interaction strength and equal mass.¹¹⁻¹³

Three-dimensional, but rather unrealistic models of particles interacting through pairwise harmonic potentials with zero equilibrium interparticle distance have been used

in the discussion of the vibration-rotational states of van der Waals molecules.¹⁴⁻¹⁶

In this paper we present a new class of three-dimensional models of many-body systems. Under adequate parametrization they can describe many-electron atoms, diatomic homo- and heteronuclear molecules, and various van der Waals complexes. These models reflect many features of real systems very well and they also allow us to obtain new information on many-body systems.

II. MODELS AND SOLUTIONS

In the calculation of the electronic energy of atoms and molecules, Gauss orbitals are commonly used as they resemble hydrogenlike orbitals, and their application significantly simplifies the calculation of atomic integrals. Gauss orbitals are the eigenfunctions of a three-dimensional harmonic oscillator. Thus a model of a Coulomb system with the attractive pairwise Coulomb potentials $-r_{ij}^{-1}$ re-

placed by the harmonic potentials $r_{i,j}^2$ constitutes a good qualitative description of the properties of the real systems. Such a model has been considered by Kesner and Sinanoğlu¹⁷ in the study of correlation effects in a two-electron atom.

In our models the repulsive Coulomb potentials $r_{i,j}^{-1}$ are also replaced by $r_{i,j}^{-2}$ terms. Thus the Hamiltonian of our models has the form

$$H = T + V^{(A)} + V^{(R)}, \quad (1)$$

where

$$T = -\frac{\hbar^2}{2} \sum_{i=1}^n m_i^{-1} \Delta_i, \quad (2a)$$

$$V^{(A)} = \sum_{(i,j) \in A} k_{i,j} (\mathbf{x}_i - \mathbf{x}_j)^2, \quad (2b)$$

and

$$V^{(R)} = \sum_{(i,j) \in R} k_{i,j} (\mathbf{x}_i - \mathbf{x}_j)^{-2}, \quad (2c)$$

where A and R are sets of pairwise attractive and repulsive particles, respectively. $\mathbf{x}_i = (x_i, y_i, z_i)$ is the Cartesian vector of the i th particle. For a given set of parameters $\{m_i, k_{i,j}\}$ the transformation A of the vectors $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\} = \mathbf{x}^T$ to the new vectors $\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n\} = \mathbf{r}^T$, where \mathbf{r}_n is the center of mass vector, can be found to be

$$\mathbf{r} = A\mathbf{x}, \quad (3)$$

such that the operators T , $V^{(A)}$, and $V^{(R)}$ take the diagonal forms, i.e.,

$$T = -\frac{\hbar^2}{2} \sum_{j=1}^{n-1} \mu_j^{-1} \Delta_j - \frac{\hbar^2}{2} \left(\sum_{j=1}^n m_j \right)^{-1} \Delta_n, \quad (4a)$$

$$V^{(A)} = \sum_{j=1}^{n-1} k_j^{(A)} r_j^2, \quad (4b)$$

and

$$V^{(R)} = \sum_{j=1}^{n-1} k_j^{(R)} r_j^{-2}. \quad (4c)$$

The last term in Eq. (4a) represents the kinetic energy operator of the system as a whole in translational motions and will not be considered any further.

In these new vector variables the Schrödinger equation

$$[H(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{n-1}) - E] \psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{n-1}) = 0 \quad (5)$$

is separable. Thus the problem is reduced to the solution of the set equations of the form

$$[-(\hbar^2/2\mu_j)\Delta_j + k_j^{(A)}r_j^2 + k_j^{(R)}r_j^{-2} - E_j] \psi_j(\mathbf{r}_j) = 0, \quad (6)$$

where

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{n-1}) = \prod_{j=1}^{n-1} \psi_j(\mathbf{r}_j) \quad (7a)$$

and

$$E = \sum_{j=1}^{n-1} E_j. \quad (7b)$$

These equations are easily solvable in the spherical coordinates $\mathbf{r}_j = (r_j, \theta_j, \varphi_j)$. Assuming $\psi_j(\mathbf{r}_j)$ as a product of the radial and angular functions,

$$\psi_j(\mathbf{r}_j) = \mathcal{R}_{n_p, l_j}(r_j) Y(\theta_j, \varphi_j), \quad (8)$$

we obtain the radial equations for the \mathcal{R}_{n_p, l_j} functions

(henceforth we will drop the index j)

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\Lambda + 2\mu k^{(R)}/\hbar^2}{r^2} \right) + k^{(A)}r^2 - E_{n,l} \right] \mathcal{R}_{n,l} = 0, \quad (9)$$

where

$$\Lambda = l(l+1). \quad (10)$$

The solutions of the above equations are well known¹⁸:

$$\mathcal{R}_{n,l} = \rho^\lambda \exp(-\rho^2/2) {}_1F_1(-n, \lambda + \frac{3}{2}, \rho^2), \quad (11)$$

where ${}_1F_1$ is the confluent hypergeometric function¹⁹ of the variable ρ^2 defined as

$$\rho^2 = \mu\omega r^2/\hbar, \quad \omega = (2k^{(A)}/\mu)^{1/2}. \quad (12)$$

The eigenvalues $E_{n,l}$ are

$$E_{n,l} = \hbar\omega(2n + \lambda + \frac{3}{2}), \quad (13)$$

where

$$\lambda = [(4\Lambda + 1 + 8\mu k^{(R)}/\hbar^2)^{1/2} - 1]/2. \quad (14)$$

Thus, if the transformation (3) exists, the solutions of the Schrödinger equation (5) are given by the formulas (7a)–(14).

III. EXAMPLES

A. Example 1: Three-body systems

Here we present some important models of three-body systems for which the transformation (3) exists. Let us consider a stable system composed of three particles making one pair of mutually repulsing and two pairs of mutually attracting particles. This system and its vectors \mathbf{x} and $\mathbf{r} = A\mathbf{x}$, where

$$A = \begin{bmatrix} 1 & -1 & 0 \\ -\tilde{\mu}_1 & \tilde{\mu}_2 & 1 \\ \nu_1 & \nu_2 & \nu_3 \end{bmatrix}, \quad (15)$$

where

$$\tilde{\mu}_i = m_i(m_1 + m_2)^{-1} \quad (16a)$$

and

$$\nu_i = m_i \left(\sum_{j=1}^n m_j \right)^{-1} \quad (16b)$$

are shown in Fig. 1. The vectors \mathbf{r}_i are the well-known Jacobi vectors.²⁰ The potentials $V^{(A)}$ and $V^{(R)}$ for this model system are as follows:

$$V^{(A)} = k_{1,3} (\mathbf{x}_1 - \mathbf{x}_3)^2 + k_{2,3} (\mathbf{x}_2 - \mathbf{x}_3)^2, \quad (17a)$$

$$V^{(R)} = k_{1,2} (\mathbf{x}_1 - \mathbf{x}_2)^{-2}. \quad (17b)$$

Under the transformation (15) these potentials take the

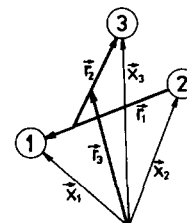


Fig. 1. The Cartesian \mathbf{x}_i and Jacobi \mathbf{r}_i vectors for the three-body system.

following forms:

$$V^{(A)} = k_1^{(A)} r_1^2 + k_2^{(A)} r_2^2 + 2k_h^{(A)} \mathbf{r}_1 \cdot \mathbf{r}_2, \quad (18a)$$

$$V^{(R)} = k_1^{(R)} r_1^{-2}, \quad (18b)$$

where

$$\begin{aligned} k_1^{(A)} &= k_{1,3} \tilde{\mu}_2^2 + k_{2,3} \tilde{\mu}_1^2, \\ k_2^{(A)} &= k_{1,3} + k_{2,3}, \\ k_h^{(A)} &= k_{2,3} \tilde{\mu}_1 - k_{1,3} \tilde{\mu}_2, \\ k_1^{(R)} &= k_{1,2}. \end{aligned} \quad (19)$$

The reduced masses μ_j in the operator T [see Eq. (4a)] are defined by the equations

$$\mu_1^{-1} = m_1^{-1} + m_2^{-1}, \quad (20)$$

$$\mu_2^{-1} = (m_1 + m_2)^{-1} + m_3^{-1}.$$

We can see that for $k_h^{(A)} = 0$ the Hamiltonian is separable. Equation $k_h^{(A)} = 0$ has two solutions:

$$\tilde{\mu}_1 = \tilde{\mu}_2, \quad k_{1,3} = k_{2,3}; \quad (21)$$

and

$$\tilde{\mu}_1 \neq \tilde{\mu}_2, \quad k_{1,3}/k_{2,3} = \tilde{\mu}_1/\tilde{\mu}_2. \quad (22)$$

The first solution defines the model of a two-electron atom or ion (when $m_1 = m_2 = m_e \ll m_3$) and the model of a homonuclear diatomic molecule ion (when $m_1 = m_2 \gg m_3 = m_e$). The second solution defines the special model of a heteronuclear diatomic molecule ion. Both solutions can also specify models of van der Waals molecules such as Ar XY with X, Y = N, O, Cl, etc.

B. Example 2: Four-body systems; a two-electron diatomic molecule

Let us consider the model system shown in Fig. 2 (only the vectors \mathbf{r}_i are presented). The operators $V^{(A)}$ and $V^{(B)}$ expressed in the vectors \mathbf{x}_i have the forms

$$V^{(A)} = k_{1,3} (\mathbf{x}_1 - \mathbf{x}_3)^2 + k_{1,4} (\mathbf{x}_1 - \mathbf{x}_4)^2 + k_{2,3} (\mathbf{x}_2 - \mathbf{x}_3)^2 + k_{2,4} (\mathbf{x}_2 - \mathbf{x}_4)^2, \quad (23a)$$

$$V^{(R)} = k_{1,2} (\mathbf{x}_1 - \mathbf{x}_2)^{-2} + k_{3,4} (\mathbf{x}_3 - \mathbf{x}_4)^{-2}. \quad (23b)$$

In the following we will take $m_3 = m_4$ and $k_{i,3} = k_{i,4}$ for $i = 1, 2$. Under the transformation

$$A = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ -\tilde{\mu}_1 & -\tilde{\mu}_2 & \frac{1}{2} & \frac{1}{2} \\ \nu_1 & \nu_2 & \nu_3 & \nu_4 \end{bmatrix}, \quad (24)$$

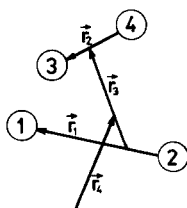


Fig. 2. The model of a two-electron diatomic molecule.

the potentials $V^{(A)}$ and $V^{(B)}$ take the following forms:

$$V^{(A)} = k_1^{(A)} r_1^2 + k_2^{(A)} r_2^2 + k_3^{(A)} r_3^2 + 4k_h^{(A)} \mathbf{r}_1 \cdot \mathbf{r}_3, \quad (25a)$$

$$V^{(R)} = k_1^{(R)} r_1^{-2} + k_2^{(R)} r_2^{-2}, \quad (25b)$$

where

$$\begin{aligned} k_1^{(A)} &= 2(k_{1,3} \tilde{\mu}_2^2 + k_{2,4} \tilde{\mu}_1^2), \quad k_1^{(R)} = k_{1,2}, \\ k_2^{(A)} &= (k_{1,3} + k_{2,4})/2, \quad k_2^{(R)} = k_{3,4}, \\ k_3^{(A)} &= 4k_2^{(A)}, \quad k_h^{(A)} = (k_{2,4} \tilde{\mu}_1 - k_{1,3} \tilde{\mu}_2). \end{aligned} \quad (26)$$

The reduced masses μ_j are given by the equations

$$\begin{aligned} \mu_1^{-1} &= m_1^{-1} + m_2^{-1}, \\ \mu_2^{-1} &= m_3^{-1} + m_4^{-1}, \\ \mu_3^{-1} &= (m_1 + m_2)^{-1} + (m_3 + m_4)^{-1}. \end{aligned} \quad (27)$$

The Hamiltonian is separable for $k_h^{(A)} = 0$. This equation has two solutions: $\tilde{\mu}_1 = \tilde{\mu}_2$, which defines the model of a two-electron homonuclear diatomic molecule; and $\tilde{\mu}_1 \neq \tilde{\mu}_2$, which defines the model of a heteronuclear diatomic molecule. Both solutions can also specify models of van der Waals and hydrogen bound complexes such as $(H_2)_2$, $(HF)_2$, etc.

C. Example 3: Four-body systems; a three-electron atom

Let us consider the model system shown in Fig. 3. The potentials $V^{(A)}$ and $V^{(R)}$ expressed in the vectors \mathbf{x}_i have the forms

$$V^{(A)} = \sum_{i=1}^3 k_{i,4} (\mathbf{x}_i - \mathbf{x}_4)^2, \quad (28a)$$

$$V^{(R)} = k_{1,2} (\mathbf{x}_1 - \mathbf{x}_2)^{-2} + k_{1,3} (\mathbf{x}_1 - \mathbf{x}_3)^{-2} + k_{2,3} (\mathbf{x}_2 - \mathbf{x}_3)^{-2}. \quad (28b)$$

In the following we will take $k_{i,4} \equiv k_4$, $k_{1,3} = k_{2,3}$, and $m_i \equiv m$, for $i = 1, 2, 3$. The transformation

$$A = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & -1 \\ \nu_1 & \nu_2 & \nu_3 & \nu_4 \end{bmatrix} \quad (29)$$

gives the potentials $V^{(A)}$ and $V^{(R)}$ in the forms

$$V^{(A)} = k_4 (3r_1^2 + 4r_2^2 + 18r_3^2)/6, \quad (30a)$$

$$V^{(R)} = k_{1,2} r_1^{-2} + k_{1,3} [(\mathbf{r}_2 - \mathbf{r}_1/2)^{-2} + (\mathbf{r}_2 + \mathbf{r}_1/2)^{-2}]. \quad (30b)$$

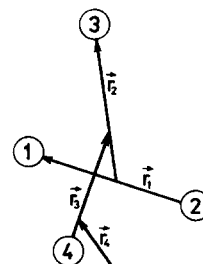


Fig. 3. The model of a two-electron atom.

The reduced masses μ_j are

$$\mu_1 = m/2, \quad \mu_2 = m/3, \quad \mu_3^{-1} = 3m^{-1} + m_4^{-1}. \quad (31)$$

For $r_2 \gg r_1$ we can write

$$|\mathbf{r}_2 \pm \mathbf{r}_1/2| \cong r_2.$$

The simplified model with

$$V^{(R)} = k_{1,2}r_1^{-2} + 2k_{1,3}r_2^{-2} \quad (32)$$

is solvable and can be used as the model of a three-electron atom with one highly excited electron.

It is also possible to construct various simplified models of this kind: for example, a model of an atom interacting with a diatomic molecule, a model of two interacting diatomic molecules, etc.

IV. DISCUSSION

The models of many-body systems presented in this paper can describe atoms, molecules, and van der Waals complexes. Many features of these systems are adequately represented in the models considered and will be examined in subsequent papers. These models allow us to illustrate many important problems of atomic and molecular physics.

The parameters m_i and $k_{i,j}$, which specify the models, can be varied enabling us to analyze the connections between the states of various systems. So far, only correlation diagrams for the electron states of atoms and molecules have been constructed. However, in such diagrams the internuclear distance is treated as a parameter and not as a dynamical variable.

It would be interesting to find out how the vibrational states of a molecule arise from the atomic states. Our models enable a continuous change of parameters, which leads to new model systems. For example, a three-body system

with $m_3 = m_{\text{He}}$ and $m_1 = m_2 = m_e$ describes the He atom. Changing m_3 from m_{He} to m_e and m_1 from m_e to m_p , we transform the model of the He atom to the model of the H_2^+ molecule. Thus, it becomes possible to construct correlation diagrams of a new type.

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SOLUTION TO THE PROBLEM ON PAGE 121

The three components of the dipole field in spherical coordinates are

$$B_r = (\mu_0/4\pi)(2M/r^3)\cos\theta,$$

$$B_\theta = (\mu_0/4\pi)(M/r^3)\sin\theta,$$

$$B_\phi = 0,$$

where M = magnetic moment of earth, θ = co-latitude of earth, and $k = \mu_0 M/4\pi$.

The magnetic induction

$$\mathbf{B} = (2k/r^3)\cos\theta\mathbf{a}_r + (k/r^3)\sin\theta\mathbf{a}_\theta + 0\mathbf{a}_\phi.$$

$$|B| = \sqrt{\frac{4k^2}{r^6}\cos^2\theta + \frac{k^2}{r^6}\sin^2\theta} = \frac{k}{r^3}\sqrt{3\cos^2\theta + 1}.$$

The magnetic energy

$$U = \frac{1}{2\mu_0} \int_{\text{volume}} B^2 dV,$$

$$U = \frac{1}{2\mu_0} \int_r \int_\phi \int_\theta B^2 r^2 \sin\theta dr d\phi d\theta,$$

$$U = \frac{2\pi}{2\mu_0} \int_{R_E}^{\infty} \frac{k^2}{r^6} r^2 dr \int_{\theta=0}^{\pi} (3\cos^2\theta + 1)\sin\theta d\theta,$$

$$U = 4\pi k^2/3\mu_0 R_E^3 = \mu_0 M^2/12\pi R_E^3.$$

Determine M by using the dipole field at the equator:

$$B_{\text{EQ}} = \frac{1}{3} * 10^{-4} \text{ T} = \mu_0 M/4\pi R_E^3,$$

where $\mu_0 = 4\pi * 10^{-7}$ mks and $R_E = 6.4 * 10^6$ m.

$$M = 4\pi R_E^3 B_{\text{EQ}}/\mu_0 = 8.74 * 10^{22} \text{ amp} \cdot \text{m}^2.$$

Then,

$$U = \mu_0 M^2/12\pi R_E^3 = 9.7 * 10^{17} \text{ J} = 230 \text{ MT},$$

where 1 MT = $4.2 * 10^{15}$ J.

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