

## FERMIONIUM IN AN EXTERNAL POTENTIAL\*

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*(Received March 30, 1994)*

The set of 16 first-order relativistic equations derived from the two-body Dirac equation is discussed for a system of two spin-1/2 particles moving in an external potential. Scalar and vector wave-function components are used in place of double-bispinor components. In general, the case of different masses is considered. In the case of equal masses, this set is explicitly reduced to four second-order equations involving "large-large" components, if terms quartic in momenta are neglected.

PACS numbers: 11.10. Qr

Consider a system of two spin-1/2 particles moving in an external potential,  $V^{\text{ex}}(\vec{r}_1, \vec{r}_2)$ , and use to describe such a system the two-body Dirac equation (called also the Breit equation [1]):

$$(E - V - \vec{\alpha}_1 \cdot \vec{p}_1 - \beta_1 m_1 - \vec{\alpha}_2 \cdot \vec{p}_2 - \beta_2 m_2) \psi(\vec{r}_1, \vec{r}_2) = 0, \quad (1)$$

where  $V(\vec{r}_1, \vec{r}_2) = V^{\text{in}}(\vec{r}_1 - \vec{r}_2) + V^{\text{ex}}(\vec{r}_1, \vec{r}_2)$  is a total potential. Here,  $\vec{\alpha}_i = \gamma_i^5 \vec{\sigma}_i$  and  $\beta_i = \gamma_i^0$  ( $i = 1, 2$ ) are the usual Dirac matrices of two particles. In particular, the system may be a fermionium *i.e.*, a fermion-antifermion pair (*e.g.* the positronium), affected by an external force (*e.g.* the Coulomb force from a heavy ion).

In order to split Eq. (1) into a set of equations for 16 spinorial (double-bispinor) wave-function components it is convenient to apply the representation

$$\psi = \begin{pmatrix} \psi_{(\beta_1 \beta_2)}^{(\gamma_1^5 \gamma_2^5)} \end{pmatrix}, \text{ where } (\beta_1 \beta_2) = \pm 1 \text{ and } (\gamma_1^5 \gamma_2^5) = \pm 1$$

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\* Work supported in part by the Polish KBN-Grant 2-P302-143-06.

are eigenvalues of (commuting) direct products of the corresponding Dirac matrices. Such a representation is connected with the double Dirac representation  $\psi = (\psi_{\beta_1\beta_2})$ , where  $\beta_1 = \pm 1$  and  $\beta_2 = \pm 1$ , through the relations

$$\psi_{\pm}^{\pm} = \frac{1}{\sqrt{2}} (\psi_{++} \pm \psi_{--}), \quad \psi_{\pm}^{\mp} = \frac{1}{\sqrt{2}} (\psi_{+-} \pm \psi_{-+}). \quad (2)$$

Then, Eq. (1) takes the form

$$\begin{aligned} (E - V)\psi_{\pm}^{\pm} - (m_1 + m_2)\psi_{\pm}^{\mp} &= \pm (\vec{\sigma}_1^P \cdot \vec{p}_1 \pm \vec{\sigma}_2^P \cdot \vec{p}_2) \psi_{\pm}^{\pm}, \\ (E - V)\psi_{\pm}^{\pm} - (m_1 - m_2)\psi_{\pm}^{\mp} &= \pm (\vec{\sigma}_1^P \cdot \vec{p}_1 \pm \vec{\sigma}_2^P \cdot \vec{p}_2) \psi_{\pm}^{\pm}, \end{aligned} \quad (3)$$

where,  $\vec{\sigma}_i = \text{diag}(\vec{\sigma}_i^P, \vec{\sigma}_i^P)$  with  $\vec{\sigma}_i^P$  ( $i = 1, 2$ ) denoting the Pauli matrices of two particles.

Making use of the spin projection operators  $P_s$  onto states with the total spin  $s = 0, 1$ ,

$$P_0 = \frac{1}{2} (1 - \vec{\sigma}_1^P \cdot \vec{\sigma}_2^P), \quad P_1 = \frac{1}{4} (3 + \vec{\sigma}_1^P \cdot \vec{\sigma}_2^P), \quad (4)$$

one may calculate the respective wave-function components  $\psi_{\pm s}^{\pm} = P_s \psi_{\pm}^{\pm}$ , and then introduce the corresponding spatial scalars  $\phi_{\pm}^{\pm}$  and vectors  $\vec{\phi}_{\pm}^{\pm}$  through the connections:

$$\delta_{a_1 a_2} \phi_{\pm}^{\pm} = (\psi_{\pm 0}^{\pm})_{a_1 a_2}, \quad \delta_{a_1 a_2} \vec{\phi}_{\pm}^{\pm} = \frac{1}{2} (\vec{\sigma}_{a_1 b_1}^P \delta_{a_2 b_2} - \delta_{a_1 b_1} \vec{\sigma}_{a_2 b_2}^P) (\psi_{\pm 1}^{\pm})_{b_1 b_2} \quad (5)$$

( $a_i = 1, 2$ ,  $b_i = 1, 2$ ). In terms of these 16 scalar and vector wave-function components, the set of equations for  $\psi_{\pm s}^{\pm}$  ( $s = 0, 1$ ) (as following from Eqs. (3)) can be rewritten in the form:

$$\begin{aligned} (E - V)\phi_{\pm}^{\pm} - (m_1 + m_2)\phi_{\pm}^{\mp} &= \pm (\vec{p}_1 \mp \vec{p}_2) \cdot \vec{\phi}_{\pm}^{\pm}, \\ (E - V)\phi_{\pm}^{\pm} - (m_1 - m_2)\phi_{\pm}^{\mp} &= \pm (\vec{p}_1 \mp \vec{p}_2) \cdot \vec{\phi}_{\pm}^{\pm}, \\ (E - V)\vec{\phi}_{\pm}^{\pm} - (m_1 + m_2)\vec{\phi}_{\pm}^{\mp} &= \pm (\vec{p}_1 \mp \vec{p}_2) \phi_{\pm}^{\pm} \pm i (\vec{p}_1 \pm \vec{p}_2) \times \vec{\phi}_{\pm}^{\pm}, \\ (E - V)\vec{\phi}_{\pm}^{\pm} - (m_1 - m_2)\vec{\phi}_{\pm}^{\mp} &= \pm (\vec{p}_1 \mp \vec{p}_2) \phi_{\pm}^{\pm} \pm i (\vec{p}_1 \pm \vec{p}_2) \times \vec{\phi}_{\pm}^{\pm}. \end{aligned} \quad (6)$$

Here, the wave-function components depend on  $\vec{r}_1$  and  $\vec{r}_2$ , while  $\vec{p}_1 = -i\partial/\partial\vec{r}_1$  and  $\vec{p}_2 = -i\partial/\partial\vec{r}_2$ . In the above derivation, the identities

$$\begin{aligned} P_0(\vec{\sigma}_1^P + \vec{\sigma}_2^P) &= 0, & P_0(\vec{\sigma}_1^P - \vec{\sigma}_2^P) &= (\vec{\sigma}_1^P - \vec{\sigma}_2^P)P_1, \\ P_1(\vec{\sigma}_1^P + \vec{\sigma}_2^P) &= (\vec{\sigma}_1^P + \vec{\sigma}_2^P)P_1, & P_1(\vec{\sigma}_1^P - \vec{\sigma}_2^P) &= (\vec{\sigma}_1^P - \vec{\sigma}_2^P)P_0, \end{aligned} \quad (7)$$

were used. The second of these four identities shows in which way the second connection (5) is true.

In the particular case when external forces are absent,  $V^{\text{ex}}(\vec{r}_1, \vec{r}_2) = 0$ , the set of 16 equations (6) takes in the centre-of-mass frame (there  $\vec{P} = \vec{p}_1 + \vec{p}_2$  assumes its eigenvalue 0) the previously discussed form [2]:

$$\begin{aligned} (E^{\text{in}} - V^{\text{in}})\phi_{\pm}^{\pm \text{in}} - (m_1 + m_2)\phi_{\pm}^{\mp \text{in}} &= \begin{cases} 2\vec{p} \cdot \vec{\phi}_{-}^{+ \text{in}} \\ 0 \end{cases}, \\ (E^{\text{in}} - V^{\text{in}})\phi_{\pm}^{\pm \text{in}} - (m_1 - m_2)\phi_{\pm}^{\mp \text{in}} &= \begin{cases} 2\vec{p} \cdot \vec{\phi}_{+}^{+ \text{in}} \\ 0 \end{cases}, \\ (E^{\text{in}} - V^{\text{in}})\vec{\phi}_{\pm}^{\pm \text{in}} - (m_1 + m_2)\vec{\phi}_{\pm}^{\mp \text{in}} &= \begin{cases} 2\vec{p}\phi_{-}^{+ \text{in}} \\ -2i\vec{p} \times \vec{\phi}_{-}^{- \text{in}} \end{cases}, \\ (E^{\text{in}} - V^{\text{in}})\vec{\phi}_{\pm}^{\pm \text{in}} - (m_1 - m_2)\vec{\phi}_{\pm}^{\mp \text{in}} &= \begin{cases} 2\vec{p}\phi_{+}^{+ \text{in}} \\ -2i\vec{p} \times \vec{\phi}_{+}^{- \text{in}} \end{cases}, \end{aligned} \quad (8)$$

where  $V(\vec{r}_1, \vec{r}_2) = V^{\text{in}}(\vec{r})$  with  $\vec{r} = \vec{r}_1 - \vec{r}_2$  (and  $\vec{p} = \vec{p}_1 = -\vec{p}_2$ , if acting on the wave function). Here, the wave-function components depend only on  $\vec{r}$ , while  $\vec{p} = -i\partial/\partial\vec{r}$ . The Reader may consult Ref. [3] for the radial equations following from Eqs. (8) when internal forces are central,  $V^{\text{in}}(\vec{r}) = V^{\text{in}}(r)$  with  $r = |\vec{r}|$  (there, the case  $m_1 = m_2$  was considered).

In the case of equal masses,  $m_1 = m_2 (= m)$ , the centre-of-mass and relative canonical variables are

$$\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2), \quad \vec{P} = \vec{p}_1 + \vec{p}_2 \quad (9)$$

and

$$\vec{r} = \vec{r}_1 - \vec{r}_2, \quad \vec{p} = \frac{1}{2}(\vec{p}_1 - \vec{p}_2), \quad (10)$$

respectively. Then, in general, the set of 16 equations (6) assumes the form

$$\begin{aligned} (E - V)\phi_{\pm}^{\pm} - 2m\phi_{\pm}^{\mp} &= \begin{cases} 2\vec{p} \cdot \vec{\phi}_{-}^{+} \\ -\vec{P} \cdot \vec{\phi}_{-}^{-} \end{cases}, \\ (E - V)\phi_{\pm}^{\pm} &= \begin{cases} 2\vec{p} \cdot \vec{\phi}_{+}^{+} \\ -\vec{P} \cdot \vec{\phi}_{+}^{-} \end{cases}, \\ (E - V)\vec{\phi}_{\pm}^{\pm} - 2m\vec{\phi}_{\pm}^{\mp} &= \begin{cases} 2\vec{p}\phi_{-}^{+} + i\vec{P} \times \vec{\phi}_{-}^{+} \\ -\vec{P}\phi_{-}^{-} - 2i\vec{p} \times \vec{\phi}_{-}^{-} \end{cases}, \\ (E - V)\vec{\phi}_{\pm}^{\pm} &= \begin{cases} 2\vec{p}\phi_{+}^{+} + i\vec{P} \times \vec{\phi}_{+}^{+} \\ -\vec{P}\phi_{+}^{-} - 2i\vec{p} \times \vec{\phi}_{+}^{-} \end{cases}, \end{aligned} \quad (11)$$

where  $V(\vec{R}, \vec{r}) = V^{\text{in}}(\vec{r}) + V^{\text{ex}}(\vec{R}, \vec{r})$ . Here, the wave-function components depend on  $\vec{R}$  and  $\vec{r}$ , while  $\vec{P} = -i\partial/\partial\vec{R}$  and  $\vec{p} = -i\partial/\partial\vec{r}$ .

Due to Eqs. (2) and (5) the wave-function components  $\phi_{\pm}^{\pm}$  and  $\bar{\phi}_{\pm}^{\pm}$  are "large-large"  $\pm$  "small-small" while  $\phi_{\pm}^{\pm}$  and  $\bar{\phi}_{\pm}^{\pm}$  are "large-small"  $\pm$  "small-large". Eliminating from Eqs. (11) the components  $\phi_{\pm}^{\pm}$  and  $\bar{\phi}_{\pm}^{\pm}$ , one can obtain the following involved set of eight second-order equations for  $\phi_{\pm}^{\pm}$  and  $\bar{\phi}_{\pm}^{\pm}$ :

$$\begin{aligned}
 & \left[ (E - V)^2 - 4m^2 - 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \cdot \vec{p} \right] \phi_{+}^{+} - \frac{2m}{E - V} \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \cdot \vec{P} \phi_{+}^{-} \\
 &= 2i \left[ \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times \vec{P} \right] \cdot \bar{\phi}_{+}^{+} + 2i \frac{2m}{E - V} \left[ \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times \vec{p} \right] \cdot \bar{\phi}_{+}^{-}, \\
 & \left[ (E - V)^2 - 4m^2 - \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \cdot \vec{P} \right] \phi_{+}^{-} - 4 \frac{2m}{E - V} \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \cdot \vec{p} \phi_{+}^{+} \\
 &= 2i \left[ \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times \vec{p} \right] \cdot \bar{\phi}_{+}^{-} + 2i \frac{2m}{E - V} \left[ \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times \vec{P} \right] \cdot \bar{\phi}_{+}^{+}, \\
 & \left[ (E - V)^2 - 4m^2 \right] \bar{\phi}_{+}^{+} - 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) (\vec{p} \cdot \bar{\phi}_{+}^{+}) + \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times (\vec{P} \times \bar{\phi}_{+}^{+}) \\
 &- \frac{2m}{E - V} \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) (\vec{P} \cdot \bar{\phi}_{+}^{-}) + 4 \frac{2m}{E - V} \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times (\vec{p} \times \bar{\phi}_{+}^{-}) \\
 &= 2i \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times \vec{p} \phi_{+}^{+} + 2i \frac{2m}{E - V} \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times \vec{P} \phi_{+}^{-}, \\
 & \left[ (E - V)^2 - 4m^2 \right] \bar{\phi}_{+}^{-} - \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) (\vec{P} \cdot \bar{\phi}_{+}^{-}) + 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times (\vec{p} \times \bar{\phi}_{+}^{-}) \\
 &- 4 \frac{2m}{E - V} \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) (\vec{p} \cdot \bar{\phi}_{+}^{+}) + \frac{2m}{E - V} \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times (\vec{P} \times \bar{\phi}_{+}^{+}) \\
 &= 2i \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \times \vec{P} \phi_{+}^{-} + 2i \frac{2m}{E - V} \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times \vec{p} \phi_{+}^{+}. \tag{12}
 \end{aligned}$$

Further, eliminating from Eqs. (12) the components  $\phi_+^-$  and  $\tilde{\phi}_+^-$  by means of Eqs. (11), we can get the following set of four second-order equations for  $\phi_+^+$  and  $\tilde{\phi}_+^+$  if we neglect terms of the order of  $Pp^3$ ,  $P^2p^2$  and  $P^3p$ :

$$\begin{aligned}
 & \left[ (E - V)^2 - 4m^2 - 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \cdot \vec{p} - \vec{P} \cdot \left( \vec{P} - \frac{[\vec{P}, V]}{E - V} \right) \right] \phi_+^+ \\
 &= 2i \left( \frac{[\vec{p}, V]}{E - V} \times \vec{P} - \vec{P} \times \frac{[\vec{p}, V]}{E - V} \right) \cdot \tilde{\phi}_+^+ + O(P^2p^2) + O(P^3p), \\
 & [(E - V)^2 - 4m^2] \tilde{\phi}_+^+ - 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) (\vec{p} \cdot \tilde{\phi}_+^+) + \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \times (\vec{P} \times \tilde{\phi}_+^+) \\
 & - \vec{P} \left[ \left( \vec{P} - \frac{[\vec{P}, V]}{E - V} \right) \cdot \tilde{\phi}_+^+ \right] + 4\vec{p} \times \left[ \left( \vec{p} - \frac{[\vec{p}, V]}{E - V} \right) \times \tilde{\phi}_+^+ \right] \\
 &= 2i \left( \frac{[\vec{P}, V]}{E - V} \times \vec{p} - \vec{p} \times \frac{[\vec{P}, V]}{E - V} \right) \phi_+^+ + O(Pp^3) + O(P^2p^2) + O(P^3p), \quad (13)
 \end{aligned}$$

where the second equation can be rewritten also as

$$\begin{aligned}
 & \left[ (E - V)^2 - 4m^2 - 4\vec{p} \cdot \left( \vec{p} - \frac{[\vec{p}, V]}{E - V} \right) - \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \cdot \vec{P} \right] \tilde{\phi}_+^+ \\
 & - \left( 4 \frac{[\vec{p}, V]}{E - V} p_l + 4p_l \frac{[\vec{p}, V]}{E - V} - \vec{P} \frac{[P_l, V]}{E - V} - \frac{[P_l, V]}{E - V} \vec{P} \right) \phi_{+l}^+ \\
 &= 2i \left( \frac{[\vec{P}, V]}{E - V} \times \vec{p} - \vec{p} \times \frac{[\vec{P}, V]}{E - V} \right) \phi_+^+ + O(Pp^3) + O(P^2p^2) + O(P^3p) \quad (14)
 \end{aligned}$$

with  $\tilde{\phi}_+^+ = (\phi_{+l}^+)_l$ . Here, the omitted term of the order of  $Pp^3$  on the rhs. of the second equation (13) or Eq. (14) is

$$-8i \left[ \vec{p}, \frac{1}{(E - V)^2} \left( \vec{p} + \frac{[\vec{p}, V]}{E - V} \right) \cdot \left( \vec{P} + \frac{[\vec{P}, V]}{E - V} \right) \right] \times \vec{p} \phi_+^+.$$

We assumed that the contribution from this term can be neglected in comparison with the contribution from the term

$$2i \left( \frac{[\vec{P}, V]}{E - V} \times \vec{p} - \vec{p} \times \frac{[\vec{P}, V]}{E - V} \right) \phi_+^+$$

which is of the order of  $Pp$ . Note that the coupling between two equations (13) is caused by the acceleration of the system's centre of mass under the influence of external forces.

In the particular case of no external forces,  $V^{\text{ex}}(\vec{R}, \vec{r}) = 0$ , one can use the centre-of-mass frame (where  $\vec{P}$  assumes its eigenvalue 0), and then the set of equations (13) (with the use of Eq. (14)) splits into two independent equations: the scalar equation

$$\left[ (E^{\text{in}} - V^{\text{in}})^2 - 4m^2 - 4 \left( \vec{p} + \frac{[\vec{p}, V^{\text{in}}]}{E^{\text{in}} - V^{\text{in}}} \right) \cdot \vec{p} \right] \phi_+^{\text{+in}} = 0 \quad (15)$$

and the vector equation

$$\begin{aligned} & \left[ (E^{\text{in}} - V^{\text{in}})^2 - 4m^2 - 4\vec{p} \cdot \left( \vec{p} - \frac{[\vec{p}, V^{\text{in}}]}{E^{\text{in}} - V^{\text{in}}} \right) \right] \vec{\phi}_+^{\text{+in}} \\ & - 4 \left( \frac{[\vec{p}, V^{\text{in}}]}{E^{\text{in}} - V^{\text{in}}} p_l + p_l \frac{[\vec{p}, V^{\text{in}}]}{E^{\text{in}} - V^{\text{in}}} \right) \phi_{+l}^{\text{+in}} = 0. \end{aligned} \quad (16)$$

Notice that these equations follow in a simpler way as an exact consequence of the nonapproximate equations (8) (with  $m_1 = m_2 (= m)$ ), where the centre-of-mass frame is also used.

When the nonrelativistic approximation is applicable both to the external and internal motion, we may put

$$(E - V)^2 \simeq 4m^2 + 4m(E - 2m - V), \quad (17)$$

where  $(E - 2m - V)^2$  is neglected. Then, in the denominators in Eqs. (12)–(14) we may write  $E - V \simeq 2m$  (if not under differentiation).

In this way, Eq. (16), for instance, takes approximately the form

$$(E^{\text{in}} - 2m) \phi_{+k}^{\text{+in}} = G_{kl} \phi_{+l}^{\text{+in}}, \quad (18)$$

where

$$\begin{aligned} G_{kl} = & \left[ \frac{1}{m} \vec{p} \cdot \left( \vec{p} - \frac{[\vec{p}, V^{\text{in}}]}{2m} \right) - \frac{1}{m} \left( \frac{[\vec{p}, V^{\text{in}}]}{2m} \right)^2 + V^{\text{in}} \right] \delta_{kl} \\ & + \frac{1}{m} \left( \frac{[p_k, V^{\text{in}}]}{2m} p_l + p_l \frac{[p_k, V^{\text{in}}]}{2m} + \frac{[p_k, V^{\text{in}}][p_l, V^{\text{in}}]}{4m^2} \right). \end{aligned} \quad (19)$$

Here, the reduced mass is  $\mu = m/2$ . We can see that for the wave-function component  $\vec{\phi}_+^{\text{+in}} = (\phi_{+l}^{\text{+in}})$  the nonrelativistic sector-energy operator  $H = (H_{kl})$  is given by the Hermitian part of  $G = (G_{kl})$ :

$$H_{kl} = \frac{1}{2} (G_{kl} + G_{lk}^\dagger), \quad (20)$$

while the respective energy-width operator  $\Gamma = (\Gamma_{kl})$  for transitions into all other wave-function components  $\phi_+^{\pm\text{in}}, \phi_-^{\pm\text{in}}, \vec{\phi}_+^{\pm\text{in}}$  and  $\vec{\phi}_-^{\pm\text{in}}$  is defined by the anti-Hermitian part of  $G = (G_{kl})$ :

$$-i\Gamma_{kl} = \frac{1}{2} (G_{kl} - G_{lk}^\dagger). \quad (21)$$

Thus, in consequence of the above approximate linearization of Eq. (16) with respect to the energy eigenvalue  $E^{\text{in}} - 2m$ , this eigenvalue gets an imaginary part (of course, in the initial equation (1) as well as in the equivalent set of equations (6)  $E$  is real, so such is also  $E^{\text{in}}$  in Eqs. (8)). If  $\Gamma$  is small, the real part of  $E^{\text{in}}$  appears in the approximate eigenvalue equation

$$(\text{Re } E^{\text{in}} - 2m) \phi_{+k}^{+\text{in}} = H_{kl} \phi_{+l}^{+\text{in}} \quad (22)$$

involving the Hermitian sector-energy operator  $H$ , whilst the imaginary part of  $E^{\text{in}}$  is given perturbatively as

$$\text{Im } E^{\text{in}} = - \int d^3\vec{r} \phi_{+k}^{+\text{in}*} \Gamma_{kl} \phi_{+l}^{+\text{in}} \quad (23)$$

in the case of state  $\vec{\phi}_+^{+\text{in}} = (\phi_{+l}^{+\text{in}})$  normalized to 1.

When the nonrelativistic approximation is applicable to the external motion (though the internal motion still may be relativistic), then writing  $E - V = E^{\text{in}} - V^{\text{in}} + E - E^{\text{in}} - V^{\text{ex}}$  we may put

$$(E - V)^2 \simeq (E^{\text{in}} - V^{\text{in}})^2 + 2(E^{\text{in}} - V^{\text{in}})(E - E^{\text{in}} - V^{\text{ex}}), \quad (24)$$

where  $(E - E^{\text{in}} - V^{\text{ex}})^2$  is neglected. Hence, in the denominators in Eqs. (12)–(14) we may insert  $E - V \simeq E^{\text{in}} - V^{\text{in}}$  (if not under differentiation).

In such a case, Eqs. (13) (with the use of Eq. (14)) take approximately the form

$$\begin{aligned} & \left\{ E - E^{\text{in}} - V^{\text{ex}} - \frac{1}{2(E^{\text{in}} - V^{\text{in}})} \left[ - (E^{\text{in}} - V^{\text{in}})^2 + 4m^2 + 4 \left( \vec{p} + \frac{[\vec{p}, V]}{E^{\text{in}} - V^{\text{in}}} \right) \cdot \vec{p} \right. \right. \\ & \left. \left. + \left( \vec{p} - \frac{[\vec{p}, V^{\text{ex}}]}{E^{\text{in}} - V^{\text{in}}} \right) \cdot \vec{p} - \frac{[p_l, [p_l, V^{\text{ex}}]]}{E^{\text{in}} - V^{\text{in}}} - \left( \frac{[\vec{p}, V^{\text{ex}}]}{E^{\text{in}} - V^{\text{in}}} \right)^2 \right] \right\} \phi_+^+ \\ & = \frac{i}{(E^{\text{in}} - V^{\text{in}})^2} \left[ [\vec{p}, V] \times \vec{p} - \left( \vec{p} + \frac{[\vec{p}, V]}{E^{\text{in}} - V^{\text{in}}} \right) \times [\vec{p}, V] \right] \cdot \vec{\phi}_+^+, \\ & \left\{ E - E^{\text{in}} - V^{\text{ex}} - \frac{1}{2(E^{\text{in}} - V^{\text{in}})} \left[ - (E^{\text{in}} - V^{\text{in}})^2 + 4m^2 + 4 \left( \vec{p} - \frac{[\vec{p}, V]}{E^{\text{in}} - V^{\text{in}}} \right) \cdot \vec{p} \right. \right. \end{aligned}$$

$$\begin{aligned}
& -4 \frac{[p_l, [p_l, V]]}{E^{\text{in}} - V^{\text{in}}} - 4 \left( \frac{[\vec{p}, V]}{E^{\text{in}} - V^{\text{in}}} \right)^2 + \left( \vec{p} + \frac{[\vec{p}, V^{\text{ex}}]}{E^{\text{in}} - V^{\text{in}}} \right) \cdot \vec{p} \Big\} \phi_+^+ - \frac{1}{2(E^{\text{in}} - V^{\text{in}})^2} \\
& \times \left[ 4 [\vec{p}, V] p_l + 4 \left( p_l + \frac{[p_l, V]}{E^{\text{in}} - V^{\text{in}}} \right) [\vec{p}, V] - [p_l, V^{\text{ex}}] \vec{p} - \left( \vec{p} + \frac{[\vec{p}, V^{\text{ex}}]}{E^{\text{in}} - V^{\text{in}}} \right) [p_l, V^{\text{ex}}] \right] \phi_{+l}^+ \\
& = \frac{i}{(E^{\text{in}} - V^{\text{in}})^2} \left[ [\vec{p}, V^{\text{ex}}] \times \vec{p} - \left( \vec{p} + \frac{[\vec{p}, V]}{E^{\text{in}} - V^{\text{in}}} \right) \times [\vec{p}, V^{\text{ex}}] \right] \phi_+^+. \quad (25)
\end{aligned}$$

Here,  $V(\vec{R}, \vec{r}) = V^{\text{in}}(\vec{r}) + V^{\text{ex}}(\vec{R}, \vec{r})$  all the time. In this way, the approximate linearization of Eqs. (13) with respect to the external energy eigenvalue  $E - E^{\text{in}}$  is carried out (while the internal energy eigenvalue  $E^{\text{in}}$  is given as in Eqs. (15) and (16)).

Consider now an effective approximation, where the factorized ansatz

$$\phi_+^+(\vec{R}, \vec{r}) \simeq \chi_0(\vec{R}) \phi_+^{\text{in}}(\vec{r}), \quad \vec{\phi}_+^+(\vec{R}, \vec{r}) \simeq \chi_1(\vec{R}) \vec{\phi}_+^{\text{in}}(\vec{r}) \quad (26)$$

is enforced (with  $\phi_+^{\text{in}}$  and  $\vec{\phi}_+^{\text{in}}$  satisfying Eqs. (15) and (16)), and where  $V^{\text{ex}}(\vec{R}, \vec{r}) \simeq \bar{V}_0^{\text{ex}}(\vec{R})$  or  $\bar{V}_1^{\text{ex}}(\vec{R})$  is assumed when commuted with momenta. Then, after projecting onto the states  $\phi_+^{\text{in}}$  and  $\vec{\phi}_+^{\text{in}}$ , Eqs. (25) tell us that

$$\begin{aligned}
& \left[ E - E^{\text{in}} - \bar{V}_0^{\text{ex}} - \frac{1}{2M_0} \vec{p} \cdot \left( \vec{p} - \frac{\xi_0}{M_0} [\vec{p}, \bar{V}_0^{\text{ex}}] \right) + \frac{\eta_0}{2M_0^3} [\vec{p}, \bar{V}_0^{\text{ex}}]^2 \right] \chi_0(\vec{R}) \\
& = \varepsilon_{klm} \left( 2e_{km} p_l + \frac{f_{km}}{\sqrt{M_0 M_1}} [p_l, \bar{V}_1^{\text{ex}}] \right) \chi_1(\vec{R}), \\
& \left[ E - E^{\text{in}} - \bar{V}_1^{\text{ex}} - \frac{1}{2M_1} \left( \vec{p} + \frac{\xi_1}{M_1} [\vec{p}, \bar{V}_1^{\text{ex}}] \right) \cdot \vec{p} \right. \\
& \quad \left. + \frac{\xi_{kl}}{2M_1^2} (p_k [p_l, \bar{V}_1^{\text{ex}}] + [p_l, \bar{V}_1^{\text{ex}}] p_k) + \frac{\eta_{kl}}{2M_1^3} [p_k, \bar{V}_1^{\text{ex}}] [p_l, \bar{V}_1^{\text{ex}}] \right] \chi_1(\vec{R}) \\
& = \varepsilon_{klm} \frac{g_{km}}{\sqrt{M_0 M_1}} [p_l, \bar{V}_1^{\text{ex}}] \chi_0(\vec{R}), \quad (27)
\end{aligned}$$

where we put  $\bar{V}_0^{\text{ex}}(\vec{R}) = \langle V^{\text{ex}} \rangle_{00}$  and  $\bar{V}_1^{\text{ex}}(\vec{R}) = \langle V^{\text{ex}} \rangle_{kk}$ , and define the constants

$$\begin{aligned}
\frac{1}{M_0} &= \left\langle \frac{1}{E^{\text{in}} - V^{\text{in}}} \right\rangle_{00} > 0, \quad \frac{\xi_0}{M_0^2} = \left\langle \frac{1}{(E^{\text{in}} - V^{\text{in}})^2} \right\rangle_{00} > 0, \quad \frac{\eta_0}{M_0^3} = \left\langle \frac{1}{(E^{\text{in}} - V^{\text{in}})^3} \right\rangle_{00} > 0, \\
\frac{1}{M_1} &= \left\langle \frac{1}{E^{\text{in}} - V^{\text{in}}} \right\rangle_{kk} > 0, \quad \frac{\xi_1}{M_1^2} = \left\langle \frac{1}{(E^{\text{in}} - V^{\text{in}})^2} \right\rangle_{kk} > 0, \\
\frac{\xi_{kl}}{M_1^2} &= \left\langle \frac{1}{(E^{\text{in}} - V^{\text{in}})^2} \right\rangle_{kl}, \quad \frac{\eta_{kl}}{M_1^3} = \left\langle \frac{1}{(E^{\text{in}} - V^{\text{in}})^3} \right\rangle_{kl}, \\
-ie_{km} &= \left\langle \frac{[p_k, V^{\text{in}}]}{(E^{\text{in}} - V^{\text{in}})^2} \right\rangle_{0m}, \quad \frac{-if_{km}}{\sqrt{M_0 M_1}} = \left\langle \frac{[p_k, V^{\text{in}}]}{(E^{\text{in}} - V^{\text{in}})^3} \right\rangle_{0m}, \\
\frac{-ig_{km}}{\sqrt{M_0 M_1}} &= \left\langle \frac{2}{(E^{\text{in}} - V^{\text{in}})^2} p_m + \frac{[p_m, V^{\text{in}}]}{(E^{\text{in}} - V^{\text{in}})^3} \right\rangle_{k0}. \quad (28)
\end{aligned}$$

Here,  $-i [\vec{P}, \bar{V}_{0,1}^{\text{ex}}] = -\partial \bar{V}_{0,1}^{\text{ex}} / \partial \vec{R}$  and  $-i [\vec{p}, V^{\text{in}}] = -\partial V^{\text{in}} / \partial \vec{r}$  give external and internal forces, whereas

$$\langle F \rangle_{\mu\nu} = \int d^3\vec{r} \phi_{+\mu}^{+\text{in}*} F(\vec{R}, \vec{r}, \vec{p}) \phi_{+\nu}^{+\text{in}} \quad (29)$$

is the internal matrix element with the states  $\phi_{+0}^{+\text{in}} \equiv \phi_+^{+\text{in}}$  and  $(\phi_{+l}^{+\text{in}}) \equiv \bar{\phi}_+^{+\text{in}}$  normalized to 1 (the case of internal bound states).

The system of two coupled effective Schrödinger equations (27) allows to estimate the external-motion factors  $\chi_0$  and  $\chi_1$  of the wave-function components  $\phi_+^+$  and  $\bar{\phi}_+^+$  in the case of external nonrelativistic approximation (although the internal motion may be relativistic).

When the nonrelativistic approximation is applicable also to the internal motion, we may write

$$E - E^{\text{in}} - V^{\text{ex}} \simeq E - 2m - V. \quad (30)$$

Then,  $E^{\text{in}} - V^{\text{in}} \simeq 2m$  everywhere in Eqs. (25) and, therefore, also within the constants (28) in Eqs. (27). In this case  $M_0 \simeq 2m \simeq M_1$ ,  $\xi_0 \simeq 1 \simeq \xi_1$ ,  $\eta_0 \simeq 1$ ,  $\xi_{kl} \simeq \frac{1}{3} \delta_{kl} \simeq \eta_{kl}$  and

$$\begin{aligned} -ie_{kn} &\simeq \frac{1}{4m^2} \langle [p_k, V^{\text{in}}] \rangle_{0n} \simeq -if_{kn}, \\ -ig_{kn} &\simeq \frac{1}{2m} \langle 2p_n + \frac{1}{2m} [p_n, V^{\text{in}}] \rangle_{k0}. \end{aligned} \quad (31)$$

Here, the reduced mass is  $\mu = m/2$ , so  $\vec{v} = 2\vec{p}/m = \vec{v}_1 - \vec{v}_2$  gives the relative velocity of two particles.

Thus, in this fully nonrelativistic approximation, Eqs. (27) take the form

$$\begin{aligned} &\left[ E - E^{\text{in}} - \bar{V}_0^{\text{ex}} + \frac{1}{4m} \Delta_R - \frac{1}{8m^2} (\text{grad}_R \bar{V}_0^{\text{ex}}) \cdot \text{grad}_R, \right. \\ &\quad \left. - \frac{1}{8m^2} \Delta_R \bar{V}_0^{\text{ex}} - \frac{1}{16m^3} (\text{grad}_R \bar{V}_0^{\text{ex}})^2 \right] \chi_0(\vec{R}) \\ &= -ie_{kln} f_{kn} \left( 2 \frac{\partial}{\partial X_l} + \frac{1}{2m} \frac{\partial \bar{V}_1^{\text{ex}}}{\partial X_l} \right) \chi_1(\vec{R}), \\ &\left[ E - E^{\text{in}} - \bar{V}_1^{\text{ex}} + \frac{1}{4m} \Delta_R + \frac{1}{24m^2} (\text{grad}_R \bar{V}_1^{\text{ex}}) \cdot \text{grad}_R \right. \\ &\quad \left. - \frac{1}{24m^2} \Delta_R \bar{V}_1^{\text{ex}} - \frac{1}{48m^3} (\text{grad}_R \bar{V}_1^{\text{ex}})^2 \right] \chi_1(\vec{R}) \\ &= -ie_{kln} \frac{g_{kn}}{2m} \frac{\partial \bar{V}_0^{\text{ex}}}{\partial X_l} \chi_0(\vec{R}), \end{aligned} \quad (32)$$

where  $\text{grad}_R = \partial/\partial \vec{R}$ ,  $\Delta_R = (\partial/\partial \vec{R})^2$  and  $\vec{R} = (X_l)$ . Since the potentials  $\bar{V}_{0,1}^{\text{ex}}$  and  $V^{\text{in}}$  must be comparatively weak in the case of fully relativistic approximation, four terms of the order of  $\bar{V}_{0,1}^{\text{ex}2}$  and  $\bar{V}_{0,1}^{\text{ex}} V^{\text{in}}$  in Eqs. (32) can be consistently neglected (here,  $V^{\text{in}}$  is involved in  $f_{kn}$  and  $g_{kn}$  through Eqs. (31)).

Eventually, when the nonrelativistic approximation is applicable to the internal motion (though the external motion may be relativistic), then writing  $E - V = E^{\text{ex}} - V^{\text{ex}} + E - E^{\text{ex}} - V^{\text{in}}$  we may approximate

$$(E - V)^2 \simeq (E^{\text{ex}} - V^{\text{ex}})^2 + 2(E^{\text{ex}} - V^{\text{ex}})(E - E^{\text{ex}} - V^{\text{in}}), \quad (33)$$

where  $(E - E^{\text{ex}} - V^{\text{in}})^2$  is neglected. In this case, in the denominators in Eqs. (12)–(14) we may substitute  $E - V \simeq E^{\text{ex}} - V^{\text{ex}}$  (if not under differentiation).

I am indebted to Sławomir Wycech for interesting discussions on the problem of positronium in external Coulomb fields of heavy ions.

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