# Hartree-Fock Theory with Correlation Effects Applied to Nuclear Reaction Rates for Charged Bose Nuclei Confined in a Harmonic Trap

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Abstract: Based on Hartree-Fock theory with correlations, approximate solutions of the many-body Schrödinger equation are examined for their use for calculations of nuclear reaction rates for charged Bose nuclei confined in a harmonic trap. It is shown that the nuclear reaction rate calculated with the Hartree-Fock mean field solution makes a significant contribution even in the presence of two-body correlations.

The nuclear reaction rates for charged Bose nuclei confined in a harmonic trap has been calculated based on the optical theorem formulation of low-energy nuclear reactions [1] using approximate solutions of the many-body Schrödinger equation [2-15]. The effect of two-body correlations are examined in the context of the Hartree-Fock theory with correlation effects [3].

For N charged Bose nuclei (Z=1) confined in a harmonic trap, the many-body Schrödinger equation is given by

$$H\Psi = E\Psi \tag{1}$$

$$H = \frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \frac{1}{2}m\omega^2\sum_{i=1}^{N}r_i^2 + \sum_{i<j}\frac{e^2}{\left|\mathrm{r}_i - \mathrm{r}_j\right|} \tag{2}$$

Since we cannot solve the above many-body Schrödinger equation to obtain the exact solution for the ground bound-state wave function Ψ, we seek approximate solutions $\overline{\Psi}_i$ for the case of N>> 1 satifying

$$H\overline{\Psi}_{(i)} \approx E_0\overline{\Psi}_{(i)} \tag{3}$$

with

$$\overline{\Psi}_{(1)} = \phi_{(1)}(\mathrm{r}_1)\phi_{(1)}(\mathrm{r}_2)\phi_{(1)}(\mathrm{r}_3)\phi_{(1)}(\mathrm{r}_4)....\phi_{(1)}(\mathrm{r}_N) \tag{4-1}$$

$$\overline{\Psi}_{(2)} = f_{(2)}(\mathrm{r}_1,\mathrm{r}_2)\phi_{(2)}(\mathrm{r}_3)\phi_{(2)}(\mathrm{r}_4).........\phi_{(2)}(\mathrm{r}_N) \tag{4-2}$$

$$\overline{\Psi}_{(3)} = f_{(3)}(\mathrm{r}_1,\mathrm{r}_2)\, f_{(3)}(\mathrm{r}_3,\mathrm{r}_4)\phi_{(3)}(\mathrm{r}_5)......\phi_{(3)}(\mathrm{r}_N) \tag{4-3}$$

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where $f_{(i)}(\mathbf{r}_1,\mathbf{r}_2)$ is a two-body correlation function.

$\bar{\Psi}_{(1)}$ is the solution of the Hartree-Fock mean field equation which has been solved analytically [4]. The solution was used to derive an analytical formula for the nuclear reaction rates [4]. The analytical formula for the nuclear reaction rates [4] agrees with the results obtained by an independent method [2] within a factor of two (the result of [4] is a factor of 2 larger than that of [2]).

For i > 1, $\bar{\Psi}_{(i)}$ have not been solved. We need to carry out numerical calculations and simulations in order to obtain numerical solutions for $\bar{\Psi}_{(i>1)}$. In the following, we make qualitative theoretical analysis of the nuclear reaction rates using $\bar{\Psi}_{(i)}$ based on expected general properties of $\bar{\Psi}_{(i)}$ without obtaining its numerical solutions.

Since $\bar{\Psi}_{(i)}$ satisfy Eq. (3), they are degenerate eigenfunctions with the same eigenvalue. They are not orthogonal in general. We can construct an orthonormal set, $\hat{\Psi}_{(i)}$ , from the set, $\bar{\Psi}_{(i)}$, using the Schmidt orthogonalization procedure:

$$H\hat{\Psi}_{(i)} \approx E_0 \hat{\Psi}_{(i)} \tag{5}$$

with
$$\hat{\Psi}_{(i)} = \sum_j \alpha_j \overline{\Psi}_{(j)}, \qquad \left\langle \hat{\Psi}_{(k)} \middle| \hat{\Psi}_{(l)} \right\rangle = \delta_{kl} \tag{6}$$

where $\alpha_j$ are determined from the Schmidt orthogonalization procedure.

In terms of $\hat{\Psi}_{(i)}$, we can construct a general solution $\Psi$ for the bound-state wave function satisfying Eq. (1) or Eq. (7):

$$H\Psi \approx E_0 \Psi \tag{7}$$

$$\Psi = \frac{1}{\sqrt{A}} \sum_{j=1}^{A} \hat{\Psi}_{(j)}, \qquad \left\langle \hat{\Psi}_{(k)} \middle| \hat{\Psi}_{(l)} \right\rangle = \delta_{kl} \tag{8}$$

where $\Psi$ is a combination of linearly independent orthonormal eigenfunctions $\Psi_{(i)}$ given by Eq. (6).

For N identical Bose nuclei, we require the total wave function $\Psi$ in Eq. (1) and also $\Psi$ in Eq. (7) to be completely symmetric. Hence we need to symmetrize $\Psi$ in Eq. (7). The completely symmetric wave function $\overset{\frown}{\Psi}$ is obtained from $\Psi$ by

$$\overset{\frown}{\Psi} = S\Psi \tag{9}$$

using the symmetrization operator S defined as

$$S = \frac{1}{N!} \sum_i P_{(i)} \tag{10}$$

where $P_{(i)}$ is the permutation operator with (i) representing an arbitrary permutation of the first N integers. We note that $\overline{\Psi}_{(1)}$ given by Eq. (4-1) is already symmetric, i. e. $S\overline{\Psi}_{(1)} = \overline{\Psi}_{(1)}$.

Using $\widehat{\Psi}$ , Eq. (9), we can now proceed to calculate the total fusion rate $R_t$ as [4].

$$R_t = -\frac{2}{\hbar}\frac{\sum_{i<j}\left\langle\widehat{\Psi}\middle|\mathrm{Im}V_{ij}^F\middle|\widehat{\Psi}\right\rangle}{\left\langle\widehat{\Psi}\middle|\widehat{\Psi}\right\rangle} \tag{11}$$

with

$$Im\, V_{ij}^F = -\frac{A\hbar}{2}\delta(\boldsymbol{r}_{ij}) \tag{12}$$

where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$.

In calculating $R_t$ from Eq. (11) with Eq. (12), we need to evaluate

$$\left\langle S\overline{\Psi}_{(i)}\middle|\sum_{k<l}\delta(\boldsymbol{r}_{kl})\middle|S\overline{\Psi}_{(i)}\right\rangle \tag{13}$$

For the case of (i) = (1), we have $\left\langle S\overline{\Psi}_{(1)}\middle|\sum_{k<l}\delta(\boldsymbol{r}_{kl})\middle|S\overline{\Psi}_{(1)}\right\rangle = \left\langle\overline{\Psi}_{(1)}\middle|\sum_{k<l}\delta(\boldsymbol{r}_{kl})\middle|\overline{\Psi}_{(1)}\right\rangle$ which were already calculated in [4].

For the case of (i) = (2), we need to evaluate many terms from $\left\langle S\overline{\Psi}_{(2)}\middle|\sum_{i<j}\delta(\boldsymbol{r}_{ij})\middle|S\overline{\Psi}_{(2)}\right\rangle$. The terms (Eqs. (14) and (15)) involving $f_{(2)}(\boldsymbol{r}_i,\boldsymbol{r}_j)$:

$$\left\langle f_{(2)}(\boldsymbol{r}_i,\boldsymbol{r}_j)\middle|\delta(\boldsymbol{r}_{ij})\middle|f_{(2)}(\boldsymbol{r}_i,\boldsymbol{r}_j)\right\rangle \propto e^{-2\pi\eta}\ (\rightarrow 0) \tag{14}$$

and

$$\left\langle f_{(2)}(\boldsymbol{r}_i,\boldsymbol{r}_j)\middle|\delta(\boldsymbol{r}_{ij})\middle|\phi_{(2)}(\boldsymbol{r}_i)\phi_{(2)}(\boldsymbol{r}_j)\right\rangle \tag{15}$$

are expected to be very small ($e^{-2\pi\eta}$ is the Gamow factor) and hence they may not contribute significantly to $R_{t,}$ Eq. (11). However, other terms (Eq. (16)) invloving

$$\left\langle \phi_{(2)}(\boldsymbol{r}_i)\phi_{(2)}(\boldsymbol{r}_j)\middle|\delta(\boldsymbol{r}_{ij})\middle|\phi_{(2)}(\boldsymbol{r}_i)\phi_{(2)}(\boldsymbol{r}_j)\right\rangle \tag{16}$$

are expected to contribute to $R_{t,}$ Eq. (11).

Therefore, the use of Eq. (4-2) in Eq. (3) is expected to provide additional contributions from the terms involving these terms (Eq. (16) to the total reaction rate $R_t$ , Eq. (11). However, it is most unlikely that contributions originating from both $\overline{\Psi}_{(1)}$ and $\overline{\Psi}_{(2)}$ could cancel exactly leading to $R_t \approx 0$ in evaluating $R_t$ , Eq. (11).

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