บทความวิชาการ

การคำนวณค่าเบื้องต้นของพลังงานสถานะพื้นของสสารประเภทเฟอร์มิออนในสองมิติที่ประกอบด้วยไฮโดรเจนหนึ่งและสองอะตอม

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บทคัดย่อ

การคำนวณเบื้องต้นของพลังงานสถานะพื้นของสสารประเภทเฟอร์มิออนในสองมิติที่ประกอบด้วยอะตอมไฮโดรเจนได้จากการพิจารณาฟังก์ชันดีเทอร์มิเนนที่สอดคล้องกับฟังก์ชันคลื่นนอร์มัลไลซ์และฟังก์ชันสปินนอร์มัลไลซ์ พลังงานสถานะพื้นสองค่าที่คำนวณได้ ได้แก่ พลังงานสถานพื้นแบบแม่นตรงของอะตอมไฮโดรเจนจำนวนหนึ่งอะตอมเท่ากับ $-\frac{3me^4}{2\hbar^2}$ ซึ่งพิจารณาภายใต้อันตรกิริยาแบบคูลอมบ์ และค่าขอบเขตบนของพลังงานสถานะพื้นของสสารประเภทเฟอร์มิออนที่ประกอบด้วยอะตอมไฮโดรเจนจำนวนสองอะตอมคือ $-2\left(\frac{3me^4}{2\hbar^2}\right)$

คำสำคัญ: พลังงานสถานะพื้น ขอบเขตบน สสารประเภทเฟอร์มิออน

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Basic Calculations of Ground-State Energy of Two Dimensional Fermionic Matter Consisting of One and Two Hydrogen Atoms

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ABSTRACT

The basic calculations of the ground-state energy of two dimensional fermionic matter consisting of hydrogen atom have been shown by considering the determinantal function with normalized wavefunction and normalized spin functions. Two ground-state energies are derived. The exact ground-state energy, based on considering the one hydrogen atom wave function in the ground-state under Coulomb interaction in two dimensions, is $-\left(\frac{3me^4}{2\hbar^2}\right)$. The upper bound of the ground-state energy, based on considering 2 hydrogen atoms with infinitely separated 2 clusters, each in its ground-state, with nuclear charges each having one electron, is $-2\left(\frac{3me^4}{2\hbar^2}\right)$.

Keywords: ground state energy, upper bound, fermionic matter

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1. Introduction

During the recent years, there has been much interest in two dimensional physics, e.g. [1,2], and the role of spin and statistics theorem to investigate the nature of matter in two dimensions relevant with the exclusion principle. E. B. Manoukian, C. Muthaporn [3] have shown in 2004 that the upper bound for the ground-state energy of bosonic matter, by using trial wavefunction, depend on $-N^2$, $E_N \leq -C_H N^2$ when C_H is positive constant. In 2010, K. Shiwongsa, S. Sirininlakul and P. Sripirom [4] have shown that the lower bound for the ground-state energy of bosonic matter in two dimensions is same depend on $-N^2$, $E_N \geq -C_L N^2$ which $-C_L < -C_H$. P.S. Sirininlakul and S. Sirininlakul [5] have shown in 2012, that the lower bound for the ground-state energy of fermionic matter with the exclusion principle, by using the density, depend on single power N, $E_N \propto N$. We hope that in the future one can find the upper bound on the ground-state energy of matter with the exclusion principle in two dimensions. So that, the purpose of this article is to provide the guideline and useful information by carrying a mathematically rigorous analysis of ground-state energy problem of two dimensionnal fermionic matter consisting one and two hydrogen atoms, by invoking, in the process, the fundamental Pauli exclusion principle which, as mentioned above, has far reaching consequences in nature relevant directly to our world. We provide basic estimates involving the upper bounds for the exact ground-state energy, corresponding to the Hamiltonian (by setting $\frac{1}{4\pi\varepsilon_0} = 1$)

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{N} \frac{e^2}{\left|\mathbf{x}_i - \mathbf{x}_j\right|} + \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{\left|\mathbf{L}_i - \mathbf{L}_j\right|} - \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{Z_j e^2}{\left|\mathbf{x}_i - \mathbf{L}_j\right|} \tag{1}$$

where Z_i and Z_j are number of protons in nucleus of hydrogen atom i and j, k is number of nucleus, N is number of electrons in the system and $\mathbf{L}_i$, $\mathbf{L}_j$ are vectors in two dimensions from the origin to nucleus $Z_i\,|e|$ and $Z_j\,|e|$ localization,

$$\mathbf{L}_i = L_0 \mathbf{n}_i, \tag{2}$$

$$\mathbf{L}_i - \mathbf{L}_{i+1} = \mathbf{L}_0 = L_0(\mathbf{n}_i - \mathbf{n}_{i+1}), \tag{3}$$

where L_0 is a constant, $\mathbf{n}_i$, $\mathbf{n}_{i+1}$ are unit vectors and

$$\left|\mathbf{L}_i - \mathbf{L}_j\right| \geq L_0 \tag{4}$$

For fermionic matter, the anti-symmetric two dimensional wavefunction in ground-state be writen as the determinantal function

$$\Psi\left(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N\right) = \frac{1}{\sqrt{N!}} \det\left[\psi_j\left(\mathbf{x}, \sigma\right)\right] \tag{5}$$

$\mathbf{x}_i$ is two dimensions vector from the origin to the i^{th} electron, $\psi_j(\mathbf{x}, \sigma) = \psi_j(\mathbf{x})\chi_j(\sigma)$ and $\chi_j(\sigma)$ is spin functions. Each orbital occurring in (5) is product of an anti-symmetric spatial state $\psi(\mathbf{x})$, and a symmetric spin state $\chi(\sigma)$. Since orbitals of different spin are automatically orthogonal, Eq. (5) reduces to the condition that space orbitals corresponding to the same spin function should be orthonormal. This assures that the normalization conditions are

$$\sum_{\sigma_1,\ldots,\sigma_N}^{n} \int d^2\mathbf{x}_1, d^2\mathbf{x}_2, \ldots, d^2\mathbf{x}_N \left|\Psi\left(\mathbf{x}_1\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N\right)\right|^2 = 1 \tag{6}$$

and

$$\sum_{\sigma} \chi_i^*(\sigma)\chi_j(\sigma) = \delta_{ij}. \tag{7}$$

We choose to consider the matter consisting hydrogen atoms because it is easy to obtain its wavefunction and we obtain $k = N$.

2. Two dimensional fermionic matter consisting one hydrogen atom

In this case, k has chosen to be 1. Let $\psi(\mathbf{x}_1 - \mathbf{L}_1)$ be the spatial state one hydrogen atom wavefunctions in ground-state and derived by using method of separation [7], we obtain two dimensions wavefunction of one hydrogen atom is

$$\Psi\left(\mathbf{x}_1, \sigma_1\right) = \psi(\mathbf{x}_1 - \mathbf{L}_1)\chi_1(\sigma) = \sqrt{\frac{2}{\pi}}\beta e^{-\beta|\mathbf{x}_1 - \mathbf{L}_1|}\chi_1(\sigma) \tag{8}$$

where

$$\beta = \frac{me^2}{\hbar^2} \tag{9}$$

and $\frac{1}{\beta}$ is the Bohr radius $\frac{\hbar^2}{me^2}$.

For one hydrogen atom, we can ignore the second and the third terms in the right-hand side of (1), and obtain the expectation value of the Hamiltonian H for a hydrogen atom :

$$\langle\Psi|H|\Psi\rangle = \langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle - \langle\Psi|\frac{e^2}{|\mathbf{x}_1 - \mathbf{L}_1|}|\Psi\rangle \tag{10}$$

To obtain $\langle\Psi|H|\Psi\rangle$, we introduce the expectation value of kinetic energy as :

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle = \frac{\hbar^2}{2m}\int d^2\mathbf{x}_1 \left(\nabla\Psi^*(\mathbf{x}_1, \sigma_1)\right)\cdot\left(\nabla\Psi(\mathbf{x}_1, \sigma_1)\right) \tag{11}$$

where

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta}, \tag{12}$$

$$\int \mathrm{d}^2\mathbf{x}\,\Psi(\mathbf{x}) = \int_0^{\infty}\int_0^{2\pi} r\mathrm{d}r\,\mathrm{d}\theta\;\Psi(r,\theta) \tag{13}$$

and the expectation value of the potential as

$$\langle\Psi|\frac{1}{|\mathbf{x}_1 - \mathbf{L}_1|}|\Psi\rangle = \int \mathrm{d}^2\mathbf{x}_1\,\Psi^*(\mathbf{x}_1,\sigma_1)\frac{1}{|\mathbf{x}_1 - \mathbf{L}_1|}\Psi(\mathbf{x}_1,\sigma_1). \tag{14}$$

2.1 The expectation value of kinetic energy for $k = 1$

To obtain the expectation value of kinetic energy of (10), we substitute (8) into (11) and let $\mathbf{r} = \mathbf{x}_1 - \mathbf{L}_1$ and $|\mathbf{r}| = r$ to obtain

$$\begin{aligned}\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle &= \frac{\hbar^2}{m}\frac{\beta^2}{\pi}\int \mathrm{d}^2\mathbf{r}\left(\nabla_r \mathrm{e}^{-\beta|\mathbf{r}|}\right)\cdot\left(\nabla_r \mathrm{e}^{-\beta|\mathbf{r}|}\right) \\ &= \frac{\hbar^2}{m}\frac{\beta^4}{\pi}\int_0^{\infty}\int_0^{2\pi}\mathrm{d}r\,\mathrm{d}\theta\; r\mathrm{e}^{-2\beta r} \\ &= \frac{2\hbar^2\beta^4}{m}\int_0^{\infty}\mathrm{d}r\, r\mathrm{e}^{-2\beta r}\end{aligned} \tag{15}$$

Now let $u = 2\beta$, the integral term on the right-hand side of (15) can be rewritten as

$$\begin{aligned}\int_0^{\infty}\mathrm{d}r\, r\mathrm{e}^{-2\beta r} &= -\frac{\partial}{\partial u}\int_0^{\infty}\mathrm{d}r\,\mathrm{e}^{-ur} = \frac{1}{u^2} \\ &= \frac{1}{4\beta^2}.\end{aligned} \tag{16}$$

In order to obtain the expectation value of kinetic energy of one hydrogen atom in two dimensions, substitute (16) into the right-hand side of (15),

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle = \frac{\hbar^2\beta^2}{2m}. \tag{17}$$

Noting that the kinetic energy in two dimensions from (17) is the same value with kinetic energy in three dimensions. So the kinetic energy of one hydrogen does not change even the dimension is changed [6].

2.2 The expectation value of nucleus-electron interaction

To obtain the expectation value of nucleus-electron interaction of one hydrogen atom in two dimensions, we substitute (16) into the second term on right-hand side of (15), then the expectation value is expressed as

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{L}_1|}|\Psi\rangle=-e^2\int d^2\mathbf{x}_1\sqrt{\frac{2}{\pi}}\beta e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}\cdot\frac{1}{|\mathbf{x}_1-\mathbf{L}_1|}\sqrt{\frac{2}{\pi}}\beta e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}$$
$$=-\frac{2e^2\beta^2}{\pi}\int d^2\mathbf{x}_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|}. \qquad (18)$$

Let $\mathbf{D}=\mathbf{x}_1-\mathbf{L}_1$, and $|\mathbf{D}|=D$, we get $d^2\mathbf{D}=d^2\mathbf{x}_1$ ($\mathbf{L}_1$ is constant vector), then substitute them into the right-hand side of (18) to obtain

$$-\frac{2e^2\beta^2}{\pi}\int d^2\mathbf{x}_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|}=-\frac{2e^2\beta^2}{\pi}\int d^2\mathbf{D}\frac{e^{-2\beta|\mathbf{D}|}}{|\mathbf{D}|}$$
$$=-\frac{2e^2\beta^2}{\pi}\int_0^\infty dD\, e^{-2\beta D}\int_0^{2\pi}d\theta$$
$$=-2e^2\beta. \qquad (19)$$

2.3 The exact ground-state energy of two dimensional one hydrogen atom

Substituting (17) and (19) into the right-hand side of (10), we have

$$\langle\Psi|H|\Psi\rangle=\frac{\hbar^2\beta^2}{2m}-2e^2\beta. \qquad (20)$$

With β defined as in (9), we obtain the following for the ground-state energy of a hydrogen atom as

$$\langle\Psi|H|\Psi\rangle=\frac{\hbar^2}{2m}\left(\frac{me^2}{\hbar^2}\right)^2-2e^2\left(\frac{me^2}{\hbar^2}\right)$$
$$=-\frac{3me^4}{2\hbar^2} \qquad (21)$$

as expected.

3. Two dimensional fermionic matter consisting two hydrogen atoms

For two hydrogen atoms, we put number of nucleus $k=2$ and number of electron $N=2$ the ground-state energy of two hydrogen atoms is formulated as

$$\langle\Psi|H|\Psi\rangle=\langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle-\langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{e^2}{|\mathbf{x}_i-\mathbf{L}_j|}|\Psi\rangle+\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}|\Psi\rangle+\langle\Psi|\frac{e^2}{|\mathbf{L}_1-\mathbf{L}_2|}|\Psi\rangle \qquad (22)$$

where the anti-symmetric wave function for $k=2$ is defined

$$\Psi\left(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2\right)=\frac{1}{\sqrt{2}}\begin{vmatrix}\psi_1\left(\mathbf{x}_1,\sigma_1\right) & \psi_1\left(\mathbf{x}_2,\sigma_2\right)\\ \psi_2\left(\mathbf{x}_1,\sigma_1\right) & \psi_2\left(\mathbf{x}_2,\sigma_2\right)\end{vmatrix} \tag{23}$$

which can be rewritten as

$$\Psi\left(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2\right)=\frac{1}{\sqrt{2}}\left[\psi_1\left(\mathbf{x}_1,\sigma_1\right)\psi_2\left(\mathbf{x}_2,\sigma_2\right)-\psi_2\left(\mathbf{x}_1,\sigma_1\right)\psi_1\left(\mathbf{x}_2,\sigma_2\right)\right] \tag{24}$$

Substituting the two dimensional hydrogen atom wavefunction into (24) yields the two dimensional anti-symmetric wavefunction as

$$\Psi\left(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2\right)=\frac{\sqrt{2}\beta^2}{\pi}\left[\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\chi_1\left(\sigma_1\right)\chi_2\left(\sigma_2\right)-\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}\chi_1\left(\sigma_2\right)\chi_2\left(\sigma_1\right)\right]. \tag{25}$$

3.1 The expectation value of kinetic energy for $k = 2$

To obtain the expectation value of kinetic energy, we introduce

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle=\langle\Psi|T_1|\Psi\rangle=\frac{\hbar^2}{2m}\int\mathrm{d}^2\mathbf{x}_1\mathrm{d}^2\mathbf{x}_2\left(\nabla_1\Psi^*\right)\cdot\left(\nabla_1\Psi\right), \tag{26a}$$

$$\langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle=\langle\Psi|T_2|\Psi\rangle=\frac{\hbar^2}{2m}\int\mathrm{d}^2\mathbf{x}_1\mathrm{d}^2\mathbf{x}_2\left(\nabla_2\Psi^*\right)\cdot\left(\nabla_2\Psi\right), \tag{26b}$$

and from (12), for no ϕ dependence and $\hat{\theta}\cdot\hat{\mathbf{x}} = 0$, gives

$$\nabla(r_1,\theta)=\hat{r}_1\frac{\partial}{\partial r_1}+\hat{\theta}\frac{1}{r_1}\frac{\partial}{\partial\theta}, \tag{27a}$$

$$\nabla(r_2,\theta)=\hat{r}_2\frac{\partial}{\partial r_2}+\hat{\theta}\frac{1}{r_2}\frac{\partial}{\partial\theta}. \tag{27b}$$

Substituting (25) into (26), to obtain

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle=\frac{\hbar^2}{2m}\frac{\beta^2}{\pi}\Big\{\int\mathrm{d}^2\mathbf{x}_1\,\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}\cdot\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}+\int\mathrm{d}^2\mathbf{x}_1\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}\cdot\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}$$
$$-2\delta_{ab}\int\mathrm{d}^2\mathbf{x}_1\left(\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}\right)\cdot\left(\nabla_1\mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}\right)\int\mathrm{d}^2\mathbf{x}_2\left(\frac{2\beta^2}{\pi}\right)\left(\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}\right)\left(\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\right)\Big\} \tag{28}$$

where

$$\int\mathrm{d}^2\mathbf{x}_2\left|\sqrt{\frac{2}{\pi}}\beta e^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\right|^2\delta_{aa}=1 \tag{29a}$$

$$\int\mathrm{d}^2\mathbf{x}_2\left|\sqrt{\frac{2}{\pi}}\beta e^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}\right|^2\delta_{bb}=1. \tag{29b}$$

To evaluate the integral term in (28), by setting $\mathbf{R}_i = \mathbf{x}_i - \mathbf{L}$, we consider in two cases :
Firstly, if $\mathbf{L} = \mathbf{L}'$:

$$\int \mathrm{d}^2\mathbf{x}_i \nabla_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{x}_1 - \mathbf{L}'|} = \beta^2 \int_0^\infty \int_0^{2\pi} \mathrm{d}R_i\, \mathrm{d}\theta R_i \mathrm{e}^{-2\beta R_i} = \frac{\pi}{2}. \tag{30}$$

Secondly, if $\mathbf{L} \neq \mathbf{L}'$:

$$\nabla_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} = \left(\hat{r}_i \frac{\partial}{\partial r_i} + \hat{\theta} \frac{1}{r_i} \frac{\partial}{\partial \theta} \right) \mathrm{e}^{-\beta\sqrt{r_i^2 - 2r_i L\cos\theta + L^2}} = -\beta \left[\frac{(r_i - L\cos\theta)\hat{r}}{|\mathbf{x}_i - \mathbf{L}|} + \frac{L\sin\theta\,\hat{\theta}}{|\mathbf{x}_i - \mathbf{L}|} \right] \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|}. \tag{31}$$

From (31), we replace $\mathbf{L}$ by $\mathbf{L}'$ to obtain

$$\nabla_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|} = -\beta \left[\frac{(r_i - L'\cos\theta)\hat{r}}{|\mathbf{x}_i - \mathbf{L}'|} + \frac{L'\sin\theta\,\hat{\theta}}{|\mathbf{x}_i - \mathbf{L}'|} \right] \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|}. \tag{32}$$

By using (31) and (32) it follows that

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}_i \nabla_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{x}_1 - \mathbf{L}'|} &= \beta^2 \int \mathrm{d}^2 x_i \left[\frac{\mathbf{x}_i \cdot (\mathbf{x}_i - \mathbf{L})\mathbf{x}_i \cdot (\mathbf{x}_i - \mathbf{L}')}{r_i^2 |\mathbf{x}_i - \mathbf{L}||\mathbf{x}_i - \mathbf{L}'|} + \frac{LL'\sin\theta\sin\theta}{|\mathbf{x}_i - \mathbf{L}||\mathbf{x}_i - \mathbf{L}'|} \right] \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|}.\\ &\leq \beta^2 \int \mathrm{d}^2\mathbf{x}_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|} + \beta^2 \int \mathrm{d}^2\mathbf{x}_i \frac{LL'}{|\mathbf{x}_i - \mathbf{L}||\mathbf{x}_i - \mathbf{L}'|} \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|}\end{aligned} \tag{33}$$

where

$$\mathbf{x}_i \cdot (\mathbf{x}_i - \mathbf{L}) \leq |\mathbf{x}_i||\mathbf{x}_i - \mathbf{L}| \tag{34a}$$

$$LL' \sin\,\theta \sin\,\theta \leq LL'. \tag{34b}$$

To evaluate the first integrals on the right hand side of inequality (33), let $\mathbf{L}_0 = \mathbf{L}' - \mathbf{L}$, $\mathbf{x}_i - \mathbf{L} = \mathbf{R}_i$, and $\mathrm{d}^2\mathbf{x}_i = \mathrm{d}^2(\mathbf{R}_i + \mathbf{L}) = \mathrm{d}^2\mathbf{R}_i$, substituting all into the right-hand side of (33) to obtain

$$\beta^2 \int \mathrm{d}^2\mathbf{x}_i \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{x}_i - \mathbf{L}'|} \leq 2\pi\beta^2 \mathrm{e}^{-\beta L_0} \frac{L_0^2}{2} + 2\pi\beta^2 e^{-\beta L_0} \left[\frac{1}{4\beta^2} + \frac{L_0}{2\beta} \right] \tag{35}$$

where

$$|\mathbf{R}_i - \mathbf{L}_0| = \sqrt{R_i^2 - 2\mathbf{R}_i \cdot \mathbf{L} + L_0^2} \geq \sqrt{R_i^2 - 2R_i L + L_0^2} \tag{36a}$$

$$\mathrm{e}^{-\beta|\mathbf{R}_i - \mathbf{L}_0|} \leq \mathrm{e}^{-\beta|R_i - L_0|}. \tag{36b}$$

Consider the second term on the right-hand side of (33), let $\mathbf{x}_i - \mathbf{L} = \mathbf{R}_i$, and $\mathrm{d}^2\mathbf{x}_i = \mathrm{d}^2(\mathbf{R}_i + \mathbf{L}) = \mathrm{d}^2\mathbf{R}_i$, then using (36), to obtain

$$\beta^2 \int d^2\mathbf{x}_i \frac{LL' e^{-\beta|\mathbf{x}_i-\mathbf{L}|} e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}||\mathbf{x}_i-\mathbf{L}'|} \le \beta^2 \int d^2\mathbf{R}_i \frac{LL' e^{-\beta R_i} e^{-\beta|R_i-L_0|}}{R_i|\mathbf{R}_i-\mathbf{L}_0|}. \tag{37}$$

By nothing the expansion in term of Legendre polynomials [8]

$$\frac{1}{|\mathbf{R}_i-\mathbf{L}_0|} = \sum_{\ell=0}^{\infty}\left(\frac{R_{i<}}{R_{i>}}\right)^{\ell} \frac{1}{R_{i>}} P_\ell(\cos\theta) \tag{38}$$

and

$$\int_0^{2\pi} d\theta\, P_\ell(\cos\theta) = 2\pi\delta_{\ell 0} \tag{39}$$

where $R_i = \max[L_0, R_i]$ and $P_0(\cos\theta) = 1$.

Substituting (39) into the right-hand side of inequality (37), we obtain

$$\beta^2 \int d^2\mathbf{x}_i \frac{LL' e^{-\beta|\mathbf{x}_i-\mathbf{L}|} e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}||\mathbf{x}_i-\mathbf{L}'|} \le \beta^2 \int_0^{\infty} dR_i \frac{R_i LL' e^{-\beta R_i} e^{-\beta|R_i-L_0|}}{R_i} \int_0^{2\pi} d\theta \sum_{\ell=0}^{\infty}\left(\frac{R_{i<}}{R_{i>}}\right)^{\ell} \frac{1}{R_{i>}} P_\ell(\cos\theta). \tag{40}$$

Applying (38), with $\ell = 0$, to the right-hand side of inequality (40), we obtain the inequality

$$\beta^2 \int d^2\mathbf{x}_i \frac{LL' e^{-\beta|\mathbf{x}_i-\mathbf{L}|} e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}||\mathbf{x}_i-\mathbf{L}|} \le \left(\frac{2\pi\beta^2 LL'L_0}{2} + \frac{2\pi\beta LL'}{2}\right) e^{-\beta L_0}. \tag{41}$$

Substituting (35) and (41) into the right-hand side of inequality (33) yields

$$\int d^2\mathbf{x}_i \nabla_i e^{-\beta|\mathbf{x}_i-\mathbf{L}|} \cdot \nabla_i e^{-\beta|\mathbf{x}_i-\mathbf{L}'|} \le 2\pi e^{-\beta L_0}\left[\frac{\beta^2 L_0^2}{2} + \frac{L_0}{2} + \frac{\beta L_0}{2} + \frac{\beta^2 LL'L_0}{2} + \frac{\beta LL'}{2} + \frac{1}{4}\right], \tag{42}$$

and

$$\int d^2\mathbf{x}_i \left(e^{-\beta|\mathbf{x}_i-\mathbf{L}|}\right)\left(e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}\right) \le 2\pi e^{-\beta L_0}\left[\frac{L_0^2}{2} + \frac{L_0}{2\beta} + \frac{1}{4\beta^2}\right]. \tag{43}$$

Using (30) and noting (28), with $i = 1$ and $\mathbf{L}_1 = \mathbf{L} = \mathbf{L}'$, we have

$$\int d^2\mathbf{x}_1 \nabla_1 e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|} \cdot \nabla_1 e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|} = \frac{\pi}{2}. \tag{44}$$

Now, with $i = 2$ and $\mathbf{L}_2 = \mathbf{L} = \mathbf{L}'$, we also have

$$\int d^2\mathbf{x}_1 \nabla_1 e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|} \cdot \nabla_1 e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|} = \frac{\pi}{2}. \tag{45}$$

Using (42) and (43), noting (28), with $i = 1$, $\mathbf{L}_1 = \mathbf{L}$, and $\mathbf{L}_2 = \mathbf{L}'$, it follows that

$$2\int \mathrm{d}^2\mathbf{x}_1 \nabla_1 \mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_2|} \cdot \nabla_1 \mathrm{e}^{-\beta|\mathbf{x}_1-\mathbf{L}_1|} \le 4\pi \mathrm{e}^{-\beta L_0}\left[\frac{\beta^2 L_0^2}{2}+\frac{L_0}{2}+\frac{\beta L_0}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}+\frac{1}{4}\right] \quad (46)$$

and with $i = 2$, $\mathbf{L}_1 = \mathbf{L}$ and $\mathbf{L}_2 = \mathbf{L}'$, we obtain

$$\int \mathrm{d}^2\mathbf{x}_1 \left(\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}\right)\left(\mathrm{e}^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\right) \le 2\pi \mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \quad (47)$$

Substituting (44), (45), (46) and (47) into the right-hand side of (28), then taking the limit $L_0 \to \infty$ yields

$$\langle \Psi | \frac{\mathbf{p}_1^2}{2m} | \Psi \rangle \le \frac{\hbar^2 \beta^2}{2m}. \quad (48)$$

Noting (26) and (28), then replacing ∇_1 by ∇_2 in the same way as (29) to (47), we obtain

$$\langle \Psi | \frac{\mathbf{p}_2^2}{2m} | \Psi \rangle \le \frac{\hbar^2 \beta^2}{2m}. \quad (49)$$

From (48) and (49), we obtain the upper bound for the expectation value of kinetic energy of hydrogen atom for $k = N = 2$ expressed as

$$\begin{aligned}\langle \Psi | \sum_{i=1}^{2} \frac{\mathbf{p}_i^2}{2m} | \Psi \rangle &= \langle \Psi | \frac{\mathbf{p}_1^2}{2m} | \Psi \rangle + \langle \Psi | \frac{\mathbf{p}_2^2}{2m} | \Psi \rangle \\ &\le 2\left(\frac{\hbar^2\beta^2}{2m}\right) \quad (50)\end{aligned}$$

3.2 The expectation value of nucleus-electron interaction for $k = 2$

To obtain the bound of nucleus-electron interaction, we choose $\mathbf{L}_j$ be the vector from the origin to the nuclei of charges $Z_j\,|e|$. For $Z_j = 1$, $k = 2$ and $N = 2$, the second term on the right-hand side of (22) gives

$$\begin{aligned}-\langle \Psi | \sum_{i=1}^{2}\sum_{j=1}^{2} \frac{e^2}{|\mathbf{x}_i - \mathbf{L}_j|} | \Psi \rangle &= -\langle \Psi | \frac{e^2}{|\mathbf{x}_1 - \mathbf{L}_1|} | \Psi \rangle - \langle \Psi | \frac{e^2}{|\mathbf{x}_2 - \mathbf{L}_2|} | \Psi \rangle \\ &\quad -\langle \Psi | \frac{e^2}{|\mathbf{x}_2 - \mathbf{L}_1|} | \Psi \rangle - \langle \Psi | \frac{e^2}{|\mathbf{x}_1 - \mathbf{L}_2|} | \Psi \rangle. \quad (51)\end{aligned}$$

Considering the first term on the right-hand side of the inequality (51), we obtain

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{L}_1|}|\Psi\rangle = -e^2\int d^2\mathbf{x}_1 d^2\mathbf{x}_2\,\Psi^*(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2)\frac{1}{|\mathbf{x}_1-\mathbf{L}_1|}\Psi(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2)$$
$$= -\frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|} - \frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_2|}}{|\mathbf{x}_1-\mathbf{L}_1|}$$
$$+\delta_{ab}\left[e^2\frac{\sqrt{2}\beta^2}{\pi}\frac{\sqrt{2}\beta^2}{\pi}\int d^2\mathbf{x}_1\frac{e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|}\int d^2\mathbf{x}_2 e^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}e^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\right]. \quad (52)$$

To obtain the expectation value in (52), we introduce the basic following integral for $\mathbf{L}=\mathbf{L}'$ and set $\mathbf{R}=\mathbf{x}_i-\mathbf{L}$

$$\int d^2\mathbf{x}_i\frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}|} = \int_0^\infty\int_0^{2\pi} dR\,d\theta\,\frac{Re^{-2\beta R}}{R} = \frac{\pi}{\beta} \quad (53)$$

and for $\mathbf{L}\neq\mathbf{L}'$, let $\mathbf{R}_i=\mathbf{x}_i-\mathbf{L}$, $\mathbf{x}_i-\mathbf{L}'=\mathbf{R}_i+\mathbf{L}-\mathbf{L}'$ and $\mathbf{L}_0'=\mathbf{L}-\mathbf{L}'$ we obtain

$$\int d^2\mathbf{x}_i\frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}|} \geq \int d^2\mathbf{R}_i\frac{e^{-2\beta|R_i+L_0'|}}{R_i}$$
$$= 2\pi e^{-2\beta L_0'}\int_0^\infty dR_i\,e^{-2\beta R_i}$$
$$= \frac{\pi}{\beta}e^{-2\beta L_0'}. \quad (54)$$

The right hand side of inequality (54) is positive number and vanishes very rapidly for $L_0\to\infty$, it obviously follows that

$$-\int d^2\mathbf{x}_i\frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}|} \leq 0\,. \quad (55)$$

In the other case for $\mathbf{L}\neq\mathbf{L}'$ let $\mathbf{L}_0=\mathbf{L}'-\mathbf{L}$, we obtain

$$\int d^2\mathbf{x}_i\frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}|}}{|\mathbf{x}_i-\mathbf{L}|} = \int d^2\mathbf{R}_i\frac{e^{-\beta|\mathbf{R}_i|}}{|\mathbf{R}_i|}e^{-\beta|\mathbf{R}_i-\mathbf{L}_0|}. \quad (56)$$

Applying (36), to the right-hand side of (56), to obtain

$$\int d^2\mathbf{x}_i \frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}|}}{|\mathbf{x}_i-\mathbf{L}|} \le 2\pi\int_0^\infty dR_i\, R_i \frac{e^{-\beta R_i}\, e^{-\beta|R_i-L_0|}}{R_i}$$
$$= 2\pi\int_0^{L_0} dR_i\, e^{-\beta R_i}\, e^{-\beta(L_0-R_i)} + 2\pi\int_{L_0}^\infty dR_i\, e^{-\beta R_i}\, e^{-\beta(R_i-L_0)}$$
$$= 2\pi e^{-\beta L_0}\left[L_0 + \frac{1}{2\beta^2}\right]. \qquad (57)$$

From (53), (55) and (57), we conclude that

$$-\int d^2\mathbf{x}_i \frac{e^{-2\beta|\mathbf{x}_i-\mathbf{L}|}}{|\mathbf{x}_i-\mathbf{L}|} = -\frac{\pi}{\beta} \qquad (58a)$$

$$-\int d^2\mathbf{x}_i \frac{e^{-2\beta|\mathbf{x}_i-\mathbf{L}'|}}{|\mathbf{x}_i-\mathbf{L}|} \le 0 \qquad (58b)$$

$$\int d^2\mathbf{x}_i \frac{e^{-\beta|\mathbf{x}_i-\mathbf{L}'|}e^{-\beta|\mathbf{x}_i-\mathbf{L}|}}{|\mathbf{x}_i-\mathbf{L}|} \le \frac{\pi}{\beta}e^{-2\beta L_0}\left[2\beta L_0 + \frac{1}{\beta}\right]. \qquad (58c)$$

Applying (58a), with $i = 1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{x}_i = \mathbf{x}_1$ to the first term on the right-hand side of inequality (52), with normalized wavefunction, gives

$$-\frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_1 \frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|} = -e^2\beta. \qquad (59)$$

Again, applying the integration in (58b), set $i = 1$, $\mathbf{L} = \mathbf{L}_1$, $\mathbf{L}' = L_2$ and $\mathbf{x}_i = \mathbf{x}_1$, to the second term on the right-hand side of inequality (52), with normalized wavefunction, we obtain the following inequality

$$-\frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_1 \frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_2|}}{|\mathbf{x}_1-\mathbf{L}_1|} \le 0. \qquad (60)$$

Now, applying (43), with $i = 2$, $\mathbf{L}=\mathbf{L}_1$, $\mathbf{L}' = \mathbf{L}_2$ and $\mathbf{x}_i = \mathbf{x}_2$, to the third term on the right-hand side of (52), we have

$$\int d^2\mathbf{x}_2 e^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}e^{-\beta|\mathbf{x}_2-\mathbf{L}_2|} \le 2\pi e^{-\beta L_0}\left[\frac{L_0^2}{2} + \frac{1}{4\beta^2} + \frac{L_0}{2\beta}\right] \qquad (61)$$

and using (58c), with $i = 1$, $\mathbf{L}=\mathbf{L}_1$, $\mathbf{L}' = \mathbf{L}_2$ and $\mathbf{x}_i = \mathbf{x}_1$, as applied to the third term on the right-hand side of (52), yields

$$\int d^2\mathbf{x}_1 \frac{e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|} \le \frac{\pi}{\beta}e^{-2\beta L_0}\left[2\beta L_0 + \frac{1}{\beta}\right]. \qquad (62)$$

Substituting of (61) and (62) into the third term on the right-hand side of (52) for $L_0 \to \infty$ gives

$$\lim_{L_0\to\infty}\left(\frac{2e^2\beta^4}{\pi^2}\int d^2\mathbf{x}_1\,\frac{e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{L}_1|}\int d^2\mathbf{x}_2 e^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}e^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\right)=0. \quad (63)$$

By substituting (59), (60) and (63) into the right-hand side of (52), taking $L_0 \to \infty$, it follows that

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{L}_1|}|\Psi\rangle \le -e^2\beta. \quad (64)$$

Referring (52)–(63), by taking the $L_0 \to \infty$ the upper bounds of some terms on the right-hand side of (51) are shown below

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_2-\mathbf{L}_2|}|\Psi\rangle \le -e^2\beta. \quad (65)$$

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_2-\mathbf{L}_1|}|\Psi\rangle \le -e^2\beta. \quad (66)$$

$$-\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{L}_2|}|\Psi\rangle \le -e^2\beta. \quad (67)$$

Substituting (64), (65), (66) and (67) into the right-hand side of (51), we obtain the following bound for the expectation value of the nucleus-electron interaction for two hydrogen atoms as

$$-\langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{e^2}{|\mathbf{x}_i-\mathbf{L}_j|}|\Psi\rangle \le -4e^2\beta. \quad (68)$$

3.3 The expectation value of electron-electron interaction for $k = 2$

Considering the the third term on the right-hand side of (22), the expectation value of electron-electron interaction for $k = 2$ hydrogen nuclei, we obtain

$$\begin{aligned}\langle\Psi|\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}|\Psi\rangle &= e^2\int d^2\mathbf{x}_1\, d^2\mathbf{x}_2\, \Psi^*(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2)\frac{1}{|\mathbf{x}_1-\mathbf{x}_2|}\Psi(\mathbf{x}_1\sigma_1,\mathbf{x}_2\sigma_2)\\ &= \delta_{aa}\frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_2 e^{-2\beta|\mathbf{x}_2-\mathbf{L}_2|}\int d^2x_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{x}_2|}+\delta_{bb}\frac{e^2\beta^2}{\pi}\int d^2\mathbf{x}_2\, e^{-2\beta|\mathbf{x}_2-\mathbf{L}_1|}\int d^2x_1\frac{e^{-2\beta|\mathbf{x}_1-\mathbf{L}_2|}}{|\mathbf{x}_1-\mathbf{x}_2|}\\ &\quad -\delta_{ab}\left[e^2\frac{\sqrt{2}\beta^2}{\pi}\frac{\sqrt{2}\beta^2}{\pi}\int d^2\mathbf{x}_2\, e^{-\beta|\mathbf{x}_2-\mathbf{L}_1|}\, e^{-\beta|\mathbf{x}_2-\mathbf{L}_2|}\int d^2x_1\frac{e^{-\beta|\mathbf{x}_1-\mathbf{L}_2|}e^{-\beta|\mathbf{x}_1-\mathbf{L}_1|}}{|\mathbf{x}_1-\mathbf{x}_2|}\right].\end{aligned} \quad (69)$$

To evaluate (69), we introduce following variables : $\mathbf{R} = \mathbf{x}-\mathbf{L}$, $\mathbf{L}_0 = \mathbf{L}'-\mathbf{L}$, $\mathbf{L}_0' = \mathbf{L}-\mathbf{L}'$. Firstly, for $\mathbf{R}' = \mathbf{x}'-\mathbf{L}'$ we have

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}|}}{|\mathbf{x}-\mathbf{x}'|} &= \int \mathrm{d}^2\mathbf{R}\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R}-(\mathbf{R}'+\mathbf{L}_0)|} \\ &= 2\pi \int_0^\infty \mathrm{d}R\, \frac{R}{R_>}\,\mathrm{e}^{-2\beta|\mathbf{R}|} \\ &= \frac{2\pi}{R'+L_0}\int_0^{R'+L_0} \mathrm{d}R\, R\,\mathrm{e}^{-2\beta R} + 2\pi \int_{R'+L_0}^\infty \mathrm{d}R\,\mathrm{e}^{-2\beta R} \\ &= \frac{2\pi}{R'+L_0}\left(\frac{1}{4\beta^2} - \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2} - \frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\right) + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta(R'+L_0)} \end{aligned} \tag{70}$$

where

$$\frac{1}{|\mathbf{R}_i-(\mathbf{R}'+\mathbf{L}_0)|} = \sum_{\ell=0}^{\infty}\left(\frac{R_{i<}}{R_{i>}}\right)^{\ell}\frac{1}{R_{i>}}P_\ell(\cos\theta), \tag{71a}$$

$$R_> = \max(R, R'+L_0), \tag{71b}$$

$$\int \mathrm{d}\Omega\, P_\ell(\cos\theta) = 2\pi. \tag{71c}$$

For $L_0 \to \infty$, the right-hand side of (70), can be rewritten as

$$\lim_{L_0\to\infty}\left(\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}|}}{|\mathbf{x}-\mathbf{x}'|}\right) = 0. \tag{72}$$

which leads to

$$\lim_{L_0\to\infty}\left(\int \mathrm{d}^2\mathbf{x}'\,\mathrm{e}^{-2\beta|\mathbf{x}'-\mathbf{L}'|}\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}|}}{|\mathbf{x}-\mathbf{x}'|}\right) = 0. \tag{73}$$

Secondly, let $\mathbf{R}' = (\mathbf{x}'-\mathbf{L})$ and $\mathbf{A} = \mathbf{x}-\mathbf{L}$,

$$\int \mathrm{d}^2\mathbf{x}'\,\mathrm{e}^{-2\beta|\mathbf{x}'-\mathbf{L}|}\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}'|}}{|\mathbf{x}-\mathbf{x}'|} = \int \mathrm{d}^2\mathbf{x}'\,\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}'|}\int \mathrm{d}^2\mathbf{R}'\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-\mathbf{A}|}. \tag{74}$$

Considering the second integral on the right-hand side of (74) to obtain

$$\begin{aligned}\int \mathrm{d}^2\mathbf{R}' \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-\mathbf{A}|} &= \int_0^\infty \mathrm{d}R'\, R'\mathrm{e}^{-2\beta R'} \int d\Omega \sum_{\ell=0}^{\infty}\left(\frac{R'_<}{R'_>}\right)^{\ell} \frac{1}{R'_>} P_\ell(\cos\theta) \\ &= 2\pi \int_0^\infty \mathrm{d}R' \frac{R'}{R'_>}\mathrm{e}^{-2\beta R'} \\ &= \frac{2\pi}{A}\int_0^A \mathrm{d}R'\, R'\mathrm{e}^{-2\beta R'} + 2\pi\int_A^\infty \mathrm{d}R'\,\mathrm{e}^{-2\beta R'} \\ &= \frac{2\pi}{A}\left(\frac{1}{4\beta^2} - \frac{\mathrm{e}^{-2\beta A}}{4\beta^2} - \frac{A\mathrm{e}^{-2\beta A}}{2\beta}\right) + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta A} \\ &= \frac{\pi}{2A\beta^2} + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta A} - \frac{2\pi}{A}\left(\frac{\mathrm{e}^{-2\beta A}}{4\beta^2} + \frac{A\mathrm{e}^{-2\beta A}}{2\beta}\right) \\ &\le \frac{\pi}{2A\beta^2} + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta A}. \end{aligned} \tag{75}$$

We substitute $A = |\mathbf{x}-\mathbf{L}|$ into the right-hand side of inequality (75), to get the inequality

$$\int \mathrm{d}^2\mathbf{R}' \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-(\mathbf{x}-\mathbf{L})|} \le \frac{\pi}{2\beta^2|\mathbf{x}-\mathbf{L}|} + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}|}. \tag{76}$$

Let $\mathbf{L}_0 = \mathbf{L}-\mathbf{L}'$ so that $L_0 = |\mathbf{L}-\mathbf{L}'|$, (76) lead to

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^2\mathbf{x}\, \mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}'|}\left(\frac{\pi}{2\beta^2|\mathbf{x}-\mathbf{L}|} + \frac{2\pi}{2\beta}\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}|}\right)\right] = 0 \tag{77}$$

and (77) can be rewritten as

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^2\mathbf{x}'\, \mathrm{e}^{-2\beta|\mathbf{x}'-\mathbf{L}|}\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-2\beta|\mathbf{x}-\mathbf{L}'|}}{|\mathbf{x}-\mathbf{x}'|}\right] = 0. \tag{78}$$

To obtain the third term on the right-hand side of (69), by using the same method, we choose $\mathbf{L}_0 = \mathbf{L}-\mathbf{L}'$ and by using the integral technique above, we obtain

$$-\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-\beta|\mathbf{x}-\mathbf{L}'|}\mathrm{e}^{-\beta|\mathbf{x}-\mathbf{L}|}}{|\mathbf{x}-\mathbf{x}'|} \le 0. \tag{79}$$

Using (43) and substituting (79) into the third term on right-hand side of inequality (69), we have

$$-\int \mathrm{d}^2\mathbf{x}'\, \mathrm{e}^{-\beta|\mathbf{x}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{x}'-\mathbf{L}'|}\int \mathrm{d}^2\mathbf{x}\, \frac{\mathrm{e}^{-\beta|\mathbf{x}-\mathbf{L}'|}\mathrm{e}^{-\beta|\mathbf{x}-\mathbf{L}|}}{|\mathbf{x}-\mathbf{x}'|} \le 0. \tag{80}$$

Noting (73), (78) and (80), let $\mathbf{L}_1 = \mathbf{L}$, $\mathbf{L}_2 = \mathbf{L}'$, $\mathbf{x}_1 = \mathbf{x}$ and $\mathbf{x}_2 = \mathbf{x}'$, we obtain the expectation value of electron-electron interaction for $k = 2$ hydrogen nuclei as

$$\langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}|\Psi\rangle = \langle\Psi|\frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|}|\Psi\rangle \leq 0. \tag{81}$$

3.4 Nucleus-nucleus interaction

To obtain the expectation value of nucleus-nucleus interaction for hydrogen nuclei, let

$$\mathbf{L}_1 - \mathbf{L}_2 = \mathbf{L}_0. \tag{82}$$

Substitution of above expression into the fourth term on the right-hand side of (22), gives us

$$\langle\Psi|\frac{e^2}{|\mathbf{L}_1 - \mathbf{L}_2|}|\Psi\rangle = \frac{e^2}{L_0}. \tag{83}$$

From (83), for $L_0 \to \infty$, the bound of the expectation value of nucleus-nucleus interaction for two $k = 2$ hydrogen nucleies is

$$\lim_{L_0\to\infty}\langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{L}_i - \mathbf{L}_j|}|\Psi\rangle = 0. \tag{84}$$

3.5 The upper bound

By referring to (22), (50), (68), (81), and (84), we obtain the upper bound for the ground-state energy of two dimensional fermionic matter consisting two hydrogen atoms :

$$\begin{aligned}\langle\Psi|H|\Psi\rangle &= \langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle - \langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{e^2}{|\mathbf{x}_i - \mathbf{L}_j|}|\Psi\rangle + \langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}|\Psi\rangle + \langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{L}_i - \mathbf{L}_j|}|\Psi\rangle \\ &\leq -2\left(\frac{3me^4}{2\hbar^2}\right).\end{aligned} \tag{85}$$

4. Conclusion

We have seen that the exact ground-state energy with one hydrogen atom in two dimensions can be computed, but the ground-state energy of fermionic matter with two hydrogen atoms need to be bounded only. This is because of the exchanging term of wave function overlabing. However in this article, we consider the case that there is no overlab of atom ($|\mathbf{L}_i - \mathbf{L}_j| \to \infty$). The results also share that the upper bound of the ground-state energy of fermionic matter with two hydrogen atoms is less than two times of the ground-state energy with one hydrogen $\left(\langle\Psi|H|\Psi\rangle \le -2\left(\frac{3me^4}{2\hbar^2}\right)\right)$.

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