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Research Article

A Self-Consistent Iterative Calculation for the Two Species of Charged Bosons Related to the Nuclear Reactions in Solids

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Abstract

Many theoretical studies on cold fusion have been done by many workers using Bose–Einstein condensation (BEC) in order to find a possible mechanism of this phenomenon. In our previous work on BEC approach to the theoretical interpretation of cold fusion, we estimated the transition temperature of BEC in palladium deuteride [1]. It was based on the Y.E.Kim's work by using equivalent linear two-body (ELTB) method to the many-body problems of charged bosons trapped in an ion trap [2]. Recently, Kim et al. tried to explain the results of Rossi's experiment [3] by using the ELTB method for a mixture of different two species of positive charged bosons trapped to the harmonic potential [4]. In this study, we verified Kim's theory and considered how to perform the numerical calculation. A self-consistent iterative calculation was introduced and the coupled two equations corresponding to the two species of positive charged bosons were solved.
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1. Introduction

Here, we briefly introduce the theory of Kim et al [4]. In their theory, the Schrödinger equation for the mixture of two different species of positive charged bosons are written as

$$\left\{-\frac{\hbar^2}{2m_i}\nabla^2 + V_i(\mathbf{r}) + W_i(\mathbf{r})\right\}\psi_i(\mathbf{r}) = \mu_i\psi_i(\mathbf{r}), \tag{1}$$

where the two species are labeled by $i = 1, 2$. The first term on the left-hand side means the kinetic energy of the boson i and the second and third terms mean the following. The potential V_i means the harmonic potential induced by the electromagnetic ion trap. In the real lattice, it corresponds to the interaction between a boson and host metal ions. The potential W_i corresponds to the electro-static potential, which means the interaction between bosons. Therefore, W_i depends on the states ψ_i and ψ_j. The energy eigenvalue μ_i means chemical potential of the system.

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The solutions of Eq. (**??**) give the number densities of each boson, which means the probability density of the particle. They are written as

$$n_i(\mathbf{r}) = |\psi_i(\mathbf{r})|^2. \tag{2}$$

The normalized states should satisfy the volume integration of the number densities over the all space, which is written as

$$\int \mathrm{d}\mathbf{r}\, n_i(\mathbf{r}) = N_i. \tag{3}$$

This means that the total number of the boson i is always N_i. We can normalize ψ_i by using Eq. (**??**).

On the other hand, it is well-known that the charge distributions in the system and the electro-static potentials should satisfy the Poisson's equation which is written as

$$\nabla^2 W_i(\mathbf{r}) = -\frac{e^2}{\varepsilon_0} Z_i \left\{ Z_i n_i(\mathbf{r}) + Z_j n_j(\mathbf{r}) \right\}, \tag{4}$$

where eZ_i is the charge of an ionized boson i and ε_0 means the dielectric constant of the vacuum.

Kim et al. have proposed the method in order to describe the states of the Bose–Einstein condensation (BEC) for the mixture of two different species of positive charged bosons by using Eqs. (1) and (4). They also emphasized the nuclear reactions in solids can be explained by using BEC, which can achieve the large overlap of the wave functions of charged bosons.

2. Self-consistent Solution

We can easily understand that Eqs. (1) and (4) for each boson are linked each other. For example, the states ψ_i and ψ_j are linked each other. The state ψ_i and the potential W_i are also linked each other. Therefore, we cannot obtain the solutions by simple method. In this study, we have tried to obtain the self-consistent solution of them by iterative substitutions.

Firstly, we introduce the Green's function for the well-known Helmholtz equation [5] ARFKEN which is written as

$$G_k(\mathbf{r}) = \frac{\mathrm{e}^{-k|\mathbf{r}|}}{4\pi|\mathbf{r}|}, \tag{5}$$

where k is a positive real constant. This function satisfies the differential equation of

$$\left(\nabla^2 - k^2\right) G_k(\mathbf{r}) = -\delta(\mathbf{r}), \tag{6}$$

where $\delta(\mathbf{r})$ is the 3-dimensional Dirac's delta function. By using this Green's function, Eq. (**??**) is translated from the differential equation into the integral equation. As a result, it is rewritten in the form of the density functional formalism as

$$W_i(\mathbf{r}) = \int \mathrm{d}\mathbf{r}' G_k(\mathbf{r} - \mathbf{r}') \times \left[\frac{e^2}{\varepsilon_0} Z_i \left\{ Z_i n_i(\mathbf{r}') + Z_j n_j(\mathbf{r}') \right\} + k^2 W_i(\mathbf{r}') \right]. \tag{7}$$

This is a typical formula for the iterative substitutions. If we regard $W_i(\mathbf{r}')$, $n_i(\mathbf{r}')$ and $n_j(\mathbf{r}')$ on the right-hand side of Eq. (**??**) as old quantities, they will make new $W_i(\mathbf{r})$ on the left-hand side through the volume integration over the

all space. Fundamentally, the constants k in Eqs. (5)–(7) are arbitrary when they are positive and real, because the subtraction of $k^2 W_i(\mathbf{r})$ from both side of Eq. (**??**) leads to Eq. (**??**). When we solve Eq. (**??**) numerically, Runge–Kutta–Gill method is used for the calculation. Usually, we start the calculation from $r = 0$ and proceed it to large r. At the final region of these calculations, the errors are accumulated larger and larger. However, these errors included in the number density n_i and n_j are eliminated by the damping factor of the Green's function in Eq. (**??**).

If we consider the ground state of the system, n_i and W_i should have spherical symmetries. Then, we can easily calculate the angular components of the volume integration in Eq. (**??**) and it becomes the function of $r = |\mathbf{r}|$ as

$$\begin{aligned} W_i(r) = & \frac{\mathrm{e}^{-kr}}{kr} \int_0^r \mathrm{d}r' r' \sinh(kr') F_i(r') \\ & + \frac{\sinh(kr)}{kr} \int_r^\infty \mathrm{d}r' r' \mathrm{e}^{-kr'} F_i(r'), \end{aligned} \tag{8}$$

where the function F_i is defined as

$$F_i(r) = \frac{e^2}{\varepsilon_0} Z_i \left\{ Z_i n_i(r) + Z_j n_j(r) \right\} + k^2 W_i(r). \tag{9}$$

The electro-static potential written in this formula has no divergence difficulties in the numerical calculations at the origin. The harmonic potential is also defined as

$$V_i(r) = \frac{1}{2} m_i \omega_i^2 r^2. \tag{10}$$

Using these potentials, the radial Schrödinger equation for s-like ground state is written as

$$\begin{aligned} & \left\{ -\frac{\hbar^2}{2m_i} \frac{1}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} \left(r^2 \frac{\mathrm{d}}{\mathrm{d}r} \right) + V_i(r) + W_i(r) \right\} \psi_i(r) \\ & \quad = \mu_i \psi_i(r), \end{aligned} \tag{11}$$

where the angular momentum term $l(l+1)\hbar^2/2m_i r^2$ is omitted because $l = 0$ for the ground state.

In order to begin the iterative calculations, we assumed the initial functions for the quantities on the right-hand side of Eq. (**??**) as

$$W_i(r') = 0 \tag{12}$$

and

$$n_i(r') = n_{0i} \theta(R_i - r'), \tag{13}$$

where the step function θ is defined as $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$. The parameters n_{0i} and R_i in Eq. (**??**) should satisfy

$$\frac{4}{3} \pi R_i^3 n_{0i} = N_i. \tag{14}$$

This means that the initial boson distributions are uniform in the sphere of radius R_i neglecting the interaction between charged bosons. Starting from these assumptions, we can solve Eq. (**??**) numerically, and the first solutions give the normalized new densities by using Eqs. (2) and (3. These densities are used for obtaining the new W_i by solving Eq. (**??**). After that, new W_i is substituted into Eq. (**??**) again and the second wave functions are obtained. These procedures will be continued until the enough self-consistency is obtained. It is checked by seeing the stability of the energy eigenvalue. The flow chart for the self-consistent calculation is shown in Fig. 1.

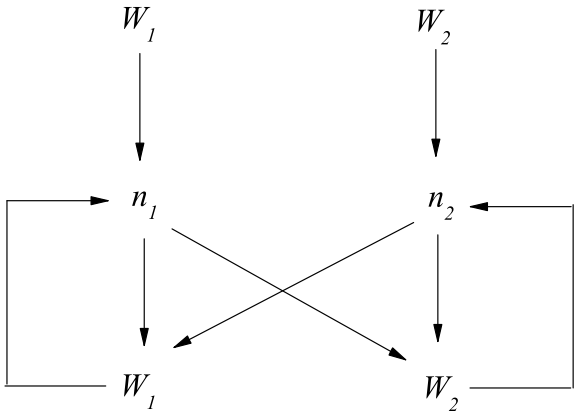

Figure 1. The flow chart for the self-consistent calculation. Using Eqs. (12)– (14), the initial function of W_i can be given by Eq. (7). The densities n_i and the electro-static potentials W_i are obtained alternatively by using Eqs. (1) and (7). The self-consistencies should be checked on the two loops in this diagram connected in parallel.

3. Units of the Calculations

We used the same unit with the pure harmonic problem. Here, they are explained briefly. It is well-known that the position r of a particle is translated into the non-dimensional quantity ξ_i by using

$$\xi_i = \alpha_i r, \tag{15}$$

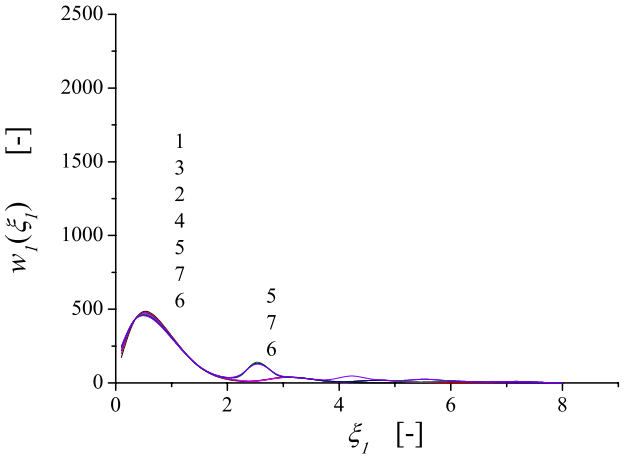

Figure 2. Change of the electro-static potential for D^+ along the iteration. The iteration numbers are also shown at the right sides of the first and second peaks. The array of them corresponds to the heights of the peaks.

where parameter α_i is given by

$$\alpha_i = \sqrt{\frac{m_i \omega_i}{\hbar}}. \tag{16}$$

In Eq. (**??**), the inverse of α_i corresponds to the classical turning point of a particle with energy $\hbar\omega_i/2$, which means the ground state energy of the quantum mechanical harmonic oscillator. Therefore, Eq. (**??**) means that ξ_i is the normalized position of the particle by the classical turning point. In Eq. (**??**), ω_i and m_i mean a frequency of the harmonic ion trap and mass of the particle, respectively. The chemical potential μ_i is also normalized by the ground state energy as

$$\varepsilon_i = \frac{2\mu_i}{\hbar\omega_i}. \tag{17}$$

By using these transformations, the radial Schrödinger equation is rewritten as

$$\left\{ -\frac{\mathrm{d}^2}{\mathrm{d}\xi_i^2} - \frac{2}{\xi_i}\frac{\mathrm{d}}{\mathrm{d}\xi_i} + \xi_i^2 + w_i(\xi_i) \right\} \psi_i(\xi_i) = \varepsilon_i \psi_i(\xi_i), \tag{18}$$

where w_i means the normalized electro-static potential. It is written as

$$\begin{aligned} w_i(\xi_i) = \; & \frac{\mathrm{e}^{-k_i\xi_i}}{k_i\xi_i} \int_0^{\xi_i} \mathrm{d}\xi_i' \, \xi_i' \sinh(k_i\xi_i') f_i(\xi_i') \\ & + \frac{\sinh(k_i\xi_i)}{k_i\xi_i} \int_{\xi_i}^{\infty} \mathrm{d}\xi_i' \, \xi_i' \mathrm{e}^{-k_i\xi_i'} f_i(\xi_i'), \end{aligned} \tag{19}$$

where function f_i is defined as

$$\begin{aligned} f_i(\xi_i) = \; & C_i Z_i \left\{ Z_i n_i(\xi_i) + Z_j n_j \left(\frac{\alpha_j}{\alpha_i}\xi_i \right) \right\} \\ & + k_i^2 w_i(\xi_i). \end{aligned} \tag{20}$$

In these equations, constants k_i and C_i are defined as

$$k_i = \frac{k}{\alpha_i} \tag{21}$$

and

$$C_i = \frac{2e^2}{\hbar\omega_i\alpha_i^2\varepsilon_0}. \tag{22}$$

In Eq. (**??**), it should be noticed that ξ_i and $\xi_j = \frac{\alpha_j}{\alpha_i}\xi_i$ indicate a same point $r = \frac{\xi_i}{\alpha_i} = \frac{\xi_j}{\alpha_j}$ in the original coordinate. Therefore, the argument of n_j in Eq. (**??**) is not ξ_i but $\frac{\alpha_j}{\alpha_i}\xi_i$. This means that the function f_i is not identical with f_j for the case of $\alpha_j \neq \alpha_i$.

Furthermore, we can obtain simpler expression by using a new function $u_i(\xi_i)$, which is defined as

$$\xi_i \psi_i(\xi_i) = u_i(\xi_i). \tag{23}$$

The new expression is written as

$$\left\{ -\frac{\mathrm{d}^2}{\mathrm{d}\xi_i^2} + \xi_i^2 + w_i(\xi_i) \right\} u_i(\xi_i) = \varepsilon_i u_i(\xi_i). \tag{24}$$

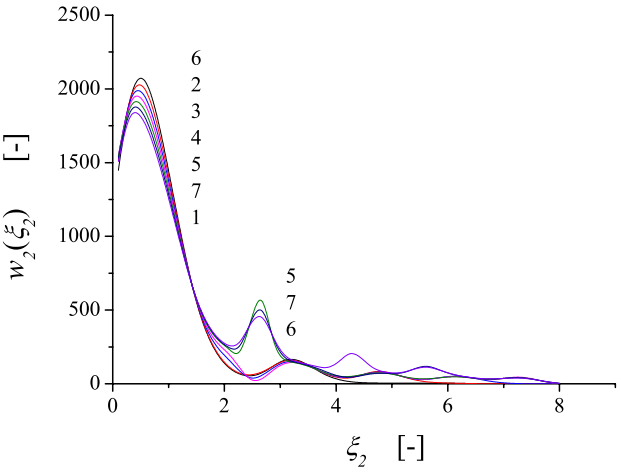

Figure 3. Change of the electro-static potential for $^6Li^+$ along the iteration. The iteration numbers are also shown at the right sides of the first and second peaks. The array of them corresponds to the heights of the peaks.

The relation between the solution of Eq. (**??**) and the number density is written as

$$n_i(\xi_i) = \left\{ \frac{u_i(\xi_i)}{\xi_i} \right\}^2 . \tag{25}$$

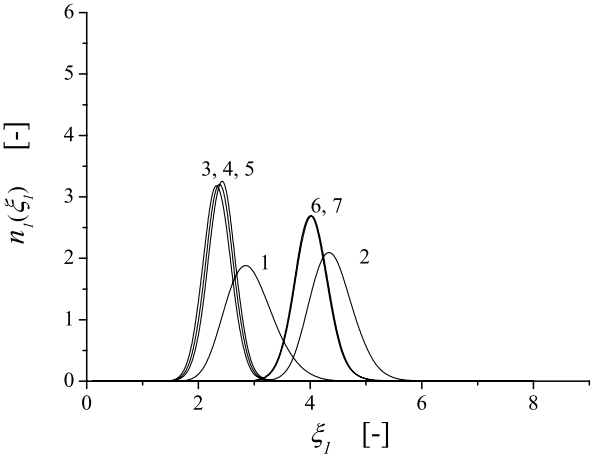

Figure 4. Change of the density for D^+ along the iteration. The iteration numbers are also shown in the figure.

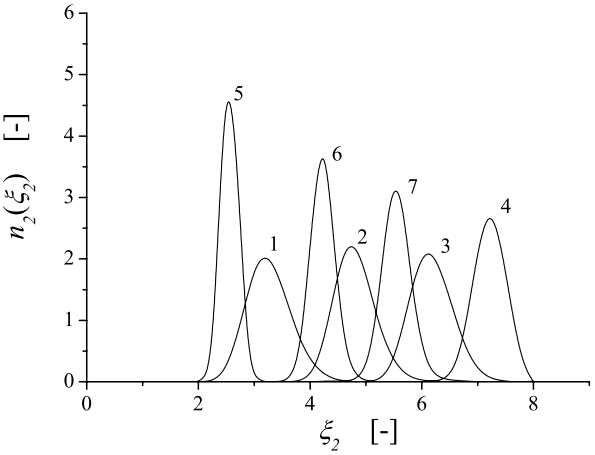

Figure 5. Change of the density for $^6Li^+$ along the iteration. The iteration numbers are also shown in the figure.

Therefore, the normalized solution of the new equation should satisfy

$$4\pi \int_0^\infty d\xi_i \, \{u_i(\xi_i)\}^2 = N_i. \tag{26}$$

In Eq. (**??**), the number density $n_i(\xi_i)$ for boson i is a non-dimensional function, because ξ_i is a dimensionless variable. If we need to know the number density in the original coordinate system, $\alpha_i^3 n_i(\alpha_i r)$ with a dimension of the reciprocal volume should be used.

The unperturbed eigenvalue of the ground state is $\varepsilon_i = 3$, because it is a radial component of a 3-dimensional problem. The unperturbed solution corresponding to $\varepsilon_i = 3$ is written as

$$u_i(\xi_i) = \xi_i H_0(\xi_i) e^{-\xi_i^2/2}, \tag{27}$$

where the function $H_0(x) = 1$ is the well-known Hermite polynomials in the 0th order [6]. At first, the eigenvalues for the perturbed system are unknown. However, we can find them by using the fact that Eq. (**??**) can be regarded as an asymptotic solution of the perturbed system for large ξ_i.

4. Results and Discussions

We have tried the calculations for $3D^+ + 3^6Li^+$ in an ion trap. In this case, D^+ and $^6Li^+$ are bosons, because they are composite particles with even number of fermions. For example, D^+ consists of a proton and a neutron, and $^6Li^+$ consists of three protons and three neutrons. The combinations of the positively charged two bosons and their numbers are arbitrary. However, we have chosen $3D^+ + 3^6Li^+$ case as a first step trial. The labels for D^+ and $^6Li^+$ are $i = 1$ and 2, respectively. In this study, $\omega_i = 4.79 \times 10^{14} s^{-1}$ is assumed for both particles. Using this frequency, the parameters α_i's for $i = 1$ and 2 are 1.23×10^{11} and $2.14 \times 10^{11} m^{-1}$, respectively. And the parameters k_i's for $i = 1$ and 2 are 29.1 and 16.8, respectively. For the initial density, we assume that $\alpha_i R_i$'s for $i = 1$ and 2 are 3.23 and 5.60, respectively.

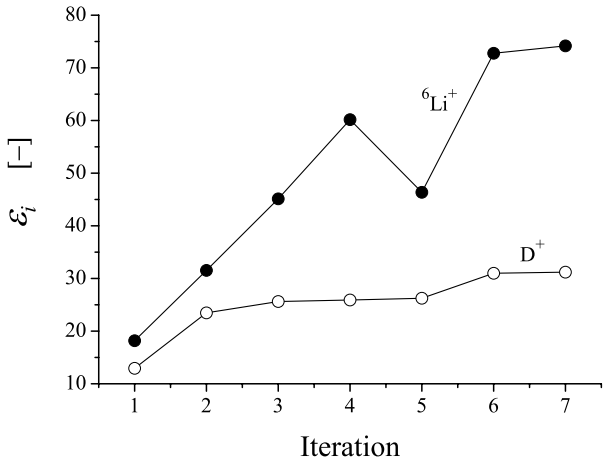

Figure 6. Energy eigenvalues for D^+ and $^6Li^+$ as a function of iterations.

Results for the electro-static potentials are plotted in Figs. 2 and 3. And results for the densities are plotted in Figs. 4 and 5. The check of self-consistency is done in Fig. 6. Seeing Figs. 2 and 3, the electro-static potentials are well converged. In both figures, changes of the first peaks are very small. And we can find the almost convergent second peak when the iteration is larger than 4.

On the other hand, seeing Figs. 4 and 5, the convergences are incomplete. In both figures, we can see the inversions of the gaussian-like peak positions. For example, the peak of n_2 suddenly shifts to the left after the 4th iteration in Fig. 5. The energy eigenvalue depression for $^6Li^+$ at the 5th iteration in Fig. 6 may cause the inversion in Fig. 5. However, the entire aspects of energy eigenvalue changes in Fig. 5 show the good convergences. If we continue the iteration, the inversion of the densities will appear again and again but gradually be smaller.

5. Conclusions

In this study, we have done the self-consistent iterative calculations for the two species of charged bosons. We have adopted $3D^+$+3^6Li^+ case for the mixtures of charged bosons and obtained the self-consistent densities. As a result, we have confirmed that $3D^+$ and 3^6Li^+ coexist at a time in an ion trap with $\omega_i = 4.79 \times 10^{14} s^{-1}$ for both particles.

In the next step, we will calculate the fusion rate by using Kim's theory [4]. The overlaps of the wave functions will make the finite value of fusion rates. In the near future, we will do it and report the results to some CF societies.

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References

[1] K.Tsuchiya, Quantum states of deuterons in Pd, *Int. J. Hydrogen Energy* **29** (2004) 1513–1519.
[2] Y.E. Kim and A.L. Zubarev, Nuclear fusion for bose nuclei confined in ion trap, *Fusion Technol*. **37** (2000) 151–156.
[3] S. Focardi and A. Rossi, *A New Energy Source from Nuclear Fusion*, March 22, 2010, *Ny Teknik*.
[4] Y.E. Kim and A.L. Zubarev, Mixtures of charged bosons confined in harmonic traps and Bose–Einstein condensation mechanism for low energy nuclear reactions and transmutation process in condensed matter, *Condensed Matter Nuclear Science, Proc. of ICCF11*, France, pp.711–717.
[5] G. Arfken, *Mathematical Methods for Physicists*, the 3rd Edition, Section 16.6, Academic Press, New York.
[6] L.I. Schiff, *Quantum Mechanics*, 3rd Edition, Section 4.13, McGraw-Hill, New York.