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Penny G. Estabrooks

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University of Wisconsin Theoretical Chemistry Institute
Madison, Wisconsin

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]

$$\Omega \Psi = 0 \qquad (1)$$

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 weak 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
$$\Psi_{ij} = \Psi_i^{I}(\underline{r}^{I})\,\Psi_j^{II}(\underline{r}^{II}) \qquad i,j = 1,2,3,4$$

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

$$\Psi^{I}(\underline{r}^{I}) = \begin{pmatrix} \Psi_u^{I} \\ \Psi_\ell^{I} \end{pmatrix} \quad \text{where } \Psi_u^{I} = \begin{pmatrix} \psi_1^{I} \\ \psi_2^{I} \end{pmatrix}; \; \Psi_\ell^{I} = \begin{pmatrix} \psi_3^{I} \\ \psi_4^{I} \end{pmatrix}$$

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

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

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 (4×4) unit matrix and $\underline{\sigma}^{I}$, $\underline{\sigma}^{II}$ are spin operators acting on electrons I, II respectively:

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

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

With this notation,

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

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

$$+ \begin{pmatrix} 0 & 0 & 0 & I \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ I & 0 & 0 & 0 \end{pmatrix} \qquad (2)$$

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

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

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

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

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:

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

+ 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:

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

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

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

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

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]

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

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

Using the operator identity:[4]

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

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

For stationary states, $\left[(W + e\phi), g_{01} \right] = 0$, 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:

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

A. For $r \gg r_0$,

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

$$l = 1,$$

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

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

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

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

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

$$H'' = 0,$$

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

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

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

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

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

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

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

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

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

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 <u>not</u> 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 $$\ell = (1 - \lambda^2 I^2 g_1^2)^{-1} \approx \left(1 - \frac{J^2}{4}\right)^{-1}$$

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 $\ell g_{01}, \ell g_{01}^2$, etc.

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

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

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.

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

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:

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

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

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

<u>Conclusions</u>: 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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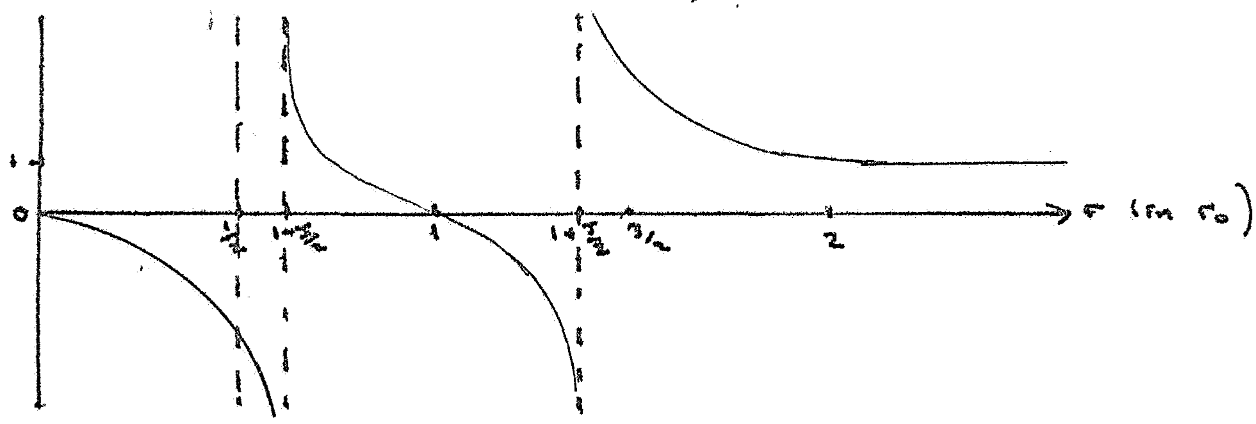
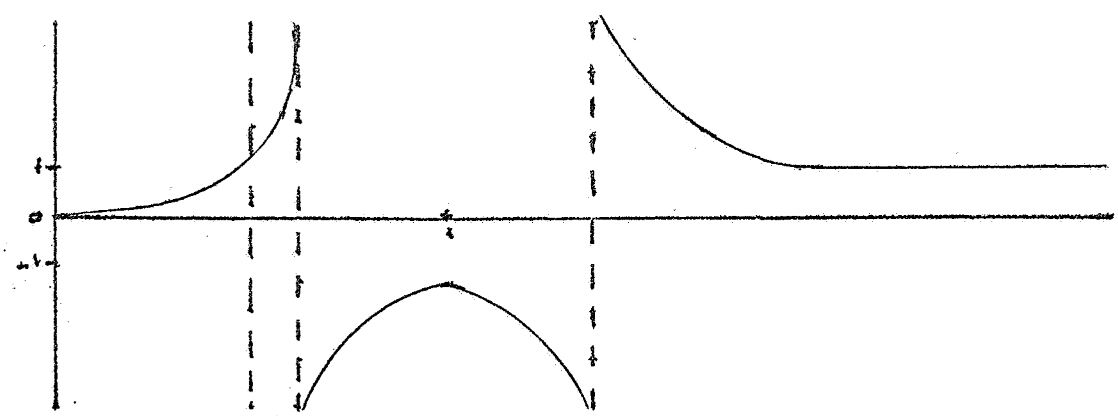
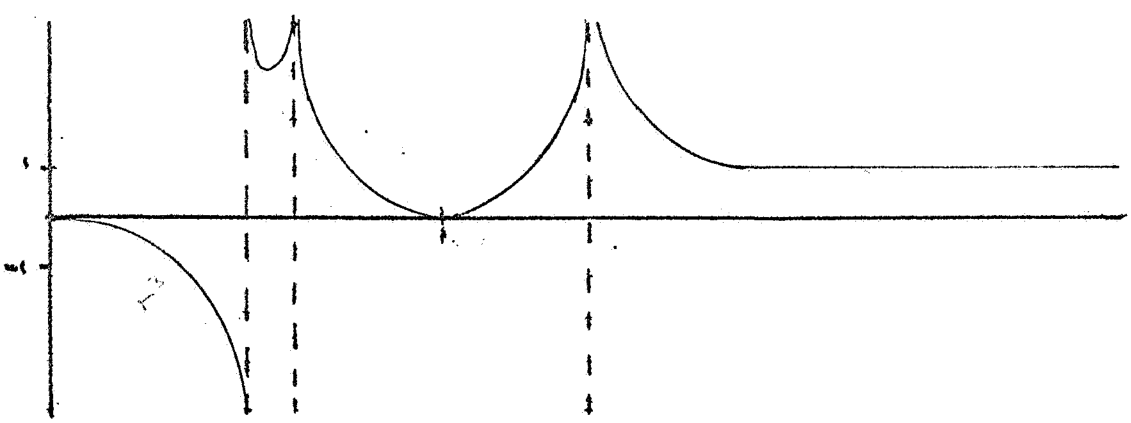
$l g_{01}$



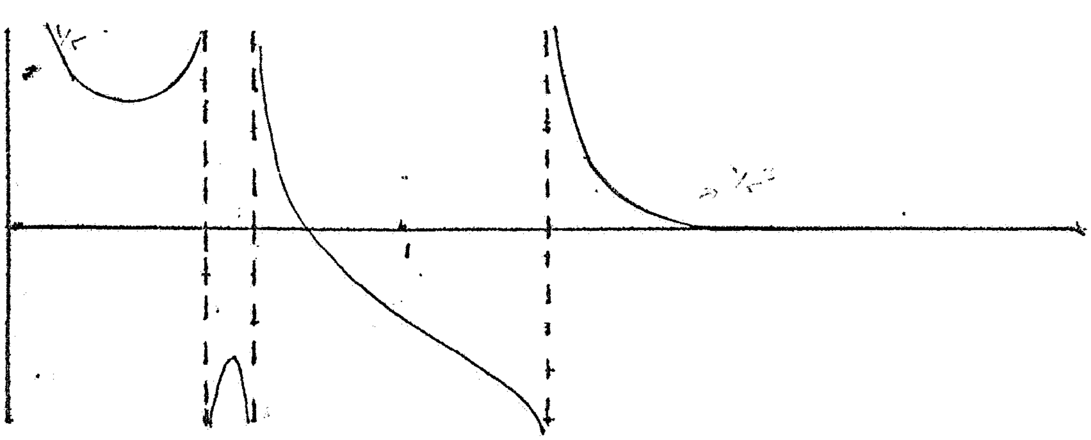
$l g_{01}^2$

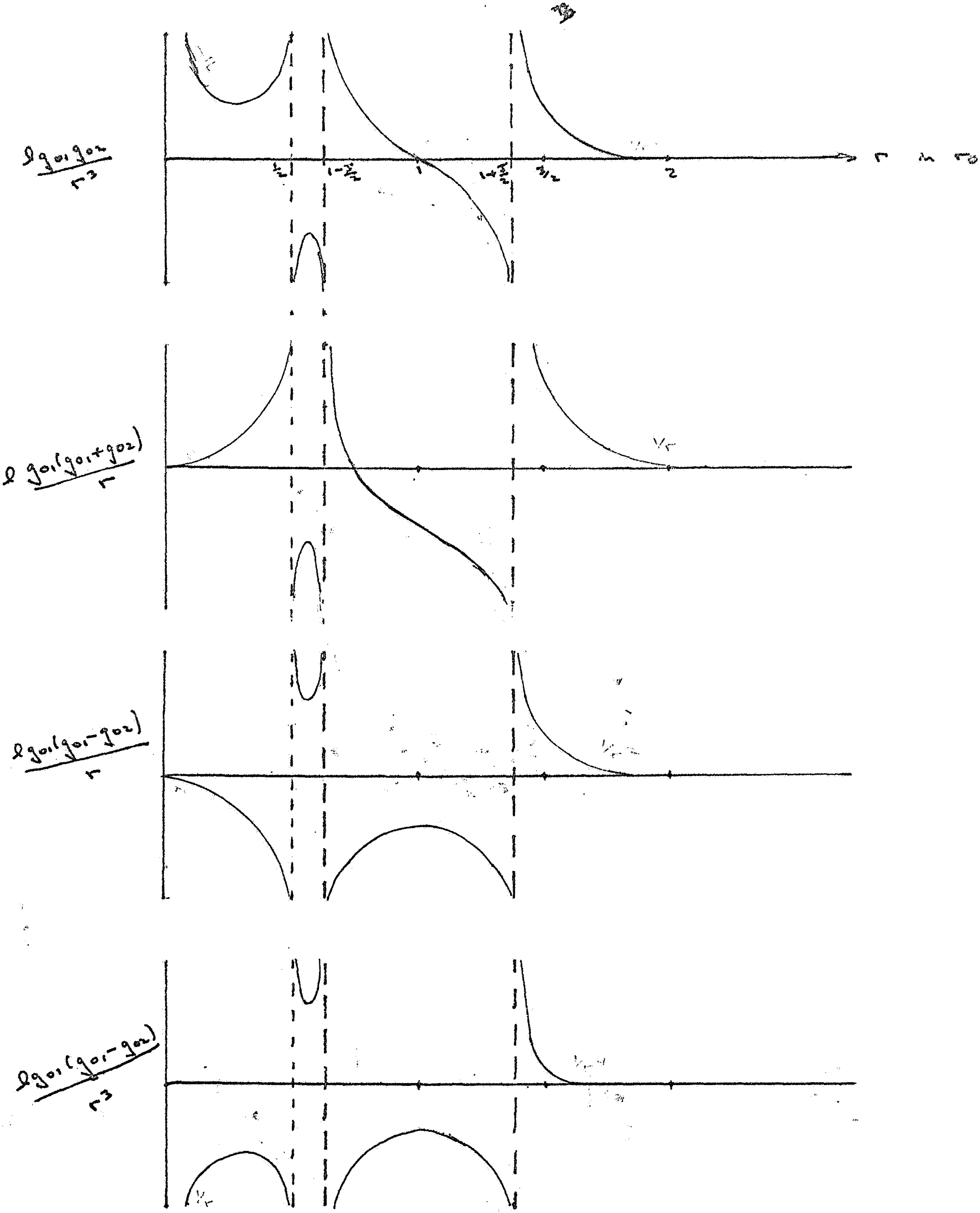


$l^2 g_{01}^2 g_{02}$



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





$\frac{l g_{01} g_{02}}{r^3}$
$\frac{1}{2}$
$1-\frac{\lambda}{2}$
1
$1+\frac{\lambda}{2}$
$3/2$
2
r in r_0
$\frac{l g_{01}(g_{01}+g_{02})}{r}$
$\frac{l g_{01}(g_{01}-g_{02})}{r}$
$\frac{l g_{01}(g_{01}-g_{02})}{r^3}$