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ABSTRACT

By means of a partitioning method similar to that applicable to the one-electron problem, the sixteen-component two-electron Breit equation is reduced to a four-component equation, involving only the "large" (i.e., positive energy) components of the wave function. The equation obtained by this method is compared to the results of a F-W transformation on the two-electron Hamiltonian.

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The Breit equation can be written as[1]

$$\Omega \Psi = 0 \tag{1}$$

where $\Omega = E - \frac{e^2}{r} - H^{I} - H^{II} + B$,

$H^{I} = -e\,\phi(\underline{r}^{I}) + \beta^{I} mc^2 + c\,\underline{\alpha}^{I} \cdot \underline{\pi}^{I}$,

E = total energy $= i\hbar\,\partial/\partial t$ for non-stationary states,

$-e$ = charge of the electron.

Superscripts I, II refer to electrons I, II respectively,

$\underline{r} = \underline{r}^{I} - \underline{r}^{II}$ = interelectron distance,

$\underline{\pi}^{I} = \underline{p}^{I} + \frac{e}{c}\underline{A}^{I}(\underline{r}^{I})$,

ϕ, $\underline{A}$ are the scalar and vector potentials of the external electromagnetic field; $\underline{\alpha}^{I}$, β^{I} are direct products of 4 x 4 Dirac matrices for electron I with the four-dimensional unit matrix for electron II, and

$$B = \frac{e^2}{2r}\left[\underline{\alpha}^{I} \cdot \underline{\alpha}^{II} + \frac{1}{r^2}(\underline{\alpha}^{I} \cdot \underline{r})(\underline{\alpha}^{II} \cdot \underline{r})\right]$$

is the Breit approximation to the relativistic interaction between two electrons[2] (neglecting quantum field effects), and, for <u>weak</u> external fields, is a good approximation to first order in perturbation theory.

The wave function $\Psi = \Psi(\underline{r}^{I}, \underline{r}^{II})$ depends on the positions of the two electrons and has sixteen spinor components. Ψ can be considered as a direct product of two one-electron, four-component spinor wave functions, $\Psi^{I}(\underline{r}^{I})$ and $\Psi^{II}(\underline{r}^{II})$.

i.e., $$\Psi(\underline{r}^{I},\underline{r}^{II}) = \Psi^{I}(\underline{r}^{I}) \otimes \Psi^{II}(\underline{r}^{II})$$

and $$\Psi_{ij} = \Psi^{I}_{i}(\underline{r}^{I})\,\psi^{II}_{j}(\underline{r}^{II})$$
$$i,j = 1,2,3,4$$

Each of Ψ^{I} and Ψ^{II} can be partitioned into large (u) and small (ℓ) components:

$$\Psi^{I}(\underline{r}^{I}) = \begin{pmatrix} \Psi^{I}_{u} \\ \Psi^{I}_{\ell} \end{pmatrix} \quad \text{where } \Psi^{I}_{u} = \begin{pmatrix} \psi^{I}_{1} \\ \psi^{I}_{2} \end{pmatrix};\ \Psi^{I}_{\ell} = \begin{pmatrix} \psi^{I}_{3} \\ \psi^{I}_{4} \end{pmatrix}$$

Consequently, $\Psi(\underline{r}^{I},\underline{r}^{II})$ can be partitioned as follows:

$$\Psi(\underline{r}^{I},\underline{r}^{II}) = \begin{pmatrix} \psi_{u,u} \\ \psi_{u,\ell} \\ \psi_{\ell,u} \\ \psi_{\ell,\ell} \end{pmatrix}, \quad \text{where } \psi_{\mu,\nu} = \Psi^{I}_{\mu}(\underline{r}^{I}) \otimes \Psi^{II}_{\nu}(\underline{r}^{II})$$
$$\mu,\nu = u,\ell.$$

Then, $$\beta^{I} = \begin{pmatrix} \mathbb{1} & 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 & 0 \\ 0 & 0 & -\mathbb{1} & 0 \\ 0 & 0 & 0 & -\mathbb{1} \end{pmatrix}, \quad \beta^{II} = \begin{pmatrix} \mathbb{1} & 0 & 0 & 0 \\ 0 & -\mathbb{1} & 0 & 0 \\ 0 & 0 & \mathbb{1} & 0 \\ 0 & 0 & 0 & -\mathbb{1} \end{pmatrix},$$

$$\underline{\alpha}^{I} = \begin{pmatrix} 0 & 0 & \underline{\sigma}^{I} & 0 \\ 0 & 0 & 0 & \underline{\sigma}^{I} \\ \underline{\sigma}^{I} & 0 & 0 & 0 \\ 0 & \underline{\sigma}^{I} & 0 & 0 \end{pmatrix}, \quad \underline{\alpha}^{II} = \begin{pmatrix} 0 & \underline{\sigma}^{II} & 0 & 0 \\ \underline{\sigma}^{II} & 0 & 0 & 0 \\ 0 & 0 & 0 & \underline{\sigma}^{II} \\ 0 & 0 & \underline{\sigma}^{II} & 0 \end{pmatrix},$$

where $\mathbb{1}$ is the (4 x 4) unit matrix and $\underline{\sigma}^{I}$, $\underline{\sigma}^{II}$ are spin operators acting on electrons I, II respectively:

$$\underline{\sigma}^{I} = \begin{pmatrix} \hat{k} & 0 & \hat{i}-i\hat{j} & 0 \\ 0 & \hat{k} & 0 & \hat{i}-i\hat{j} \\ \hat{i}+i\hat{j} & 0 & -\hat{k} & 0 \\ 0 & \hat{i}+i\hat{j} & 0 & -\hat{k} \end{pmatrix}, \quad \underline{\sigma}^{II} = \begin{pmatrix} \hat{k} & \hat{i}-i\hat{j} & 0 & 0 \\ \hat{i}+i\hat{j} & -\hat{k} & 0 & 0 \\ 0 & 0 & \hat{k} & \hat{i}-i\hat{j} \\ 0 & 0 & \hat{i}+i\hat{j} & -\hat{k} \end{pmatrix}$$

where $\hat{i}$, $\hat{j}$, $\hat{k}$ are unit vectors in the x, y, z directions.

With this notation,

$$\Omega = E + e\varphi - \frac{e^2}{r} - 2mc^2 \begin{pmatrix} \mathbb{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathbb{1} \end{pmatrix}$$

$$- c \begin{pmatrix} 0 & 0 & \underline{\sigma}^{I}\cdot\underline{\pi}^{I} & 0 \\ 0 & 0 & 0 & \underline{\sigma}^{I}\cdot\underline{\pi}^{I} \\ \underline{\sigma}^{I}\cdot\underline{\pi}^{I} & 0 & 0 & 0 \\ 0 & \underline{\sigma}^{I}\cdot\underline{\pi}^{I} & 0 & 0 \end{pmatrix} - c \begin{pmatrix} 0 & \underline{\sigma}^{II}\cdot\underline{\pi}^{II} & 0 & 0 \\ \underline{\sigma}^{II}\cdot\underline{\pi}^{II} & 0 & 0 & 0 \\ 0 & 0 & 0 & \underline{\sigma}^{II}\cdot\underline{\pi}^{II} \\ 0 & 0 & \underline{\sigma}^{II}\cdot\underline{\pi}^{II} & 0 \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & 0 & 0 & I \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ I & 0 & 0 & 0 \end{pmatrix} \tag{2}$$

where

$$I = \frac{e^2}{2r}\left[\underline{\sigma}^{I}\cdot\underline{\sigma}^{II} + \frac{1}{r^2}(\underline{\sigma}^{I}\cdot\underline{r})(\underline{\sigma}^{II}\cdot\underline{r})\right] \equiv \frac{e^2}{2r} J .$$

Equation 1 can now be written as four equations involving only (4 x 4) matrices and four-component spinors:

$$\left(W + e\phi - \frac{e^2}{r}\right)\psi_{u,u} - c(\sigma^{I}\cdot\pi^{I})\psi_{\ell,u} - c(\sigma^{II}\cdot\pi^{II})\psi_{u,\ell} + I\,\psi_{\ell,\ell} = 0 \qquad (3,a)$$

$$\left(2mc^2 + W + e\phi - \frac{e^2}{r}\right)\psi_{u,\ell} - c(\sigma^{I}\cdot\pi^{I})\psi_{\ell,\ell} - c(\sigma^{II}\cdot\pi^{II})\psi_{u,u} + I\,\psi_{\ell,u} = 0 \qquad (3,b)$$

$$\left(2mc^2 + W + e\phi - \frac{e^2}{r}\right)\psi_{\ell,u} - c(\sigma^{I}\cdot\pi^{I})\psi_{u,u} - c(\sigma^{II}\cdot\pi^{II})\psi_{\ell,\ell} + I\,\psi_{u,\ell} = 0 \qquad (3,c)$$

$$\left(4mc^2 + W + e\phi - \frac{e^2}{r}\right)\psi_{\ell,\ell} - c(\sigma^{I}\cdot\pi^{I})\psi_{u,\ell} - c(\sigma^{II}\cdot\pi^{II})\psi_{\ell,u} + I\,\psi_{\ell,\ell} = 0 \qquad (3,d)$$

where $W \equiv E - 2mc^2$.

If we write $\lambda = 1/2mc^2$ and define operators

$$g_1 = \left[1 + \lambda(W + e\phi) - \lambda\, e^2/r\right]^{-1}, \quad \ell = \left[1 - \lambda^2 I^2 g_1^{\,2}\right]^{-1}$$

and

$$g_2 = \Big[1 + \frac{\lambda}{2}(W + e\phi) - \frac{\lambda}{2}\frac{e^2}{r} - \frac{\lambda}{4m}\left\{(\sigma^{I}\cdot\pi^{I})\,\ell g_1 (\sigma^{I}\cdot\pi^{I}) + (\sigma^{II}\cdot\pi^{II})\,\ell g_1 (\sigma^{II}\cdot\pi^{II})\right\}$$
$$+ \frac{\lambda^2}{4m}\left\{(\sigma^{I}\cdot\pi^{I})\,\ell\, I g_1^{\,2}\,(\sigma^{II}\cdot\pi^{II}) + (\sigma^{II}\cdot\pi^{II})\,\ell\, I g_1^{\,2}\,(\sigma^{I}\cdot\pi^{I})\right\}\Big]^{-1},$$

then equations 3,b and 3,c can be solved formally for $\psi_{u,\ell}$ and $\psi_{\ell,u}$ in terms of $\psi_{u,u}$ and $\psi_{\ell,\ell}$. If these are substituted into equation 3,d , an expression for $\psi_{\ell,\ell}$ as a function of $\psi_{u,u}$ is obtained, and hence $\psi_{u,\ell}$ and $\psi_{\ell,u}$ can also be expressed in terms of $\psi_{u,u}$. Substitution of these expressions into equation 3,a yields an equation involving only

$\Psi_{u,u}$, namely

$$H' \Psi_{u,u} = \left(W + e\phi - \frac{e^2}{r} \right) \Psi_{u,u} \qquad (4)$$

Since the Breit equation is a good approximation only to first order, it is sufficient to include only those terms in H' which involve λ and I to zeroth or first order. In this approximation:

$$\begin{aligned}
H' = {} & \frac{1}{2m} (\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{I}\cdot\pi^{I}) + \frac{1}{2m} (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{II}\cdot\pi^{II}) \\
& + \frac{1}{16m^3c^2} \Big[(\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II})\, g_2 (\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II}) \\
& + (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I})\, g_2 (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I}) \\
& + (\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II})\, g_2 (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I}) \\
& + (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I})\, g_2 (\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II}) \Big] \\
& - \frac{1}{4m^2c^2} \Big[(\sigma^{I}\cdot\pi^{I})\, \ell I g_1^2 (\sigma^{II}\cdot\pi^{II}) + (\sigma^{II}\cdot\pi^{II})\, \ell I g_1^2 (\sigma^{I}\cdot\pi^{I}) \Big] \\
& - \frac{1}{8m^2c^2} \Big[(\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II})\, g_2 I + (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I})\, g_2 I \\
& + I g_2 (\sigma^{I}\cdot\pi^{I})\, \ell g_1 (\sigma^{II}\cdot\pi^{II}) + I g_2 (\sigma^{II}\cdot\pi^{II})\, \ell g_1 (\sigma^{I}\cdot\pi^{I}) \Big] \qquad (5)
\end{aligned}$$

+ higherorder terms involving λI^2, $\lambda^2 I$, $\lambda^2 I^2$, and $\lambda^3 I^2$.

As would be expected, H' is symmetric with respect to interchange of the two electrons, and is a hermitian operator.

If F is any arbitrary operator, then[3]

$$[F, g_1] = g_1 \, [g_1^{-1}, F] \, g_1 = \lambda g_1 \left[\left(W + e\phi - \frac{e^2}{r} \right), F \right] g_1 .$$

Since all terms in H' involving g_2 are already multiplied by λ, then $[F, g_2]$ need only be considered to zeroth order in λ, and, to this order, $[F, g_2] = 0$. To first order in λ, $[F, \ell] = 0$. Then, to first order in λ and I, for stationary states, equation 5 reduces to:

$$
\begin{aligned}
H' = {} & \frac{1}{2m} \, \ell g_1 \left(p^{I\,2} + p^{II\,2} \right) + \frac{e^2}{2mc^2} \, \ell g_1 \left(A^{I\,2} + A^{II\,2} \right) \\
& + \frac{e}{mc} \, \ell g_1 \left(A^{I} \cdot p^{I} + A^{II} \cdot p^{II} \right) + \mu_B \, \ell g_1 \left(\underline{\sigma}^{I} \cdot \underline{H}^{I} + \underline{\sigma}^{II} \cdot \underline{H}^{II} \right) \\
& - i \frac{\mu_B}{2mc} \, \ell g_1^2 \left(\underline{\mathcal{E}}^{I} \cdot p^{I} + \underline{\mathcal{E}}^{II} \cdot p^{II} \right) \\
& + \frac{\mu_B}{2mc} \, \ell g_1^2 \left[\sigma^{I} \cdot \left(\underline{\mathcal{E}}^{I} \times p^{I} \right) + \sigma^{II} \cdot \left(\underline{\mathcal{E}}^{II} \times p^{II} \right) \right] \\
& - \frac{e \mu_B}{2mc} \, \frac{\ell g_1^2}{r^3} \left[\sigma^{I} \cdot \left(\underline{r} \times p^{I} \right) - \sigma^{II} \cdot \left(\underline{r} \times p^{II} \right) \right] \\
& + \frac{i e \mu_B}{2mc} \, \frac{\ell g_1 (2 g_1 + g_2)}{r^3} \, \underline{r} \cdot \left(p^{I} - p^{II} \right) + \frac{1}{4 m^3 c^2} \ell^2 g_1^2 g_2 \, p^{I\,2} p^{II\,2} \\
& + \frac{e \mu_B}{2mc} \, \frac{\ell g_1 (g_1 + g_2)}{r^3} \left[\sigma^{I} \cdot \left(\underline{r} \times p^{II} \right) - \sigma^{II} \cdot \left(\underline{r} \times p^{I} \right) \right] \\
& + \mu_B^2 \, \frac{\ell g_1 g_2}{r^3} \left[\sigma^{I} \cdot \sigma^{II} - \frac{3}{r^2} \left(\sigma^{I} \cdot \underline{r} \right) \left(\sigma^{II} \cdot \underline{r} \right) \right] \\
& + 4 \mu_B^2 \, \ell g_1 g_2 \, \pi \, \delta(\underline{r}) \left[1 - \left(\sigma^{I} \cdot \sigma^{II} \right) \right] \\
& - \frac{e^2}{(2mc)^2} \, \ell g_1 (g_1 + g_2) \left[\frac{p^{I} \cdot p^{II}}{r} + \frac{1}{r^3} \, \underline{r} \cdot \left(\underline{r} \cdot p^{I} \right) p^{II} \right] \\
& + H''
\end{aligned}
\qquad (6)
$$

where $\underline{\mathcal{E}}^{i}$ and $\underline{H}^{i}$ are the electric and magnetic fields at electron i, $\quad i = I, II$;

$$\mu_B = \frac{e\hbar}{2mc} ,$$

$$H'' = -\frac{e^2}{(2mc)^2} \lambda g_1 (g_1 - g_2) \left\{ \frac{\hbar}{r^3} [\sigma^{I} \cdot (\underline{r} \times p^{I}) - \sigma^{II} \cdot (\underline{r} \times p^{II})] - \frac{i\hbar}{r^3} (\sigma^{I} \cdot \sigma^{II}) \underline{r} \cdot (p^{I} - p^{II}) - \frac{1}{r} (\sigma^{I} \cdot p^{II})(\sigma^{II} \cdot p^{I}) + \frac{1}{r} (\sigma^{I} \cdot \sigma^{II})(p^{I} \cdot p^{II}) + \frac{i\hbar}{r^3} [(\sigma^{I} \cdot \underline{r})(\sigma^{II} \cdot p^{I}) - (\sigma^{II} \cdot \underline{r})(\sigma^{I} \cdot p^{II})] + \frac{1}{r^3} \sigma^{I} \cdot (\underline{r} \times [\sigma^{II} \cdot (\underline{r} \times p^{II})] p^{I}) \right\} \quad (7)$$

I. Consider the case where both electrons are a large distance, i.e., $\gg \lambda e^2 \equiv r_0 = 1.409 \times 10^{-13}$ cm. from any point sources. In this case, φ is a well-behaved function (no singularities), and the operators g_1 and g_2 can be expanded as follows:[5]

$$g_1 = [g_{01}^{-1} + \lambda (W + e\varphi)]^{-1}$$

where $g_{01} \equiv \left(1 - \lambda \frac{e^2}{r}\right)^{-1}$.

Using the operator identity:[4]

$$(A - B)^{-1} = A^{-1} \sum_{n=0}^{\infty} (BA^{-1})^n ,$$

this becomes $g_1 = g_{01} \sum_{n=0}^{\infty} [-\lambda (W + e\varphi) g_{01}]^n$.

For stationary states, $[(W + e\varphi), g_{01}] = 0$, so that, to first order in λ,

$$g_1 = g_{01} - \lambda g_{01}^2 (W + e\phi)$$

To zeroth order in λ, $g_2 = g_{02} \equiv \left(1 - \lambda \frac{e^2}{2r}\right)^{-1}$.

These substitutions yield equation 6 with g_1 and g_2 everywhere replaced by g_{01} and g_{02}, and the additional term:

$$-\frac{1}{(2mc)^2} \ell g_{01}^2 (W + e\phi)(p^{I\,2} + p^{II\,2}).$$

A. For $r \gg r_0$,

$$g_{01} = \left(1 - \lambda \frac{e^2}{r}\right)^{-1} = 1 + \lambda \frac{e^2}{r} \qquad \text{to first order in } \lambda,$$

$$\ell = 1,$$

and $g_{02} = 1$ to zeroth order in λ. Also, to zeroth order in λ, $H' = \frac{1}{2m}(p^{I\,2} + p^{II\,2}) = W + e\phi - \frac{e^2}{r}$

so that:

$$\frac{1}{2m}(p^{I\,4} + p^{II\,4} + 2p^{I\,2}p^{II\,2}) = \left(W + e\phi - \frac{e^2}{r}\right)(p^{I\,2} + p^{II\,2})$$

$$+ ie\hbar\,(\mathcal{E}^{I}\cdot p^{I} + \mathcal{E}^{II}\cdot p^{II} + p^{I}\cdot \mathcal{E}^{I} + p^{II}\cdot \mathcal{E}^{II})$$

$$- 2i\,\frac{e^2\hbar}{r^3}\,\mathbf{r}\cdot(p^{I} - p^{II}).$$

Substitution of these values for g_1, g_2, ℓ, and $p^{I\,2}p^{II\,2}$ into equations 6 and 7 yields:

$$H'' = 0,$$

$$H' = \frac{1}{2m}\left(p^{I\,2} + p^{II\,2}\right) + \frac{e^2}{2mc^2}\left(A^{I\,2} + A^{II\,2}\right)$$

$$+ \frac{e}{mc}\left(A^I \cdot p^I + A^{II} \cdot p^{II}\right) + \mu_B\left(\sigma^I \cdot \underline{H}^I + \sigma^{II} \cdot \underline{H}^{II}\right)$$

$$+ \frac{ie\mu_B}{2mc}\,\frac{\underline{r}}{r^3} \cdot \left(p^I - p^{II}\right) - \frac{e\mu_B}{2mc}\,\frac{1}{r^3}\left[\sigma^I \cdot (\underline{r} \times p^I)\right.$$

$$\left. - \sigma^{II} \cdot (\underline{r} \times p^{II})\right] + \frac{i\mu_B}{2mc}\left(p^I \cdot \underline{E}^I + p^{II} \cdot \underline{E}^{II}\right)$$

$$- \frac{1}{8m^3c^2}\left(p^{I\,4} + p^{II\,4}\right) + \frac{\mu_B}{2mc}\left[\sigma^I \cdot \left(\underline{E}^I \times p^I\right) + \sigma^{II} \cdot \left(\underline{E}^{II} \times p^{II}\right)\right]$$

$$+ \frac{e\mu_B}{mc}\,\frac{1}{r^3}\left[\sigma^I \cdot \left(\underline{r} \times p^{II}\right) - \sigma^{II} \cdot \left(\underline{r} \times p^I\right)\right]$$

$$+ \frac{\mu_B^2}{r^3}\left[\sigma^I \cdot \sigma^{II} - \frac{3}{r^2}\left(\sigma^I \cdot \underline{r}\right)\left(\sigma^{II} \cdot \underline{r}\right)\right]$$

$$+ 4\pi\mu_B^2\,\delta(\underline{r})\left[1 - \left(\sigma^I \cdot \sigma^{II}\right)\right] - \frac{e^2}{2(mc)^2}\left[\frac{p^I \cdot p^{II}}{r}\right.$$

$$\left. + \frac{1}{r^3}\,\underline{r} \cdot \left(\underline{r} \cdot p^I\right) p^{II}\right] \qquad (8)$$

This agrees with the results obtained using the Foldy-Wouthuysen (FW) transformation,[6,7] except that in the FW method, the terms involving I^2 were not neglected. The FW transformation also led to a term of the form $\delta(\underline{r})\ \underline{r} \cdot (p^I - p^{II})$ which was not obtained using this partitioning method, and, according to Barker and Glover[7], the term involving $\delta(\underline{r})(\sigma^I \cdot \sigma^{II})$ should be multiplied by a factor of $2/3$.

B. For $r \ll r_0$,

$$g_{01} = \left(1 - \frac{r_0}{r}\right)^{-1} \approx - r/r_0 ,$$

$$g_{02} = \left(1 - \frac{r_0}{2r}\right)^{-1} \approx 2r/r_0 ,$$

and $\ell = \left(1 - \lambda^2 I^2 g_1^2\right)^{-1} \approx \left(1 - \frac{J^2}{4}\right)^{-1}$

Therefore, in the limit as $r \to 0$, the leading term in H' is :

$$2\mu_B^2 \left(1 - \frac{J^2}{4}\right)^{-1} \frac{1}{r_0^2 r} \left[(\sigma^I \cdot \sigma^{II}) - \frac{3}{r^2} (\sigma^I \cdot \underline{r})(\sigma^{II} \cdot \underline{r}) \right].$$

The terms involving the delta function of $\underline{r}$ do not contribute to H' in this limit, as they contain a factor of

$$\ell g_1 g_2 \to 2 \frac{r^2}{r_0^2} \left(1 - \frac{J^2}{4}\right)^{-1}$$

C. For r of the order of r_0 :

$g_{01} = \left(1 - \frac{r_0}{r}\right)^{-1}$ is well-behaved (as a function of r), except in the neighbourhood of $r = r_0$;

$g_{02} = \left(1 - \frac{r_0}{2r}\right)^{-1}$ has a pole at $r = \frac{r_0}{2}$;

and $\ell = \left(1 - \frac{r_0^4}{4r^2} J^2 g_{01}^2\right)^{-1} = (r - r_0)^2 L$, where

$L \equiv \left[(r - r_0)^2 - \frac{J^2}{4} r_0^2\right]^{-1}$ is well-behaved except

at $r = r_0 \pm \frac{J}{2} r_0.$

Thus, the weighting factors of the various terms of equation 6 are well-behaved functions of r for $r \gg r_0$ or for $r \ll r_0$, but exhibit strange singularities when $r \approx r_0$. This can be seen in the graphs of $l g_{01}, l g_{01}^2$, etc.

II. Consider the case where the electrons are in the neighbourhood of a spinless nucleus of charge Ze. Then,

$$\varphi^i = \varphi^i_{int} + \varphi^i_{ext} \qquad , \qquad i = \mathrm{I} \text{ or } \mathrm{II},$$

where φ^i_{int} is the electric potential at electron i due to the nuclear charge, and φ^i_{ext} is the electric potential at i due to the external field.

$$\varphi^{\mathrm{I}}_{int} = \frac{Ze}{r^{\mathrm{I}}} \quad , \quad \varphi^{\mathrm{II}}_{int} = \frac{Ze}{r^{\mathrm{II}}} \quad .$$

Then, in equation 6, $\mathcal{E}^{\mathrm{I}}$ is replaced by $\mathcal{E}^{\mathrm{I}}_{ext}$, $\mathcal{E}^{\mathrm{II}}$ by $\mathcal{E}^{\mathrm{II}}_{ext}$, and the following additional terms must be included:

$$- i \; \frac{Ze\mu_B}{2mc} \; l g_1^2 \left(\frac{1}{r^{\mathrm{I}3}} \, \underline{r}^{\mathrm{I}} \cdot p^{\mathrm{I}} + \frac{1}{r^{\mathrm{II}3}} \, \underline{r}^{\mathrm{II}} \cdot p^{\mathrm{II}} \right)$$

$$+ \frac{Ze\mu_B}{2mc} \; l g_1^2 \left[\frac{1}{r^{\mathrm{I}3}} \, \sigma^{\mathrm{I}} \cdot (\underline{r}^{\mathrm{I}} \times p^{\mathrm{I}}) \right.$$

$$\left. + \frac{1}{r^{\mathrm{II}3}} \, \sigma^{\mathrm{II}} \cdot (\underline{r}^{\mathrm{II}} \times p^{\mathrm{II}}) \right] .$$

Conclusions: It can be seen that, for interelectronic separations other than those of the order of $r_0 = 1.409 \times 10^{-13}$ cm, this partitioning technique yields results which agree with the results obtained using the FW type transformation. Apart from numerical factors multiplying delta functions and the non-occurrence of some delta functions in the partitioning method, the chief discrepancies are the singularities of the inverse operators at interelectronic separations of the order of r_0. It is not obvious what, if any, physical significance should be attached to this behaviour.

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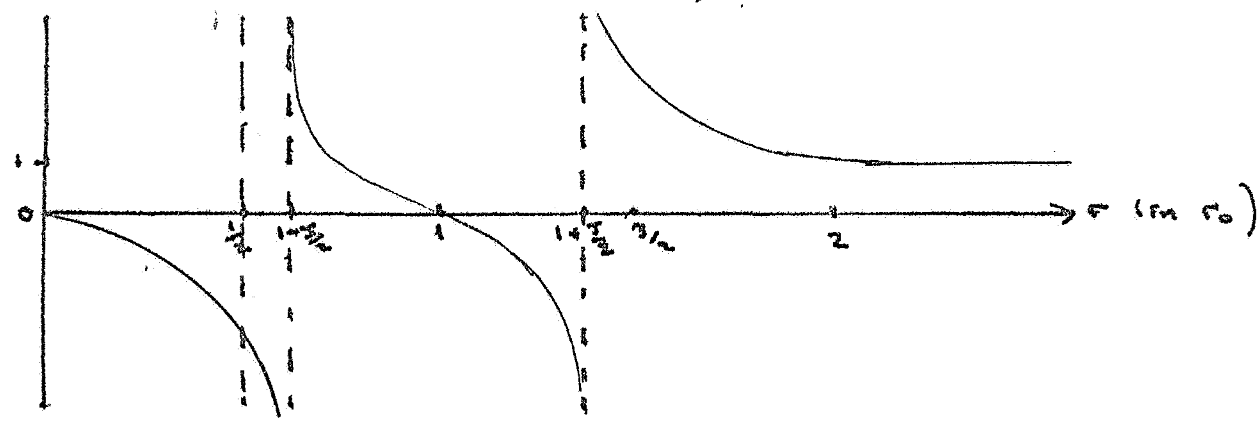
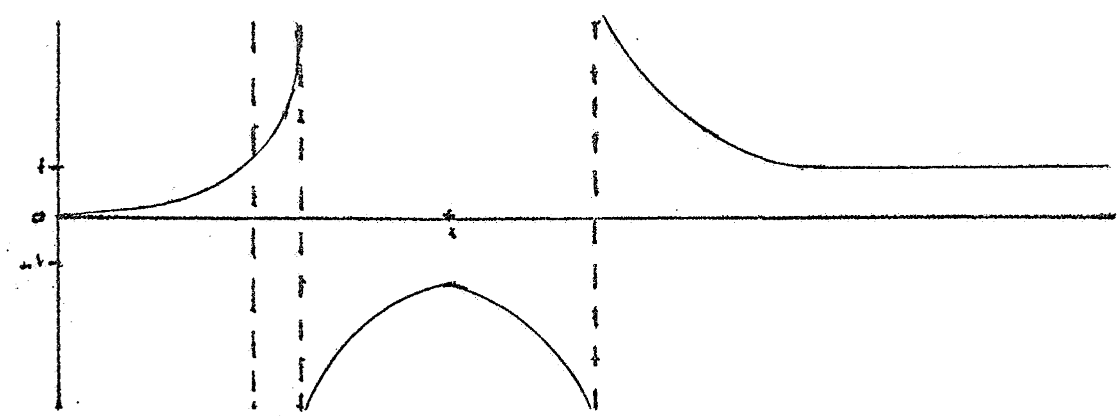
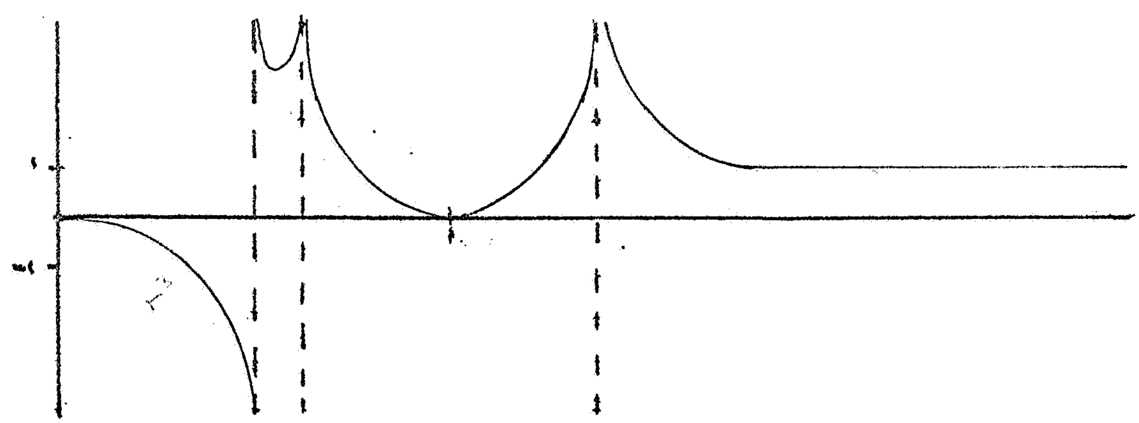
lg_{01}



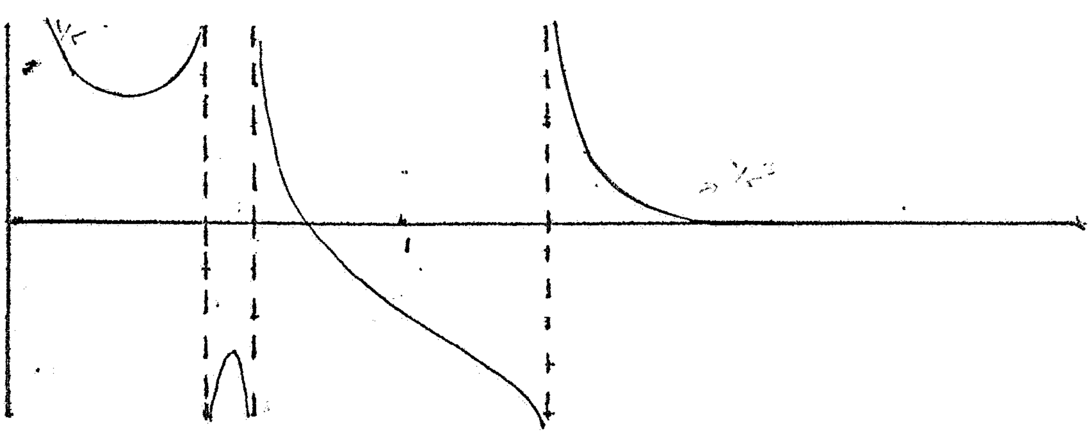
lg_{01}^2

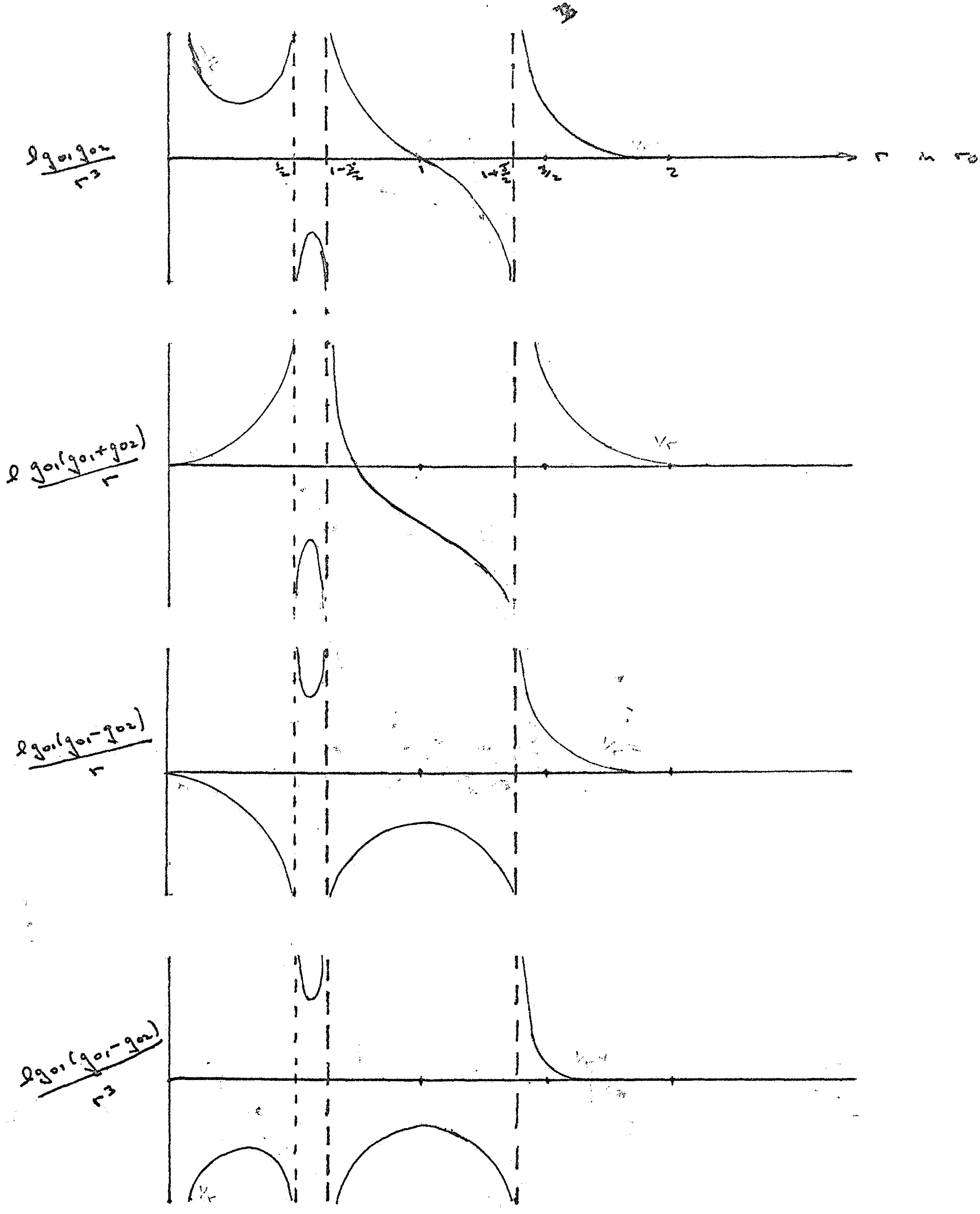


$l^2 g_{01}^2 g_{02}$



$\frac{l g_{01}(g_{01}+g_{02})}{r^3}$





lg01g02 / r3
lg01(g01+g02) / r
lg01(g01-g02) / r
lg01(g01-g02) / r3
r in r0
1/2
1
3/2
2