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MULTIPOLE EXPANSION OF THE RETARDED INTERATOMIC POTENTIAL ENERGY

IV. INDUCTION ENERGY FOR DEGENERATE GROUND-STATE ATOMS

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Synopsis

The inductive contribution to the retarded interatomic potential energy of two atoms in degenerate ground states is calculated up to all multipole orders on the basis of quantum electrodynamics. The result, which is found to have nonretarded character, is written in such a way as to show the induction effects brought about in each of the atoms by the electrostatic and magnetostatic fields of the other.

1. *Introduction.* In a previous paper[1]) we derived an expression for the multipole expansion of the retarded interatomic dispersion energy of two atoms in nondegenerate ground states. It was obtained by applying perturbation theory to the interaction hamiltonian of the atoms and the radiation field. The expression was shown to contain as its short-range limit the nonretarded dispersion energy that follows from the electrostatic part of that hamiltonian alone.

If the ground state of at least one of the atoms is degenerate, the total interatomic potential energy contains apart from a dispersion contribution also an induction energy, as is well known for the electrostatic case[2]). From the derivation given in paper I it will be shown that the expression for the retarded interatomic dispersion energy found there is valid for degenerate ground-state atoms as well; in that case the result represents the retarded dispersion energy averaged over these ground states. In addition the perturbation formulae will yield then the

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complete nondispersive part of the averaged retarded interatomic potential energy, due to electrostatic as well as photon interactions. This part will be evaluated, to all multipole orders, in the present paper. The result, which turns out to have nonretarded character, will be written in a form that justifies the interpretation as an induction energy.

2. *Averaged perturbation corrections for degenerate energy levels.* According to Rayleigh–Schrödinger perturbation theory the corrections on the energy of a degenerate level, averaged over all states belonging to this level, may be expressed in forms closely analogous to those valid for nondegenerate energy levels. In fact the lowest-order averaged corrections on the unperturbed level $E_0^{(0)}$ are[3])

$$E^{(1)} = \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_0)}{\mathrm{Tr}\,P_0},$$

$$E^{(2)} = -\sum_{n(\neq 0)} \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_nH_{\mathrm{int}}P_0)}{(\mathrm{Tr}\,P_0)\,\Delta E_n^{(0)}},$$

$$E^{(3)} = \sum_{n,n'(\neq 0)} \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_nH_{\mathrm{int}}P_{n'}H_{\mathrm{int}}P_0)}{(\mathrm{Tr}\,P_0)\,\Delta E_n^{(0)}\,\Delta E_{n'}^{(0)}} - \sum_{n(\neq 0)} \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_0H_{\mathrm{int}}P_nH_{\mathrm{int}}P_0)}{(\mathrm{Tr}\,P_0)\,(\Delta E_n^{(0)})^2}, \quad (1)$$

$$E^{(4)} = -\sum_{n,n',n''(\neq 0)} \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_nH_{\mathrm{int}}P_{n'}H_{\mathrm{int}}P_{n''}H_{\mathrm{int}}P_0)}{(\mathrm{Tr}\,P_0)\,\Delta E_n^{(0)}\,\Delta E_{n'}^{(0)}\,\Delta E_{n''}^{(0)}}$$

$$+ \sum_{n,n'(\neq 0)} \frac{\mathrm{Tr}\,(H_{\mathrm{int}}P_nH_{\mathrm{int}}P_0H_{\mathrm{int}}P_{n'}H_{\mathrm{int}}P_0)}{(\mathrm{Tr}\,P_0)\,\Delta E_n^{(0)}\,(\Delta E_{n'}^{(0)})^2}$$

[*cf.* (I.7)], where traces appear of products of the perturbation hamiltonian H_{int} and the projection operators P_n on the set of unperturbed states with energy $E_n^{(0)} = E_0^{(0)} + \Delta E_n^{(0)}$. Here the terms of $E^{(4)}$ that do not contribute have been omitted for brevity; these terms have been left out in (I.7) as well.

The above formulae will be applied now to the interaction hamiltonian for two atoms, labelled a and b, and the radiation field:

$$H_{\mathrm{int}} = H_{\mathrm{es}} + H_{1a} + H_{1b} + H_{2a} + H_{2b}. \quad (2)$$

Here the electrostatic interaction H_{es} of the atoms is given by:

$$H_{\mathrm{es}} = \frac{z_az_be^2}{|\boldsymbol{R}_a - \boldsymbol{R}_b|} - \sum_j \frac{z_be^2}{|\boldsymbol{R}_a + \boldsymbol{r}_{aj} - \boldsymbol{R}_b|}$$

$$- \sum_j \frac{z_ae^2}{|\boldsymbol{R}_b + \boldsymbol{r}_{bj} - \boldsymbol{R}_a|} + \sum_{j,j'} \frac{e^2}{|\boldsymbol{R}_a + \boldsymbol{r}_{aj} - \boldsymbol{R}_b - \boldsymbol{r}_{bj'}|}, \quad (3)$$

while the one-photon interaction H_{1a} and the two-photon interaction H_{2a} for atom a read:

$$H_{1a} = \sum_j \frac{e}{mc} \boldsymbol{p}_{aj} \cdot \boldsymbol{A}(\boldsymbol{R}_a + \boldsymbol{r}_{aj}), \tag{4}$$

$$H_{2a} = \sum_j \frac{e^2}{2mc^2} \boldsymbol{A}^2(\boldsymbol{R}_a + \boldsymbol{r}_{aj}), \tag{5}$$

respectively; $\boldsymbol{A}$ is the vector potential in Coulomb gauge [see (I.4)]. In (3)–(5) $\boldsymbol{R}_a$ and $\boldsymbol{R}_b$ are the positions of the (fixed) nuclei and $\boldsymbol{r}_{aj}, \boldsymbol{p}_{aj}$ ($j = 1, \ldots, z_a$) the positions and the momenta of the z_a electrons (with charge $-e$ and mass m) of atom a.

The averaged shift to order e^4 of the ground-level energy of the system may be evaluated now on the basis of (1), with (2) inserted. In particular, the terms depending on the interatomic separation $R = |\boldsymbol{R}_b - \boldsymbol{R}_a|$ represent the interatomic potential energy averaged over the ground states of both atoms. These terms will be calculated in the following.

Due to the rotation invariance of the (unperturbed) projection operators on the set of ground states of each of the atoms several terms are found to drop out from the expressions for the energy shifts. In fact, one may prove along similar lines as in paper I [see (I.8)–(I.9)] that the following relations hold true:

$$\sum_{\alpha_0} \langle \alpha_0 | H_{es} | \alpha_0 \rangle = 0, \tag{6}$$

$$\sum_{\alpha_0} \langle \alpha_0 | H_{1a} | \alpha_0 \rangle = 0; \tag{7}$$

here α_0 labels the ground states of atom a (α will label an arbitrary state of atom a).

Employing the relations (6) and (7) we obtain for the interatomic potential energy in the first place the terms represented by the set of diagrams in fig. 1 of paper I. Evaluation of these diagrams leads to an interaction energy that may be split into two parts, one of which has the same structure as the dispersion energy for nondegenerate ground-state atoms, given in (I.57)–(I.60) as a sum over excited intermediate atomic states, the only difference being that in the present case an average over the ground states appears. Therefore this part, which is the averaged dispersion energy for degenerate ground-state atoms, need not be considered any more. In addition, the diagrams in fig. 1 of paper I give rise to terms with ground-level intermediate states, since now such intermediate states can no longer be excluded on the basis of the arguments employed in paper I.

Apart from the additional terms just mentioned, extra contributions to the inter-

atomic potential energy arise from a different origin, *viz.* the second parts of $E^{(3)}$ and $E^{(4)}$. These contributions have the form:

$$-\sum_{n(\neq 0)} \frac{\mathrm{Tr}\,(H_{es}P_0H_{1a}P_nH_{1b}P_0)}{(\mathrm{Tr}\,P_0)\,(\Delta E_n^{(0)})^2} + (a \leftrightarrow b), \tag{8}$$

$$\sum_{n,n'(\neq 0)} \frac{\mathrm{Tr}\,[H_{1a}P_nH_{1b}P_0\,(H_{1a}P_{n'}H_{1b}P_0 + H_{1b}P_{n'}H_{1a}P_0)]}{(\mathrm{Tr}\,P_0)\,\Delta E_n^{(0)}\,(\Delta E_{n'}^{(0)})^2} + (a \leftrightarrow b). \tag{9}$$

Here the symbol $(a \leftrightarrow b)$ stands for the terms obtained from the preceding ones by an interchange of the labels a and b. Furthermore, the intermediate states of the system are labelled by the index n; the latter stands for the set of indices $\{\alpha; \beta; \boldsymbol{k}_1, \lambda_1; \ldots; \boldsymbol{k}_m, \lambda_m\}$, where $\boldsymbol{k}_i, \lambda_i$ are the wave vector and polarization of the ith photon. As a consequence of the occurrence of the projection operators P_0 only ground-level intermediate states for both atoms contribute to (8) and (9).

The total (averaged) interatomic potential energy thus consists of the (averaged) dispersion energy, with excited intermediate states for both atoms, and a non-dispersive energy, with ground-level intermediate states for at least one of the atoms. The latter contribution, which drops out in the special case of non-degenerate ground-state atoms, will be evaluated in the following section. There it is shown that in fact only the terms with one atom in a ground-level intermediate state remain. This part of the interatomic potential energy may be interpreted as the interatomic induction energy.

3. *Evaluation of the induction energy.* The induction energy will be found by calculating, in a fashion closely analogous to that of paper I, the five types of contributions following from the diagrams in fig. 1 of paper I, and moreover the contributions given in (8) and (9).

The first, electrostatic diagram leads to an inductive energy of the form:

$$\begin{aligned} V_1^{\mathrm{ind}}(R) = & -\frac{1}{g_a g_b} \sum_{\alpha_0', \beta_0'} \sum_{\alpha_0, \beta(\neq \beta_0)} \frac{e^4}{\hbar c k_\beta} \\ & \times \langle \alpha_0' |\, \mathrm{e}^{-r_a \cdot \nabla_1} - 1 \,| \alpha_0 \rangle \langle \alpha_0 |\, \mathrm{e}^{-r_a \cdot \nabla_2} - 1 \,| \alpha_0' \rangle \\ & \times \langle \beta_0' |\, \mathrm{e}^{r_b \cdot \nabla_1} - 1 \,| \beta \rangle \langle \beta |\, \mathrm{e}^{r_b \cdot \nabla_2} - 1 \,| \beta_0' \rangle \, (1/R_1 R_2) + (a, \alpha \leftrightarrow b, \beta) \end{aligned} \tag{10}$$

[*cf.* (I.10)]; here g_a and g_b are the orders of degeneracy of the ground levels of the atoms a and b. (For nondegenerate ground-state atoms $|\alpha_0\rangle$ and $|\alpha_0'\rangle$ both denote the rotationally invariant ground state of atom a; then (6) may be applied so that V_1^{ind} vanishes.)

The second type of diagrams in fig. 1 of paper I gives no extra contribution in addition to the dispersive energy written in (I.12); thus we have:

$$V_2^{\mathrm{ind}} = 0. \tag{11}$$

In the nondispersive terms following from the third type of diagrams a product of matrix elements of the form:

$$\sum_{\alpha_0'} \sum_{\alpha_0} \langle \alpha_0' | \, \mathrm{e}^{-\boldsymbol{r}_a \cdot \nabla_1} - 1 \, | \alpha_0 \rangle \langle \alpha_0 | \, \{ \boldsymbol{p}_a, \mathrm{e}^{-\boldsymbol{r}_a \cdot \nabla_2} \} \, | \alpha_0' \rangle \tag{12}$$

occurs for at least one of the atoms. With the help of a reasoning similar to that used in arriving at (I.24) expression (12) may be shown to be equal to its opposite, so that no contribution to the induction energy arises. The extra energy correction (8) contains the same combination of matrix elements (12) and hence does not contribute either. As a consequence we find for the total inductive interaction energy of the third type:

$$V_3^{\mathrm{ind}}(R) = 0. \tag{13}$$

We now turn to the fourth type of diagrams in fig. 1 of paper I. Inspection of (I.32) leads to the following expression for the partial induction energy:

$$\begin{aligned} V_4^{\mathrm{ind}}(R) = {} & \frac{1}{g_a g_b} \sum_{\alpha_0', \beta_0'} \sum_{\alpha_0} \frac{e^4}{4\pi^2 m^3 c^4} \langle \alpha_0' | \, \{ \boldsymbol{p}_a, e^{-\boldsymbol{r}_a \cdot \nabla_1} \} \, | \alpha_0 \rangle \cdot (\nabla_1 \nabla_1 - \mathrm{U} \Delta_1) \\ & \cdot (\nabla_2 \nabla_2 - \mathrm{U} \Delta_2) \cdot \langle \alpha_0 | \, \{ \boldsymbol{p}_a, \mathrm{e}^{-\boldsymbol{r}_a \cdot \nabla_2} \} \, | \alpha_0' \rangle \langle \beta_0' | \, \mathrm{e}^{\boldsymbol{r}_b \cdot (\nabla_1 + \nabla_2)} \, | \beta_0' \rangle \\ & \times \int \frac{\mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{k}'}{(4\pi)^2 \, k^3 (k')^3} (\mathrm{e}^{-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_1} - 1)(\mathrm{e}^{-\mathrm{i}\boldsymbol{k}' \cdot \boldsymbol{R}_2} - 1) \frac{2}{kk'} + (a, \alpha \leftrightarrow b, \beta). \end{aligned} \tag{14}$$

By commuting $\exp(-\boldsymbol{r}_a \cdot \nabla_1)$ with the free atomic hamiltonian [see (I.47) and (I.48)] the matrix element $\langle \alpha_0 | \, \{ \nabla_1 \cdot \boldsymbol{p}_a, \exp(-\boldsymbol{r}_a \cdot \nabla_1) \} \, | \alpha_0' \rangle$ may be proved to vanish; hence only the terms with the operator $\Delta_1 \Delta_2$ in front of the integral contribute to (14); this operator yields a factor $k^2 (k')^2$ in the integrand. Performing now first the angular integrations with the help of (I.16) and then the radial integrations by employing the relation:

$$\int_0^\infty \mathrm{d}k \int_0^\infty \mathrm{d}k' \, \frac{\sin kR_1}{kR_1} \frac{\sin k'R_2}{k'R_2} = \frac{\pi^2}{4R_1 R_2}, \tag{15}$$

we get for the induction energy (14):

$$\begin{aligned} V_4^{\mathrm{ind}}(R) = {} & \frac{1}{g_a g_b} \sum_{\alpha_0', \beta_0'} \sum_{\alpha_0} \frac{e^4}{8m^3 c^4} \langle \alpha_0' | \, \{ \boldsymbol{p}_a, \mathrm{e}^{-\boldsymbol{r}_a \cdot \nabla_1} \} \, | \alpha_0 \rangle \\ & \cdot \langle \alpha_0 | \, \{ \boldsymbol{p}_a, \mathrm{e}^{-\boldsymbol{r}_a \cdot \nabla_2} \} \, | \alpha_0' \rangle \langle \beta_0' | \, \mathrm{e}^{\boldsymbol{r}_b \cdot (\nabla_1 + \nabla_2)} \, | \beta_0' \rangle \, (1/R_1 R_2) \\ & + (a, \alpha \leftrightarrow b, \beta). \end{aligned} \tag{16}$$

In the expression for the nondispersive energy originating from the fifth type of diagrams two different terms show up, with ground-level intermediate states for one and for both of the atoms, respectively:

$$
\begin{aligned}
&-\frac{1}{g_a g_b}\sum_{\alpha_0',\beta_0'}\sum_{\alpha_0,\beta(\neq\beta_0)}\frac{e^4}{16\pi^2\hbar m^4c^5}\\
&\times\langle\alpha_0'|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_1}\}|\alpha_0\rangle\langle\beta_0'|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_1}\}|\beta\rangle:(\nabla_1\nabla_1-\mathsf{U}\Delta_1)\\
&\times\langle\alpha_0|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_2}\}|\alpha_0'\rangle\langle\beta|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_2}\}|\beta_0'\rangle:(\nabla_2\nabla_2-\mathsf{U}\Delta_2)\\
&\times\int\frac{d\boldsymbol{k}\,d\boldsymbol{k}'}{(4\pi)^2k^3(k')^3}(\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_1}-1)(\mathrm{e}^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2}-1)\frac{4}{k_\beta kk'}+(a,\alpha\leftrightarrow b,\beta)\\
&-\frac{1}{g_a g_b}\sum_{\alpha_0',\beta_0'}\sum_{\alpha_0,\beta_0}\frac{e^4}{16\pi^2\hbar m^4c^5}\\
&\times\langle\alpha_0'|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_1}\}|\alpha_0\rangle\langle\beta_0'|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_1}\}|\beta_0\rangle:(\nabla_1\nabla_1-\mathsf{U}\Delta_1)\\
&\times\langle\alpha_0|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_2}\}|\alpha_0'\rangle\langle\beta_0|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_2}\}|\beta_0'\rangle:(\nabla_2\nabla_2-\mathsf{U}\Delta_2)\\
&\times\int\frac{d\boldsymbol{k}\,d\boldsymbol{k}'}{(4\pi)^2k^3(k')^3}(\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_2}-1)(\mathrm{e}^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2}-1)\frac{4}{k^2k'}
\end{aligned}
\tag{17}
$$

[see (I.37) with (I.38)–(I.41)]. The extra term (9) leads to an expression containing the same product of matrix elements as occurring here, with ground-level intermediate states for both atoms. Upon evaluating this term it is found to cancel the second part of (17), so that only the first part remains. When this part is dealt with in the same way as V_4^{ind}, we arrive at the following formula for the total induction energy of the fifth type:

$$
\begin{aligned}
V_5^{\mathrm{ind}}(R) = &-\frac{1}{g_a g_b}\sum_{\alpha_0',\beta_0'}\sum_{\alpha_0,\beta(\neq\beta_0)}\frac{e^4}{16\hbar m^4c^5k_\beta}\\
&\times\langle\alpha_0'|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_1}\}|\alpha_0\rangle\cdot\langle\beta_0'|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_1}\}|\beta\rangle\\
&\cdot\langle\alpha_0|\{\boldsymbol{p}_a,\mathrm{e}^{-r_a\cdot\nabla_2}\}|\alpha_0'\rangle\cdot\langle\beta|\{\boldsymbol{p}_b,\mathrm{e}^{r_b\cdot\nabla_2}\}|\beta_0'\rangle(1/R_1R_2)\\
&+(a,\alpha\leftrightarrow b,\beta).
\end{aligned}
\tag{18}
$$

The complete averaged induction energy for two atoms in degenerate ground states has been found now as the sum of three contributions:

$$
V^{\mathrm{ind}}(R) = V_1^{\mathrm{ind}}(R) + V_4^{\mathrm{ind}}(R) + V_5^{\mathrm{ind}}(R). \tag{19}
$$

The formulae (10), (16) and (18) for these three contributions show that the induction energy has nonretarded character: the radial dependence of the partial induction energies V_4^{ind} and V_5^{ind}, which arise from photon interactions, is determined by the function $(R_1R_2)^{-1}$, just as that of the purely electrostatic induction energy V_1^{ind}.

4. *Expansion in multipole matrix elements.* The expression for the induction energy obtained so far may be written in terms of matrix elements of electric and magnetic multipole-moment operators, defined as

$$\mu^{(n)}_{\alpha'\alpha} = -e\,\langle\alpha'|\,\frac{1}{n!}\sum_j \boldsymbol{r}_{aj}^n\,|\alpha\rangle, \tag{20}$$

$$\nu^{(n)}_{\alpha'\alpha} = -\frac{e}{2mc}\,\langle\alpha'|\,\frac{n}{(n+1)!}\sum_j \{\boldsymbol{r}_{aj}^{n-1}, \boldsymbol{r}_{aj}\wedge\boldsymbol{p}_{aj}\}\,|\alpha\rangle. \tag{21}$$

In fact the matrix elements occurring in the electrostatic energy (10) can be expanded in the following way:

$$-e\,\langle\alpha'|\,\mathrm{e}^{-\boldsymbol{r}_a\cdot\nabla_i} - 1\,|\alpha\rangle = \sum_{n=1}^{\infty}(-\nabla_i)^n \,\vdots\, \mu^{(n)}_{\alpha'\alpha}, \tag{22}$$

while the matrix elements in (16) and (18), arising from one-photon interactions, may be expressed as

$$\frac{e}{2mc}\,\langle\alpha'|\,\{\boldsymbol{p}_a, \mathrm{e}^{-\boldsymbol{r}_a\cdot\nabla_i}\}\,|\alpha\rangle = \sum_{n=1}^{\infty}(-\nabla_i)^{n-1} \,\vdots\, \{\mathrm{i}\,(k_\alpha - k_{\alpha'})\,\mu^{(n)}_{\alpha'\alpha} + \nu^{(n)}_{\alpha'\alpha}\wedge\nabla_i\}, \tag{23}$$

with $i = 1, 2$. Inserting these relations into (10), (16) and (18) we obtain:

$$\begin{aligned} V_1^{\text{ind}} = &-\frac{1}{g_a g_b}\sum_{\alpha_0',\beta_0'}\sum_{\alpha_0,\beta(\neq\beta_0)}\sum_{n_1,m_1,n_2,m_2=1}^{\infty}\frac{1}{\hbar c k_\beta} \\ &\times (-\nabla_1)^{n_1} \,\vdots\, \mu^{(n_1)}_{\alpha_0'\alpha_0}\nabla_1^{m_1} \,\vdots\, \mu^{(m_1)}_{\beta_0'\beta}(-\nabla_2)^{n_2} \,\vdots\, \mu^{(n_2)*}_{\alpha_0'\alpha_0}\nabla_2^{m_2} \,\vdots\, \mu^{(m_2)*}_{\beta_0'\beta}\,\frac{1}{R_1R_2} \\ &+ (\alpha\leftrightarrow\beta), \end{aligned} \tag{24}$$

$$\begin{aligned} V_4^{\text{ind}}(R) = &\frac{1}{g_a g_b}\sum_{\alpha_0',\beta_0'}\sum_{\alpha_0}\sum_{n_1,n_2=1}^{\infty}\frac{e^2}{2mc^2} \\ &\times \{(-\nabla_1)^{n_1-1} \,\vdots\, \nu^{(n_1)}_{\alpha_0'\alpha_0}\wedge\nabla_1\}\cdot\{(-\nabla_2)^{n_2-1} \,\vdots\, \nu^{(n_2)*}_{\alpha_0'\alpha_0}\wedge\nabla_2\} \\ &\times \langle\beta_0'|\,\mathrm{e}^{\boldsymbol{r}_b\cdot(\nabla_1+\nabla_2)}\,|\beta_0'\rangle\,(1/R_1R_2) + (a,\alpha\leftrightarrow b,\beta), \end{aligned} \tag{25}$$

$$V_5^{\mathrm{ind}}(R) = -\frac{1}{g_a g_b} \sum_{\alpha_0',\beta_0'} \sum_{\alpha_0,\beta(\neq\beta_0)} \sum_{n_1,m_1,n_2,m_2=1}^{\infty} \frac{1}{\hbar c k_\beta}$$
$$\times \{(-\nabla_1)^{n_1-1} \vdots \nu_{\alpha_0'\alpha_0}^{(n_1)} \wedge \nabla_1\} \cdot \{\nabla_1^{m_1-1} \vdots (-\mathrm{i}k_\beta \mu_{\beta_0'\beta}^{(m_1)} + \nu_{\beta_0'\beta}^{(m_1)} \wedge \nabla_1)\}$$
$$\times \{(-\nabla_2)^{n_2-1} \vdots \nu_{\alpha_0'\alpha_0}^{(n_2)*} \wedge \nabla_2\}$$
$$\cdot \{\nabla_2^{m_2-1} \vdots (\mathrm{i}k_\beta \mu_{\beta_0'\beta}^{(m_2)*} + \nu_{\beta_0'\beta}^{(m_2)*} \wedge \nabla_2\} (1/R_1R_2) + (\alpha \leftrightarrow \beta). \tag{26}$$

By making use of the sum rule [see (I.53) with (I.63)]

$$\frac{e^2}{mc^2} \nabla_1 \langle\beta_0'| \mathrm{e}^{r_b \cdot (\nabla_1 + \nabla_2)} |\beta_0'\rangle$$
$$= -\sum_{\beta(\neq\beta_0)} \sum_{m_1,m_2=1}^{\infty} \frac{2\mathrm{i}}{\hbar c} \nabla_1^{m_1} \vdots \mu_{\beta_0'\beta}^{(m_1)} \nabla_2^{m_2-1} \vdots (\mathrm{i}k_\beta \mu_{\beta_0'\beta}^{(m_2)*} + \nu_{\beta_0'\beta}^{(m_2)*} \wedge \nabla_2) \tag{27}$$

the last matrix element in V_4^{ind} may be written in terms of multipole matrix elements as well. Then the induction energy is expressed completely in terms of these matrix elements. A better insight in the result is obtained, however, by employing a different sum rule, *viz.*

$$\frac{e^2}{mc^2} \mathsf{U} \langle\beta_0'| \mathrm{e}^{r_b \cdot (\nabla_1 + \nabla_2)} |\beta_0'\rangle$$
$$= \sum_{\beta(\neq\beta_0)} \sum_{m_1,m_2=1}^{\infty} \frac{2\mathrm{i}}{\hbar c} \{(\nabla_1^{m_1-1} \vdots \nu_{\beta_0'\beta}^{(m_1)} \wedge \nabla_1) (\nabla_2^{m_2-1} \vdots \mu_{\beta_0'\beta}^{(m_2)*})$$
$$+ (\nabla_1^{m_1-1} \vdots \mu_{\beta_0'\beta}^{(m_1)*}) (\nabla_2^{m_2-1} \vdots \nu_{\beta_0'\beta}^{(m_2)} \wedge \nabla_2)$$
$$- \mathrm{i}k_\beta (\nabla_1^{m_1-1} \vdots \mu_{\beta_0'\beta}^{(m_1)}) (\nabla_2^{m_2-1} \vdots \mu_{\beta_0'\beta}^{(m_2)*})\} + \mathsf{M}_{\beta_0'\beta_0'} \tag{28}$$

[see (I.B9)] with the matrix element

$$\mathsf{M}_{\beta_0'\beta_0'} = \frac{e^2}{mc^2} \langle\beta_0'| \sum_{m_1,m_2=1}^{\infty} \frac{m_1 m_2}{(m_1+1)!\,(m_2+1)!} (r_b \cdot \nabla_1)^{m_1-1} (r_b \cdot \nabla_2)^{m_2-1}$$
$$\times (r_b r_b \nabla_1 \cdot \nabla_2 - r_b \nabla_1 r_b \cdot \nabla_2 - \nabla_2 r_b r_b \cdot \nabla_1 + \mathsf{U} r_b \cdot \nabla_1 r_b \cdot \nabla_2) |\beta_0'\rangle \tag{29}$$

[see (I.B6)]. If (28) is inserted into (25) an expression results of which several terms occur in (26) with the opposite sign. As a consequence the following formula

is found for the sum of the partial induction energies (24)–(26):

$$
\begin{aligned}
V^{\mathrm{ind}}(R) = & -\frac{1}{g_a g_b} \sum_{\alpha_0', \beta_0'} \sum_{\alpha_0, \beta (\neq \beta_0)} \sum_{n_1, m_1, n_2, m_2 = 1}^{\infty} \frac{1}{\hbar c k_\beta} \\
& \times \{(-\nabla_1)^{n_1} \vdots \mu^{(n_1)}_{\alpha_0' \alpha_0} \nabla_1^{m_1} \vdots \mu^{(m_1)}_{\beta_0' \beta} (-\nabla_2)^{n_2} \vdots \mu^{(n_2)*}_{\alpha_0' \alpha_0} \nabla_2^{m_2} \vdots \mu^{(m_2)*}_{\beta_0' \beta} \\
& + (-\nabla_1)^{n_1} \vdots \nu^{(n_1)}_{\alpha_0' \alpha_0} \nabla_1^{m_1} \vdots \nu^{(m_1)}_{\beta_0' \beta} (-\nabla_2)^{n_2} \vdots \nu^{(n_2)*}_{\alpha_0' \alpha_0} \nabla_2^{m_2} \vdots \nu^{(m_2)*}_{\beta_0' \beta}\} \, (1/R_1 R_2) \\
& + \frac{1}{2 g_a g_b} \sum_{\alpha_0', \beta_0'} \sum_{\alpha_0} \sum_{n_1, n_2 = 1}^{\infty} \{(-\nabla_1)^{n_1 - 1} \vdots \nu^{(n_1)}_{\alpha_0' \alpha_0} \wedge \nabla_1\} \\
& \cdot \mathsf{M}_{\beta_0' \beta_0'} \cdot \{(-\nabla_2)^{n_2 - 1} \vdots \nu^{(n_2)*}_{\alpha_0' \alpha_0} \wedge \nabla_2\} \, (1/R_1 R_2) + (\alpha \leftrightarrow \beta). \qquad (30)
\end{aligned}
$$

This expression may be interpreted in terms of a hamiltonian similar to that derived recently by Atkins and Woolley[4,5]). These authors found, as an extension of a result obtained earlier by Power and Zienau[6]), that from the hamiltonian for neutral atoms in a radiation field the vector potential may be eleminated in favour of the transverse electric and magnetic fields by employing a canonical transformation (see also appendix B of paper I). Likewise, the hamiltonian for a single neutral atom b in static external electromagnetic fields $\boldsymbol{E} = -\nabla\varphi$, $\boldsymbol{B} = \nabla \wedge \boldsymbol{A}$ may be brought into the form:

$$
\begin{aligned}
\hat{H} = & \sum_j \frac{\boldsymbol{p}_{bj}^2}{2m} + \sum_{j \neq j'} \frac{e^2}{|\boldsymbol{r}_{bj} - \boldsymbol{r}_{bj'}|} - \sum_{m=1}^{\infty} \nabla_b^{m-1} \vdots \mu_b^{(m)} \cdot \boldsymbol{E}(\boldsymbol{R}_b) \\
& - \sum_{m=1}^{\infty} \nabla_b^{m-1} \vdots \nu_b^{(m)} \cdot \boldsymbol{B}(\boldsymbol{R}_b) + \sum_j \frac{e^2}{2mc^2} \\
& \times \left\{ \sum_{m=1}^{\infty} \frac{m}{(m+1)!} (\boldsymbol{r}_{bj} \cdot \nabla_b)^{m-1} \boldsymbol{r}_{bj} \wedge \boldsymbol{B}(\boldsymbol{R}_b) \right\}^2 . \qquad (31)
\end{aligned}
$$

If the static fields are generated by a neutral atom a, with multipoles $\mu_a^{(n)}$, $\nu_a^{(n)}$, we may insert into (31):

$$
\boldsymbol{E}(\boldsymbol{R}_b) = -\nabla_b \sum_{n=1}^{\infty} \nabla_a^n \vdots \mu_a^{(n)} \frac{1}{|\boldsymbol{R}_a - \boldsymbol{R}_b|}, \qquad (32)
$$

$$
\boldsymbol{B}(\boldsymbol{R}_b) = \nabla_b \wedge \sum_{n=1}^{\infty} (\nabla_a^{n-1} \vdots \nu_a^{(n)} \wedge \nabla_a) \frac{1}{|\boldsymbol{R}_a - \boldsymbol{R}_b|}. \qquad (33)
$$

The expression (31), with (32) and (33), reveals the mechanism that leads to the potential-energy contribution (30): each atom induces, through its static electric and magnetic fields, multipole moments in the other. Since only static fields come into play, the ensuing induction energy shows no retardation effects.

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