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Quantum states of deuterons in palladium

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Bose-Einstein condensation (BEC) is one of the candidates to induce the nuclear fusions in solids, because d-d repulsions are screened by conduction electrons and deuterons can be condensed at defects in solids. In this work, d-d fusion rate in Pd induced by BEC is estimated. The equivalent linear two-body method, which is based on an approximate reduction of many-body problems by variational principle, is used for the calculation. Thomas-Fermi and non-linear screening potentials are used as d-d interactions.

1 Introduction

Using equivalent linear two-body (ELTB) method to the many-body problems of charged bosons trapped in an ion trap [1], Y.E.Kim and A.L.Zubarev [2] derived the ground-state wave function and the nucleus-nucleus fusion rate. In this work, Kim-Zubarev theory is modified in the following two points. Firstly, vacancies in solid are regarded as harmonic ion traps and the frequency of this potential is estimated by using spherical approximation. The ELTB solution is obtained numerically and also the rate of d-d nuclear fusion in Pd lattice defect is obtained. Secondly, the critical temperature of this phenomenon is introduced.

2 Application of Kim-Zubarev Method to the Phenomenon in Solids

In Kim-Zubarev method, an isotropic harmonic potential is used for the ion trap potential. Then the Hamiltonian of the system including N charged particle is

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \frac{m\omega^2}{2}\sum_{i=1}^{N}\mathbf{r}_i^2 + \sum_{i<j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{1}$$

where $\mathbf{r}_i$ is the position of the particle. Using ELTB method, the ground state of this many-body problem is written as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \approx \frac{\phi(\rho)}{\rho^{(3N-1)/2}}, \tag{2}$$

$$\rho = \left(\sum_{i=1}^{N}\mathbf{r}_i^2\right)^{1/2}. \tag{3}$$

The wave function ϕ in eq.(2) satisfies

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{d\rho^2} + \frac{\hbar^2}{2m}\frac{(3N-1)(3N-3)}{4\rho^2} + \frac{m\omega^2\rho^2}{2} + \frac{2N\Gamma\left(\frac{3N}{2}\right)}{3\sqrt{2\pi}\,\Gamma\left(\frac{3(N-1)}{2}\right)}\frac{e^2}{\rho}\right\}\phi(\rho) = E\phi(\rho). \tag{4}$$

The fourth term is the translated form of the summation $\sum_{i<j} \mathrm{v}(|\mathbf{r}_i - \mathbf{r}_j|)$ in eq.(1) into ρ space by

$$V(\rho) = \frac{N(N-1)\Gamma\left(\frac{3N}{2}\right)}{\sqrt{2\pi}\Gamma\left(\frac{3(N-1)}{2}\right)\rho^3} \int_0^{\sqrt{2}\rho} dr r^2 \mathrm{v}(r) \left(1 - \frac{r^2}{2\rho^2}\right)^{\frac{3N-5}{2}}. \tag{5}$$

Using $x = \sqrt{m\omega/\hbar}\, r$ and $\varepsilon = 2E/\hbar\omega$, eq.(4) is rewritten as

$$\left(-\frac{d^2}{dx^2} + x^2 + \frac{p}{x^2} + \frac{q}{x}\right)\phi(x) = \varepsilon\phi(x), \tag{6}$$

$$p = \frac{(3N-1)(3N-3)}{4} \quad \text{and} \quad q = \alpha\sqrt{\frac{mc^2}{\hbar\omega}} \frac{4N\Gamma\left(\frac{3N}{2}\right)}{3\sqrt{2\pi}\Gamma\left(\frac{3(N-1)}{2}\right)}, \tag{7}$$

where α is the fine structure constant.

Now the application of Kim-Zubarev method to the phenomenon in solid is shown here. In eqs.(4) and (6), harmonic term is the electro magnetically induced potential in the ion trap device. [1] In crystalline solids, this term corresponds to the interaction between host ions and impurity deuterons. The Hamiltonian of this system is written as

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2 + \sum_{ij} \frac{Ze^2 \exp(-K|\mathbf{R}_j - \mathbf{r}_i|)}{|\mathbf{R}_j - \mathbf{r}_i|} + \sum_{i<j} \frac{e^2 \exp(-k|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{8}$$

where $\mathbf{R}_j$ is the Bravais lattice vector and Z is the effective charge of a host ion. By intuitive estimation, the second term in eq.(8) is approximately harmonic at the center of the defects in the crystalline solids. This can be explained as following. The i-th component of the second term in eq.(8) can be expanded into spherical harmonics as

$$\sum_j \frac{Ze^2 \exp(-K|\mathbf{R}_j - \mathbf{r}_i|)}{|\mathbf{R}_j - \mathbf{r}_i|} = \sum_{lm} A_{lm}(r_i) Y_{lm}(\theta, \phi). \tag{9}$$

If this is approximately spherical function, dominant term in the expansion is the $l = m = 0$ component, which is written as

$$A_{00}(r_i)Y_{00}(\theta,\phi) = Ze^2 \frac{\sinh Kr_i}{Kr_i} \sum_j \frac{\exp(-KR_j)}{R_j} \approx Ze^2 \left\{1 + \frac{(Kr)^2}{6}\right\} \sum_j \frac{\exp(-KR_j)}{R_j}. \tag{10}$$

Therefore, if we define ω as

$$\frac{Ze^2K^2}{6} \sum_j \frac{\exp(-KR_j)}{R_j} \equiv \frac{1}{2} m\omega^2, \tag{11}$$

the second term in eq.(8) becomes $\text{constant} + \frac{1}{2}m\omega^2 \sum_i \mathbf{r}_i^2$ for small Kr. This means that transformed form of the second term in eq.(8) into ρ space is similar to the third term in eq.(4). On the other hand, transformed form of the third term in eq.(8) into ρ space is not similar to the fourth term in eq.(4) because of the existence of the screening factor $\exp(-k|\mathbf{r}_i - \mathbf{r}_j|)$. If we transform eq.(8) into x space, it is written as

$$\left(-\frac{d^2}{dx^2} + x^2 + \frac{p}{x^2} + \frac{q}{x} f(x)\right)\phi(x) = \varepsilon\phi(x), \tag{12}$$

where f is a screening function. For Thomas-Fermi potential it is given by

$$f_{TF}(x) = 3(N-1)\int_0^{\frac{\pi}{2}} d\theta \sin\theta \cos^{3N-4}\theta \exp\left(-k\sqrt{\frac{2\hbar}{m\omega}} x \sin\theta\right). \tag{13}$$

3 Non-Linear Screening Potential

It is well known that deuterons provide very strong potentials to the electron gas. This effect is introduced by using the density functional formalism of Hohenberg-Kohn-Sham.[3,4] From the variational principle, they have derived the one body equation;

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + \Phi(\mathbf{r}) + V_{xc}(\mathbf{r})\right\}\psi_k(\mathbf{r}) = \varepsilon_k\psi_k(\mathbf{r}), \tag{14}$$

where Φ and V_{xc} are electrostatic and exchange-correlation potential, respectively. From the self consistent solutions of eq.(14), the density of the non-linear screening cloud induced around a deuteron in the electron gas can be obtained. The non-linear screening d-d interaction is obtained by considering the change in energy due to the embedding of two deuterons in electron gas. It is written as

$$V_{NL}(r) = \frac{e^2}{r} - 2\mathrm{v}_s(r) + \int d\mathbf{r}' \Box n(\mathbf{r}')\{\mathrm{v}_s(|\mathbf{r}-\mathbf{r}'|) + \phi_{xc}(|\mathbf{r}-\mathbf{r}'|)\}, \tag{15}$$

where $\Box n$, v_s and ϕ_{xc} are deviation of electron density from mean density , induced static potential and exchange-correlation potential, respectively. They are defined as

$$\mathrm{v}_s(|\mathbf{r}_1 - \mathbf{r}_2|) = \int d\mathbf{r}\frac{e^2 \Box n(|\mathbf{r}-\mathbf{r}_1|)}{|\mathbf{r}-\mathbf{r}_2|}, \tag{16}$$

$$\phi_{xc}(r) = \mathrm{v}_{xc}(n_0 + \Box n(r)) - \mathrm{v}_{xc}(n_0) \quad \text{and} \quad \mathrm{v}_{xc} = \frac{d(\varepsilon_{xc} n)}{dn}, \tag{17}$$

where $\mathbf{r}_i$ is the position of a deuteron and ε_{xc} is the exchange-correlation energy per one electron. The calculated results of d-d pair potential using non-linear and Thomas-Fermi screenings are plotted in Figure 1.

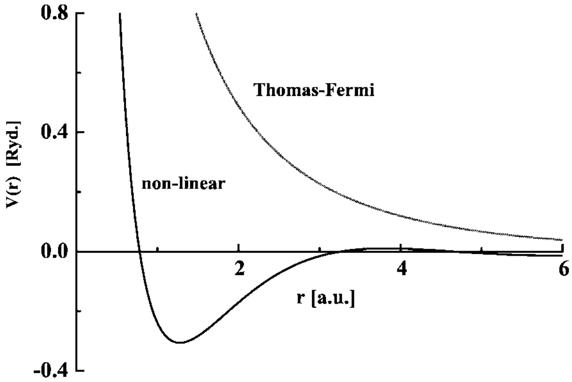

Figure1. Screened d-d pair potential

The screening function for non-linear screening potential V_{NL} is given by

$$f_{NL}(x) \;=\; 3(N-1)\int_0^{\frac{\pi}{2}} d\theta \sin\theta \cos^{3N-4}\theta \, V_{NL}\left(\sqrt{\frac{2\hbar}{m\omega}}x\sin\theta\right)\frac{1}{e^2}\sqrt{\frac{2\hbar}{m\omega}}x\sin\theta. \tag{18}$$

4 Nuclear Reaction Rate

The ELTB solution gives the nuclear reaction rate by

$$R = -\frac{2}{\hbar}\frac{\sum_{i<j} \langle \Psi | Im V_{ij}^F | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \tag{19}$$

where $ImV_{ij}^{F} = -A\hbar\,\delta(\mathbf{r}_i - \mathbf{r}_j)/2$ is imaginary part of Fermi pseudopotential.[2] The short-range interactions of nuclear forces between two bose nuclei are introduced by using δ function. The constant $A = 2Sr_B / \pi\hbar$ is determined by the S factor of the nuclear reaction between two nuclei. If the ELTB solution is obtained, the critical temperature of BEC is estimated by

$$T_c = \frac{h^2}{2\pi m k_B}\left(\frac{n}{\zeta(3/2)}\right)^{2/3}, \tag{20}$$

where n is the number density of bose particles. The probability of the ground-state occupation is given by $\Omega=1-(T/T_c)^{2/3}$ for $T<T_c$. If the ground state occupation is accounted, the fusion rate is given by $R\Omega$.

5 Results and Discussions

In this work, ELTB solutions for N deuterons trapped in Pd defects have been obtained, and d-d nuclear reaction rate has been estimated. The calculations were performed within the following conditions. (a) The octahedral void constructed by 6 vacancies (VacO) is adopted as an ion trap in solid. The radius R_v is 3.37 Å. The frequency ω is 0.86x10^{14}sec^{-1}. (b) In eq.(11), the convergences of the lattice summations are kept to be smaller than 1%. (c) Thomas-Fermi and non-linear screening potentials are used to describe d-d interactions. The screening constant in eq.(11) is 2/(1st NN distance). (d) The effective charge of a host Pd is one. (e) The S factor is 110kevb. This is consistent with Kim and Zubarev [2].

The ELTB solutions are plotted in Figures 2 and 3. The results for nuclear reaction rates are given in Table 1. In eq.(3), if all the particles exist at the same radial component r, ρ would become $\sqrt{N}r$. Therefore, if a position of a sharp peak is smaller than $\sqrt{N}R_V$, where R_v is the radius of the defect, the condensed deuterons are trapped in the defect. These values are also given in Table 1. Seeing the ELTB ground state solutions in Figures 2 and 3, sharp peak exists. For the non-linear screening in Figure 3, the peak exists in the negative region of the total potential. The peak position in Figure 3 is smaller than that in Figure 2. They are the results from the difference between two potentials plotted in Figure 1. Seeing Table1, positions of the sharp peak are completely included in the defects. For Thomas-Fermi screening, T_c's are lower than the room temperature. In contrast to them, for non-linear screening, they are higher than room temperature. Nuclear reaction rates are extremely high. If a nuclear fusion happens, immediately temperature becomes higher than T_c. Then Ω becomes zero. And the reaction will be stopped. These results lead us to the conclusion that BEC of condensed deuterons trapped in the Pd defect induces cold and calm fusion.

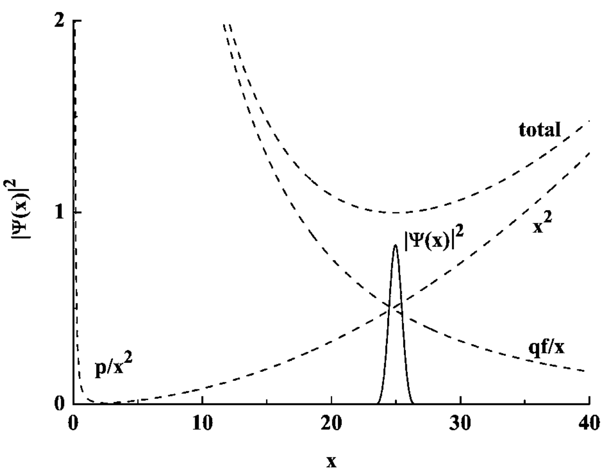

Figure 2. The ELTB solution for the system including 5 deuterons in VacO in fcc Pd. Thomas-Fermi screening potential is used as the d-d interaction. The nondimensional quantity x is defined as $x = \sqrt{m\omega/\hbar}\, r$, where $\omega = 0.86 \times 10^{14}\ \mathrm{sec}^{-1}$. The screening constant in eq.(13) is defined as $k=1/(2R_{dd})$, where R_{dd} (=0.74Å) is the d-d separation of D_2 molecule. The solid line means the ELTB solution. The dashed lines mean each potential in eq.(12) normalized by ε.

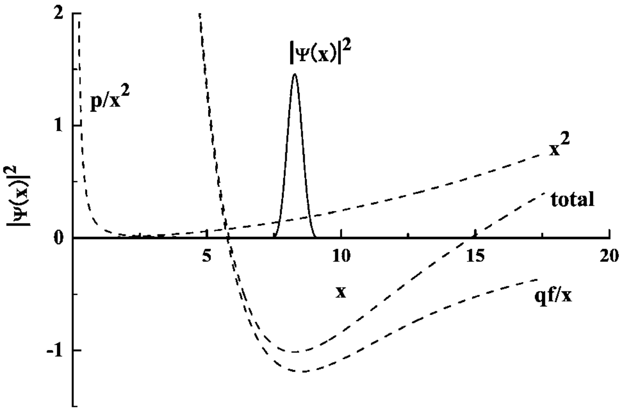

Figure 3. The ELTB solution for the system including 5 deuterons in VacO in fcc Pd. Non-linear screening potential is used for the d-d interaction. The nondimensional quantity x is defined as $x = \sqrt{m\omega/\hbar}\,\rho$, where $\omega = 0.86 \times 10^{14}\ \mathrm{sec}^{-1}$. The solid line means the ELTB solution. The dashed lines mean each potential in eq.(12) normalized by ε .

Table 1. Nuclear reaction rates as a function of N for trapped deuterons in VacO in Pd.

		Thomas-Fermi screening				non-linear screening			
N	$\sqrt{N}R_V$	ρ_{max}	ρ_2	T_c	R	ρ_{max}	ρ_2	T_c	R
3	5.83	3.01	3.15	49	1.8	1.13	1.21	256	33.7
4	6.74	3.93	4.07	55	2.8	1.37	1.45	328	66.2
5	7.53	4.78	4.92	62	3.9	1.58	1.66	402	108.2
6	8.25	5.58	5.72	69	5.1	1.77	1.85	478	159.7
7	8.91	6.34	6.48	75	6.4	1.95	2.02	556	220.7

N: the number of the trapped deuterons R_V: radius of the defect [Å]
ρ_{max}: position of a peak in ELTB solution [Å] T_c: critical temp. of BEC [K]
ρ_2: position of the right side foot of the peak [Å] R: nuclear reaction rate [$10^7 \mathrm{sec}^{-1}$]

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