A Orthonormality and Expectation Values

The orthonormality relations (1.197) for two solutions ψ_i and ψ_j of the KG equation are

$$\int r^2 dr R_j R_i (E_j/2 + E_i/2 - V) = mc^2 \delta_{ij}. \tag{A.1}$$

The resulting normalization for $i = j,\ R_i = R_j = R$ is

$$\int r^2 dr R^2 (1 - V/E) = mc^2/E. \tag{A.2}$$

In the following we set $V = -Ze^2/r = -\alpha_Z \hbar c/r$, and $l_\alpha = [(l+\frac{1}{2})^2 - \alpha_Z^2]^{\frac{1}{2}} - \frac{1}{2}$:

$$R = N_{\rm KG} e^{-z/2} z^{l_\alpha} F, \quad z = 2\kappa r, \quad F = F(-n_r, b, z), \quad b = 2l_\alpha + 2. \tag{A.3}$$

The value of $N_{\rm KG}$ follows from insertion into (A.3):

$$N_{\rm KG}^2 (2\kappa)^{-3} \int_0^\infty dz e^{-z} z^b (1 + 2\alpha_Z \hbar c \kappa / zE) F^2 = mc^2/E. \tag{A.4}$$

This and similar integrals for $\langle r^{-s} \rangle$ follow from the formula

$$J_s = \int dz e^{-z} z^{b-s} F^2(-n_r, b, z) = n_r! \Gamma^{-1}(b + n_r) \Gamma(b) \Gamma(b + 1 - s)[1 + X], \tag{A.5}$$

$$X = n_r \frac{(s-2)(s-1)}{b} \left[1 + (n_r - 1) \frac{(s-3)s}{2^2(b+1)} \left(1 + (n_r - 2) \frac{(s-4)(s+1)}{3^2(b+2)} \right) \right], \tag{A.6}$$

where X is complete for $-3 < s < 6$. Using $\Gamma(b+1) = b\Gamma(b)$ and $b/2 + n_r = l_\alpha + 1 + n_r = n_\beta$, both J_0 and J_1 contain the following combination of gamma functions:

$$\Pi_\Gamma = \Gamma^2(b)/\Gamma(b + n_r). \tag{A.7}$$

The nonrelativistic limit of Π_Γ is

$$\Pi_{\Gamma,nr} = [(2l+1)!]^2/(l+n)!. \tag{A.8}$$

The first three values of J_s are

$$J_0 = n_r! 2 n_\beta \Pi_\Gamma, \quad J_1 = n_r! \Pi_\Gamma, \quad J_2 = n_r! \Pi_\Gamma/(b-1). \tag{A.9}$$

Insertion of J_0 and J_1 into (A.4) gives

$$N_{\mathrm{KG}}^{-2} mc^2/E = (2\kappa)^{-3} n_r!2(n_\beta + \alpha_Z \hbar c\kappa/E)\Pi_\Gamma. \tag{A.10}$$

The general definition of κ is $\hbar\kappa = (m^2c^2 - E^2/c^2)^{1/2}$. For bound states, $\hbar\kappa$ is quantized according to (1.129),

$$\hbar c\kappa = \alpha_Z E/n_\beta, \tag{A.11}$$

such that the second term in the bracket is α_Z^2/n_β. By means of (1.129), $1 + \alpha_Z^2/n_\beta^2 = m^2c^4/E^2$, N_{KG}^2 gets simplified:

$$N_{\mathrm{KG}}^2 = 4\kappa^3 [n_r! n_\beta \Gamma^2(b)]^{-1} \Gamma(b + n_r) E/mc^2. \tag{A.12}$$

The nonrelativistic limit has

$$N_{\mathrm{KG}}^2 \approx N^2 = 4\kappa^3 (n + l)!/[(2l + 1)!^2 n n_r!]. \tag{A.13}$$

The following expectation values are defined as in (1.206), $\langle r^{-s}\rangle \equiv \int \psi^* r^{-s} \psi d^3r$. For $s = 1, 2, 3, 4$, and with $l_\alpha(l_\alpha + 1) = L_\alpha^2$, they are

$$\langle r^{-1}\rangle = \kappa^2 a_B = \kappa^2/\alpha_Z m, \tag{A.14}$$

$$\langle r^{-2}\rangle = \kappa^3 a_B/(l_\alpha + \tfrac{1}{2}) = \kappa^3/\alpha_Z m(l_\alpha + \tfrac{1}{2}), \tag{A.15}$$

$$\langle r^{-3}\rangle = n_\beta \kappa^4 a_B/(l_\alpha + \tfrac{1}{2}) L_\alpha^2 = \alpha_Z E \langle r^{-2}\rangle / L_\alpha^2, \tag{A.16}$$

$$\langle r^{-4}\rangle = \kappa^5 a_B [3n_\beta^2 - L_\alpha^2 - 1]/L_\alpha^2 (l_\alpha^2 - 1/4)(l_\alpha + 3/2). \tag{A.17}$$

The last expression in each line sets $\hbar = c = 1$. The nonrelativistic approximations of $\langle r^{-s}\rangle$ are given in Sect. 2.8. $\langle r^{-3}\rangle_{l=0}$ and $\langle r^{-4}\rangle_{l=0}$ are only to be used in connection with an additional factor l_α. Note however that the first-order energy shift E^1 is not necessarily $\langle r^{-s}\rangle$: The KG perturbation theory is a special case of the Kramers perturbation theory of Sect. 2.9, where E^1 is given by (2.292). If the Coulomb potential is modified by a small V_{per}, then the $c^2\pi^{02}$ of (2.287) is generalized to

$$c^2\pi^{02} = (E^0 - V + E^1 - V_{\mathrm{per}})^2 \approx (E^0 - V)^2 + 2(E^1 - V_{\mathrm{per}})(E^0 - V). \tag{A.18}$$

In this case, the K_{per} of (2.288) is $V_{\mathrm{per}}(E^0 - V)$, and (2.292) becomes

$$E^1 = \langle V_{\mathrm{per}}(1 - V/E^0)\rangle = \int R^2 r^2 dr V_{\mathrm{per}}(E^0 - V)/mc^2. \tag{A.19}$$

For $V = -\alpha_Z/r$, this integral diverges for $V_{\mathrm{per}} \approx r^{-2}$. Physically relevant modifications of the point Coulomb potential have the Yukawa form, see Appendix C.

The Dirac-Coulomb equation has two types of solutions which are equivalent only for $j = n - \frac{1}{2}$. According to the orthogonality relations (2.207), the normalization constants $N_\pm$ of the solutions (2.145) equal the Klein-Gordon constant N_{KG}, taken at the appropriate value of b in Π_Γ (A.7):

$$N_\pm = N_{\mathrm{KG}}(b_\pm), \quad b_\pm = 2l_{\alpha\pm} + 2, \quad b_+ = 2\gamma + 2,\ b_- = 2\gamma. \tag{A.20}$$

The radial wave function components (g, f) of the parity eigenstates are normalized according to (2.196), $\int (g^2 + f^2) r^2 dr = 1$. A normalization constant N_γ has been defined in (2.195). However, it is customary to remove the square roots $x_\pm$ such that $F_- = F(1 - n_r, b_D, z)$ occurs with a factor $-n_r$ $(n_r = 0, 1, 2 \ldots)$ in the square bracket:

$$(g, f) = N_D (1 \pm E/m)^{1/2} e^{-z/2} z^{\gamma - 1} [\pm (m_\beta - \kappa_D) F(-n_r, b_D, z) - n_r F_-]. \tag{A.21}$$

The resulting N_D^2 is, with $m_\beta = \alpha_Z m/\kappa$ according to (2.184), and $b_D = 2\gamma + 1$,

$$N_D^2 = 4\kappa^3 [n_r! \Pi_\Gamma(b_D, n_r)[(m_\beta - \kappa_D)^2 + n_r(2\gamma + n_r)]]^{-1}. \tag{A.22}$$

Rewriting n_r as $n_\beta - \gamma$, one finds $n_r(2\gamma + n_r) = n_\beta^2 - \gamma^2 = m_\beta^2 - \kappa_D^2$, using $n_\beta^2 = m_\beta^2 - \alpha_Z^2$ according to (2.184). This allows one to simplify N_D^2 as follows:

$$\begin{gathered} N_D^2 = 2\kappa^3 [n_r! \Pi_\Gamma(b_D, n_r) m_\beta (m_\beta - \kappa_D)]^{-1}, \\ \kappa \approx \kappa_n [1 + \tfrac{1}{2}\alpha_Z^2 / n (1/(j + \tfrac{1}{2}) - 1/n)]. \end{gathered} \tag{A.23}$$

The approximate value of κ comes from (2.164). Insertion of the definition (2.184), $m_\beta = \alpha_Z m/\kappa$, gives

$$N_D^2 = 2\kappa^4 [\alpha_Z m n_r! \Gamma^2(b_D)(m_\beta - \kappa_D)]^{-1} \Gamma(b_D + n_r). \tag{A.24}$$

For $l = 0$, approximate expressions both for N_D^2 and N_{KG}^2 will be given in Appendix C. The Dirac expectation values of r^{-s} are, with $\kappa_D = (l - j)(2j + 1)$ and $\gamma = \sqrt{\kappa_D^2 - \alpha_Z^2}$,

$$\langle r^{-1} \rangle_D = \kappa^3 (\kappa_D^2 + n_r \gamma) / \gamma \alpha_Z^2 m^2 = (1 + \alpha_Z^2 / \gamma n_\beta) \langle r^{-1} \rangle, \tag{A.25}$$

$$\langle r^{-2} \rangle_D = 2\kappa^3 \kappa_D (2\kappa_D E/m - 1)[\gamma(4\gamma^2 - 1)\alpha_Z m]^{-1} E/m, \tag{A.26}$$

$$\langle r^{-3} \rangle_D = \frac{2\kappa^3}{\gamma(4\gamma^2 - 1)} \left[3\kappa_D E \frac{\kappa_D E/m - 1}{m(\gamma^2 - 1)} - 1 \right]. \tag{A.27}$$

The first-order energy shift caused by a perturbative potential $V^1 \approx r^{-s}$ is proportional to $\langle r^{-s} \rangle_D$. The corresponding energy shift in the KG equation is proportional to $\langle r^{-s}(1 + \alpha_Z / Er) \rangle$, according to (A.19). For $s = 1$, one finds from (A.14) and (A.15), $\delta E(s = 1) = \langle r^{-1} \rangle [1 + \alpha_Z^2 / n_\beta (l_\alpha + \frac{1}{2})]$, which is in fact close to the Dirac expression (A.25).

Nondiagonal matrix elements are given by Shabaev (1991), and by Martinez-y-Romero et al. (2001).

The expectation values of other operators follow from the "virial theorem" and its generalizations (Friar and Negele 1976, Goldman and Drake (1982), Shabaev, Martinez-y-Romero). Some relations are trivial, for example

$$\langle H\rangle = E, \quad H = V + \boldsymbol{p\alpha} + m\beta. \tag{A.28}$$

Others follow from an operator $\hat{O}$ as

$$\langle [H, \hat{O}]\rangle = \langle E\hat{O} - \hat{O}E\rangle = 0. \tag{A.29}$$

In particular, with $\hat{O} = \boldsymbol{rp}$ and $\hat{\boldsymbol{r}}\boldsymbol{p} = p_r$, one obtains

$$\langle \boldsymbol{p\alpha}\rangle = \langle rV'\rangle, \quad V' \equiv [\partial_r, V], \tag{A.30}$$

$$\langle r^{-1}(\boldsymbol{\alpha p} - \alpha_r p_r)\rangle = \langle V'\rangle, \tag{A.31}$$

The point Coulomb potential $V_C = -\alpha_Z/r$ has $rV_C' = -V_C$,

$$\langle \boldsymbol{p\alpha}\rangle = -\langle V_C\rangle. \tag{A.32}$$

This is the virial theorem. Insertion into (A.28) cancels V_C,

$$\langle \beta\rangle = E/m: \quad \int (g^2 - f^2) = E/m. \tag{A.33}$$

Taking for $\hat{O}$ any local function $f(r)$, one finds

$$\langle [\boldsymbol{\alpha\nabla}, f(r)]\rangle = 0. \tag{A.34}$$

Expectation values involving $\boldsymbol{p}^2$ follow most easily from the Kramers equation (2.135), as the expectation value of the anti-Hermitian operator $[\boldsymbol{\sigma p}, V]$ vanishes:

$$\langle \boldsymbol{p}^2\rangle = E^2 - m^2 - 2E\langle V\rangle + \langle V^2\rangle. \tag{A.35}$$

This applies again for any shape of V. Its nonrelativistic limit is obtained by setting $E \to E/c = mc + E_N/c$ and neglecting both E_N^2/c^2 and $\langle V^2\rangle$, $\langle \boldsymbol{p}^2/2m\rangle = E_N - \langle V\rangle$. It is identical with the expectation value of the nonrelativistic Schrödinger operator (1.49) and has nothing to do with the nonrelativistic virial theorem $\langle \boldsymbol{p}^2/2m\rangle \approx -\langle V_C/2\rangle$, which uses the Schrödinger expectation value of $\hat{O} = \boldsymbol{rp}$.

For $V = -\alpha_Z/r$, the orthogonality relations (A.1) are simplified by the transformation (1.143) of the distance variable, $\boldsymbol{r}_\epsilon = E\alpha_Z \boldsymbol{r}$.

$$\boldsymbol{r}_\epsilon = E\alpha_Z \boldsymbol{r}, \quad \int_0^\infty r_\epsilon^2 dr_\epsilon R_j(r_\epsilon/E_j) R_i(r_\epsilon/E_i) = \delta_{ij}. \tag{A.36}$$

The Dirac wave functions are normalized according to (2.203), $\int \psi_j^\dagger \psi_i = \delta_{ij}$, which is already as simple as possible. Introduction of $\boldsymbol{r}_\epsilon$ leaves $\beta m/E$ as the only energy-dependent operator. The resulting orthogonality relations are

$$\int d^3 r_\epsilon \psi_j^\dagger(\boldsymbol{r}_\epsilon/E_j)\beta\psi_i(\boldsymbol{r}_\epsilon/E_i) = 0 \quad \text{for } j \neq i. \tag{A.37}$$

The orthogonality relations of the solutions of the n_e-electron Dirac-Coulomb equation are in the standard Dirac form

$$\int d^3r_1 d^3r_2 \ldots \psi_j^\dagger(\boldsymbol{r}_1, \boldsymbol{r}_2 \ldots)\psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2 \ldots) = \delta_{ij}. \tag{A.38}$$

The form analogous to (A.37) contains the total electronic energies E_j and E_i and has β replaced by $\Sigma\beta_e$. The method can be extended to the solutions of the Dirac-Breit equation, but the Breit operator of Sect. 3.4 can only be used as a first-order perturbation, of course.

The Kramers orthogonality relations have already been presented in (2.207). They have the same form as the KG orthogonality relations, except that $\psi_j^\dagger$ must be specified as the lefthanded $\psi_{l,j}^\dagger$ if ψ_i is taken as a righthanded Kramers spinor $\psi_{r,i}$:

$$\int \psi_{l,j}^\dagger (E_i + E_j - 2V)\psi_{r,i} = 2E\delta_{ij}. \tag{A.39}$$

The $\psi_l^\dagger$ is necessary because the Kramers operator K_r^0 is not Hermitian.

As long as hyperfine operators are treated perturbatively, the most convenient form of binary equations uses the variable $\boldsymbol{\rho} = \mu\boldsymbol{r}$, because the orthogonality relations (4.211)

$$\int \rho^2 d\rho R_j(\rho)R_i(\rho)(\epsilon_i/\mu_i + \epsilon_j/\mu_j - 2V_\rho) = 2\delta_{ij}\epsilon_i/\mu_i. \tag{A.40}$$

of the Todorov equation and (4.277) $\int d^3\rho \psi_j^\dagger \psi_i = \delta_{ij}$ of the leptonium equation are then form-identical with those of the single-particle equation, all differences being concentrated in the physical meaning of the single parameter μ. Equations (A.11, A.14, A.15) and (A.16) are generalized as follows:

$$\kappa = \alpha_Z\epsilon/\mu, \quad \langle\rho^{-1}\rangle = \kappa^2/\alpha_Z\mu^2 = \alpha_Z(\epsilon/n_\beta\mu)^2, \tag{A.41}$$

$$\langle\rho^{-2}\rangle = \kappa^3/\alpha_Z\mu^3(l_\alpha + 1/2) = \alpha_Z^2(\epsilon/n_\beta\mu)^3/(l_\alpha + 1/2), \tag{A.42}$$

$$\langle\rho^{-3}\rangle = \alpha_Z(\epsilon/\mu)\langle\rho^{-2}\rangle/L_\alpha^2. \tag{A.43}$$

In the Dirac case, (A.25) and (A.26) read

$$\langle\rho^{-1}\rangle_D = (\kappa/\mu)^3(\kappa_D^2 + n_r\gamma)/\gamma\alpha_Z^2, \tag{A.44}$$

$$\langle\rho^{-2}\rangle_D = 2(\kappa/\mu)^3\kappa_D[2\kappa_D(1 + \alpha_Z^2/n_\beta^2)^{-1/2} - 1]/\gamma(4\gamma^2 - 1), \tag{A.45}$$

with $\kappa/\mu = \alpha_Z(n_\beta^2 + \alpha_Z^2)^{-1/2}$ independent of μ.

The full leptonium equation (4.275) contains E^2, E^0 and E^{-2}. The E^{-2} in the hyperfine operator makes $\boldsymbol{\rho} = \mu\boldsymbol{r}$ inappropriate for orthogonality relations. Dividing the equation by E^2 and introducing $\boldsymbol{r}_\epsilon$ as a new independent variable, one obtains

$$[\tfrac{1}{2}(1 - m_+^2/E^2) + \alpha_Z^2/r_\epsilon - \alpha_Z\gamma^5\boldsymbol{p}_\epsilon\boldsymbol{\sigma}_1 + i(\alpha_Z^2/r_\epsilon)\gamma^5\boldsymbol{\sigma}_{12}^\times\alpha_Z\boldsymbol{p}_\epsilon]\psi_1 = 0. \tag{A.46}$$

The resulting orthogonality relations are

$$\int d^3 r_\epsilon \chi_j^\dagger(\boldsymbol{r}_\epsilon/E_j) m_+^2 \psi_i(\boldsymbol{r}_\epsilon/E_i) = 0 \quad \text{for } j \neq i. \tag{A.47}$$

χ are the eight components defined in (3.173); as in the Kramers equation, they appear because one of the operators (in this case the hyperfine operator) is not Hermitian. The $m_+^2 = m_1^2 + m_2^2 + 2m_1 m_2 \beta$ is the generalization of the β of the Dirac equation.

Without hyperfine interaction, the Kramers form of the leptonium equation has the following standard form in the variable $\boldsymbol{r}_\epsilon$:

$$K = 2/r_\epsilon + \alpha_Z^2/r_\epsilon^2 + [\boldsymbol{\sigma}_1 \boldsymbol{p}_\epsilon, \alpha_Z/r_\epsilon] - \boldsymbol{p}_\epsilon^2, \quad K\psi_r = n_\beta^{-2}\psi_r. \tag{A.48}$$

One of the early arguments against the KG equation was that the integrand of its normalization integral (A.1) can be negative at small r, whereas that of the Dirac equation is always positive, which is necessary for a probability interpretation. It is amusing to see that the opposite is true for the corresponding integrals (A.36) and (A.37).

B Coulomb Greens Functions

In nonrelativistic quantum mechanics, the higher-order effects of a perturbation H' (2.208)

$$(H + H_{\rm per})\psi = (E^0 + E^1 + E^{(2)} \ldots)\psi \tag{B.1}$$

may be calculated by means of a Greens function G which is defined by the following inhomogenenous differential equation

$$(E - H(\boldsymbol{r}, \boldsymbol{p}))G(\boldsymbol{r}, \boldsymbol{r}', E) = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{B.2}$$

In atomic theory, $H = -\nabla^2/2m - \alpha_Z/r$ leads to the Coulomb Greens function. Its radial component is normally sufficient:

$$(E - H_l)G_l(\boldsymbol{r}, \boldsymbol{r}', E) = \delta(r - r'), \quad \nabla_l^2 = \partial_r^2 + (2/r)\partial_r - l(l+1)/r^2. \tag{B.3}$$

The use of these equations rests on the completeness (1.250) of the solutions ψ_n of the unperturbed equation $H\psi_n = E_n\psi_n$ (the upper index ^{0} is now suppressed)

$$\delta(\boldsymbol{r} - \boldsymbol{r}') = \Sigma_k \psi_k(\boldsymbol{r})\psi_k^*(\boldsymbol{r}'). \tag{B.4}$$

Using this expression in (B.2), one can for example calculate $E^{(2)}$ (2.223). Remember that the Coulomb spectrum includes a continuum of unbound electrons, which adds an $\int d^3k$ to the $\sum_k$ in (B.4). For G, on the other hand, one can construct forms in which the whole expression is reduced to a sum. The first such form was found by Schwinger, see the review by Maquet (1977). We shall consider the form of Hostler (1970),

$$G_l(\boldsymbol{r}, \boldsymbol{r}', E) = \Sigma_{n=l+1}^{\infty} R_{nlE}(r)R_{nlE}(r')(1 - \kappa_E/\kappa_n)^{-1}, \tag{B.5}$$

with $\kappa_n = \alpha_Z m/n$ and $\kappa_E = (-2mE)^{-1/2}$. R_{nlE} is the nonrelativistic limit of (A.3), but with κ_n replaced by κ_E:

$$R_{nlE}(r) = N(E)e^{-\kappa_E r}(2\kappa_E r)^l F(l + 1 - n,\ 2l + 2,\ 2\kappa_E r). \tag{B.6}$$

F is a polynomial of degree n_r.

The Dirac-Coulomb Greens function has also the nonrelativistic form, see (2.213) with $H_0 = H_C$ and (2.223). Its completeness relation has $\psi_k^*(\boldsymbol{r}')$ replaced by $\psi_k^\dagger(\boldsymbol{r}')$ to account for spin:

$$S(\boldsymbol{r}, \boldsymbol{r}', E) = \Sigma_k \psi_k(\boldsymbol{r}')\psi_k^\dagger(\boldsymbol{r}')(E - E_k)^{-1}. \tag{B.7}$$

However, the price of this formal simplicity is a 4×4 matrix. It seems easier to work with a 2×2 matrix G in spin space (Zon et al. 1972, Sapirstein and Yennie, in the book edited by Kinoshita (1990)). Instead of (B.1), one then has an implicit eigenvalue equation, $(K + K_{\rm per})\psi = 0$, where K is the KG or Kramers operator, and $K_{\rm per}$ is a perturbation. The Kramers operator is

$$K = E^2 - m^2 + 2E\alpha_Z/r + \nabla^2 + (\alpha_Z^2 + i\alpha_Z\sigma_r)/r^2, \tag{B.8}$$

and the relativistic Coulomb Greens function G is defined by

$$KG(\boldsymbol{r}, \boldsymbol{r}', E) = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{B.9}$$

The Dirac-Coulomb Greens function S follows from G as

$$S(\boldsymbol{r}, \boldsymbol{r}', E) = (E - V + i\gamma^5\boldsymbol{\sigma}\boldsymbol{\nabla} + m\beta)G(\boldsymbol{r}, \boldsymbol{r}', E). \tag{B.10}$$

The more complicated E-dependence of K in (B.9) prevents simple solutions of the type (B.7). G satisfies the following integral equation:

$$G = G_S - \int d^3x G_S(\boldsymbol{r}, \boldsymbol{x})(\alpha_Z^2 + i\alpha_Z\boldsymbol{\sigma}\hat{\boldsymbol{x}})/x^2 G(\boldsymbol{x}, \boldsymbol{r}'), \tag{B.11}$$

where G_S satisfies (B.9) without the last two terms in K. G_S is a Schrödinger-Coulomb Greens function with relativistic kinematics. The method yields a closed expression for most of the Bethe logarithm.

The difficulties of relativistic Coulomb Greens functions should disappear with the use of the KG and Dirac equations in the dimensionless form (1.144). The interval $0 < r_\epsilon < \infty$ need not be expressed in terms of r. The perturbative expansion for K may be taken in the form

$$(K_0 + K_{\rm per})\psi_E = [(\kappa^2/E^2)^{(0)} + (\kappa^2/E^2)^{(1)} + \ldots]\psi_E. \tag{B.12}$$

The corresponding Greens function satisfies (B.3) in the form

$$(k^2/E^2 - p_{\epsilon,l\alpha}^2 - 2V_E + V_E^2)G_{E,l}(r_\epsilon, r'_\epsilon) = \delta(r_\epsilon - r'_\epsilon), \tag{B.13}$$

where $p_{\epsilon,l\alpha}^2$ has $l(l+1)/r^2$ replaced by $l_\alpha(l_\alpha+1)/r_\epsilon^2$. It has a Hostler solution (B.5) with new parameters, l_α and $\kappa_\epsilon = \kappa/E = \alpha_Z/n_\beta$,

$$R_{nlm_E} = N(m^2/E^2)e^{-\kappa_\epsilon r_\epsilon}(2\kappa_\epsilon r_\epsilon)^{l_\alpha} F(-n_r, 2l_\alpha + 2, 2\kappa_\epsilon r_\epsilon). \tag{B.14}$$

However, this formalism remains to be applied.

C Yukawa Expectation Values

Yukawa expectation values $\langle e^{-xr}/r\rangle$ are needed for the Uehling potential (5.83). More generally, they are useful for all interactions that can be written as dispersion integrals. For fermions, this includes the electric and magnetic form factor potentials. x is the integration variable of the dispersion relation, $x = x_{\rm th}\xi$; with the threshold value $x_{\rm th} = 2m_e$ both for the Uehling potential and for the electron's form factor potentials. First-order relativistic corrections are obtained by the Pauli reduction of Sect. 2.8, with the electric potential V_C+V_U (Pachucki 1996). Beyond the first order, one needs the fully relativistic expectation values. For the KG equation, the energy shift E^1 of first-order perturbation theory is obtained from (A.19)

$$\begin{aligned} E^1(\xi) &= \int R^2 e^{-xr}(r+\alpha_Z/E)dr(E/m) \\ &= (2\kappa)^{-2}\int R^2 e^{-zx/2\kappa}(z+2\kappa\alpha_Z/E)E/mdz. \end{aligned} \tag{C.1}$$

With R from (A.3), the total exponential becomes $e^{-\lambda z}$,

$$\lambda \equiv 1 + m_e\xi/\kappa \equiv 1 + 1/y, \tag{C.2}$$

$$E^1(\xi) = (2\kappa)^{-2} N_{\rm KG}^2 (J_{\lambda 1} + J_{\lambda 2})E/m \tag{C.3}$$

$$\begin{aligned} J_{\lambda 1} &= \int e^{-\lambda z} z^{b-1} F^2(-n_r, b, z)dz, \\ J_{\lambda 2} &= (2\kappa\alpha_Z/E)\int e^{-\lambda z} z^{b-2} F^2(-n_r, b, z)dz. \end{aligned} \tag{C.4}$$

The integral $J_{\lambda 1}$ is evaluated in closed form (Landau and Lifshitz 1977, Gradshteyn and Ryzhik 1980),

$$J_{\lambda 1} = \Gamma(b)\lambda^{-b-2n_r}(\lambda-1)^{2n_r} F(-n_r, -n_r, b; (\lambda-1)^{-2}), \tag{C.5}$$

where F is the hypergeometric function,

$$F(a, a', b; y) = 1 + aa'y/b + a(a+1)a'(a'+1)y^2/2!b(b+1) + \ldots \tag{C.6}$$

In (C.5), F is a polynomial of degree n_r. Insertion of $\lambda = 1 + 1/y$ gives

$$J_{\lambda 1} = \Gamma(b)(1+1/y)^{-b-2n_r} y^{-2n_r} F(-n_r, -n_r, b, y^2). \tag{C.7}$$

With $b = 2l_\alpha + 2,\ b + 2n_r$ gives $2n_\beta$. The integral $J_{\lambda 2}$ is more complicated. The two-body case has $\kappa = \alpha_Z\epsilon/n_\beta$; when ϵ is of the order of m_e, $m_e\xi/\kappa$

is much larger than 1. It is then useful to express $J_{\lambda 1}$ and $J_{\lambda 2}$ in powers of y,

$$F^2 = 1 - 2zn_r/b + z^2 n_r[n_r/b + (n_r - 1)/(b+1)]/b + \ldots, \tag{C.8}$$

and then use the basic integral

$$\int e^{-\lambda z} z^\nu dz = \Gamma(\nu+1)\lambda^{-\nu-1}: \tag{C.9}$$

$$J_{\lambda 1} = \Gamma(b) y^b [1 - 2n_\beta y + y^2(2n_\beta^2 + n_\beta)](1 + n_r^2 y^2/b). \tag{C.10}$$

The extra factor $2\kappa\alpha_Z/m \approx 2\alpha_Z^2/n$ in $J_{\lambda 2}$ is sufficient to make the y^2-terms negligible:

$$J_{\lambda 2} = 2(\kappa\alpha_Z/E)[\Gamma(b-1)y^{b-1} - 2n_r y^b \Gamma(b)/b]. \tag{C.11}$$

The last term is conveniently combined with the y^b of $J_{\lambda 1}$ into

$$J'_{\lambda 1} = \Gamma(b) y^b [1 - 4\alpha_Z^2 n_r/nb - 2ny + y^2(2n^2 + n + n_r^2/b)], \tag{C.12}$$

where we have also approximated n_β by n in the higher powers of y. In the remainder $J'_{\lambda 2}$ of $J_{\lambda 2}$, use of $\Gamma(b-1) = \Gamma(b)/(b-1) \approx \Gamma(b)/(2l+1)$ gives

$$J'_{\lambda 2} = 2\alpha_Z^2 n^{-1} \Gamma(b) y^{2l+1}/(2l+1). \tag{C.13}$$

The $\Gamma(b)$ is combined with the $(2\kappa)^{-2} N_{\mathrm{KG}}^2$ of (C.3) into

$$(2\kappa)^{-2} N_{\mathrm{KG}}^2 = (E/m)\kappa[n_r! n_\beta]^{-1} \Gamma(b + n_r)/\Gamma(b). \tag{C.14}$$

The KG energy shift of the Yukawa potential $e^{-2m_e\xi r}/r$ is thus

$$E^1(\xi) = \kappa \left(\frac{E}{m}\right) \frac{\Gamma(b+n_r)}{n_r! n_\beta \Gamma(b)} y^b \left[1 - 4\alpha_Z^2 \frac{n_r}{nb} - 2ny + y^{-1} \frac{2\alpha_Z^2}{n(2l+1)} + y^2(\ldots)\right]. \tag{C.15}$$

The energy shift of the Uehling potential is given by (5.83),

$$E_U^1 = -\tfrac{2}{3}\alpha_\pi (2\kappa)^{-2} N_{\mathrm{KG}}^2 \int_1^\infty d\xi (J'_{\lambda 1} + J'_{\lambda 2})(\xi^2 - 1)^{1/2}(\xi^{-2} + \tfrac{1}{2}\xi^{-4}). \tag{C.16}$$

The nonrelativistic limit of this integral has been calculated for the ground state ($n_r = 0$, $b = 2$), and recurrence relations have been constructed for other, not too large values of n_r and b (Pustovalov 1957). The corresponding Dirac ground state integral has been calculated by Karshenboim (1999). A convenient transformation of variable for this purpose is

$$\xi = (1 - v^2)^{-1/2}, \quad d\xi(\xi^2 - 1)^{1/2}\xi^{-2} = 2v^2 dv. \tag{C.17}$$

Approximate expressions for all $j = n - \frac{1}{2}$ are given in the limit of large κ/m_e. Such integrals are needed for antiprotonic and other exotic atoms

(Sect. 5.6). The ξ-integration in (C.16) results in integrals (Gradshtein and Ryzhik 1980),

$$\int d\xi(\xi^2-1)^{1/2}\xi^{-\nu} = \tfrac{1}{2}B(\tfrac{3}{2},\tfrac{\nu}{2}-1) = \tfrac{1}{2}\Gamma(\tfrac{3}{2})\Gamma(\tfrac{\nu}{2}-1)/\Gamma(\tfrac{\nu}{2}+\tfrac{1}{2}). \quad \text{(C.18)}$$

In (C.16), the ξ-integrals appear as

$$I_{U,\nu} = \int d\xi(\xi^2-1)^{1/2}\xi^{-\nu}(1+\tfrac{1}{2}\xi^{-2}) = \tfrac{3}{4}\frac{\nu}{\nu+1}B(\tfrac{3}{2},\tfrac{1}{2}\nu-1). \quad \text{(C.19)}$$

Neglecting the y^2-terms of (C.12),

$$E_U^1 = -\tfrac{2}{3}\alpha_\pi\kappa\frac{\kappa^b\Gamma(b+n_r)}{m_e^b n_r! n_\beta\Gamma(b)}\left[I_{U,b+2} - 2\alpha_Z\left(\frac{m}{m_e}I_{U,b+3} - \frac{1}{2l+1}\frac{m_e}{m}I_{U,b+1}\right)\right]. \quad \text{(C.20)}$$

Insertion of $b+2 = 2(l+2-\beta)$ leads to

$$I_{U,b+2} = \Gamma(3/2)\frac{\Gamma(l+1-\beta)}{\Gamma(l+5/2-\beta)}\frac{3}{4}\frac{l+2-\beta}{l+5/2-\beta}. \quad \text{(C.21)}$$

The index $_l$ of β_l is suppressed here, to facilitate the comparison with the Dirac case below. For $l=0$, (C.21) becomes

$$I_{U,4-\beta} = \Gamma(3/2)\frac{\Gamma(1-\beta)}{\Gamma(3/2-\beta)}\frac{3}{4}\frac{2-\beta}{(3/2-\beta)(5/2-\beta)}. \quad \text{(C.22)}$$

The expansion of Γ in powers of β introduces the function $\Psi = \Gamma'/\Gamma$; use of $\Psi(3/2) = -\gamma_{\rm Eu} - 2\log 2 + 2$ and $\Psi(1) = -\gamma_{\rm Eu}$ lead to

$$I_{U,\,l=0} \approx \tfrac{2}{5}[1+\beta(-2\log 2 + 2 - \tfrac{1}{2} + \tfrac{2}{3} + \tfrac{2}{5})]. \quad \text{(C.23)}$$

For $\nu = b+3$ and $b+1$, we only consider $l=0$ and take the limit $\alpha_Z^2 = 0$,

$$I_{U,b+3} = \tfrac{3}{4}\cdot\tfrac{5}{6}\Gamma^2(\tfrac{3}{2})/\Gamma(3) = \tfrac{5}{64}\pi, \quad I_{U,b+1} = \tfrac{18}{64}\pi. \quad \text{(C.24)}$$

with $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$. Its contribution to E_U^1 is

$$E_U^1 = \tfrac{4}{3}\alpha_\pi\alpha_Z^2(\kappa/m_e)^3 m_e\pi(\tfrac{5}{64} - \tfrac{18}{64}m_e^2/m^2). \quad \text{(C.25)}$$

The presence of an extra π leads to the combination $\alpha_\pi\pi\alpha_Z^5 = \alpha\alpha_Z^5$, which shows that one-loop graphs do produce some terms without π^{-1}. Next, we expand the factors in front of the I_U in (C.20). For $l=0$, $n_r = n-1$, and to first order in α_Z^2, $b = 2-2\beta$, $n_\beta = n-\beta$:

$$\Gamma(b+n_r) = \Gamma(n+1-2\beta) = n![1-2\beta\Psi(n+1)], \quad \text{(C.26)}$$

$$(4\kappa^3)^{-1}\Gamma(b)N_{\rm KG}^2 = 1 - 2\beta[\Psi(n+1) - \Psi(2) - 1/2n] - \alpha_Z^2/2n^2, \quad \beta = \alpha_Z^2, \quad \text{(C.27)}$$

with $\Psi(n+1)-\Psi(2)=\Sigma_{i=2}^{n} i^{-1}$, see (2.228). The factor $(\kappa/m_e)^b$ of (C.15) is expanded as follows:

$$\kappa(\kappa/m_e)^b = m_e(\kappa/m_e)^{2l+3}(\kappa/m_e)^{-2\beta}, \tag{C.28}$$

$$(\kappa/m_e)^{-2\beta} = e^{-2\beta\log(\kappa_{nr}/m_e)} \approx 1-2\beta\log(\kappa_{nr}/m_e), \tag{C.29}$$

with $\kappa_{nr}=\alpha_Z\mu_{nr}/n$ (here and in the following, the one-body parameters E and m are replaced by the two-body quantities ϵ and μ). We can now check the correction $1-2\beta\log(2\alpha_Z/n)$, which has been guessed in Sect. 2.7 from the divergence of R^2/N^2 at $r=0$. The $-2\beta\log 2$ which is missing in (C.29) is provided by (C.23),

$$[1-2\beta\log(\kappa/m_e)]I_{U0} = \tfrac{2}{5}\{1+\beta[2\log(m_e/2\kappa)+\tfrac{3}{2}+\tfrac{2}{3}+\tfrac{2}{5}]\}. \tag{C.30}$$

The logarithmic correction is now complete, including the recoil factor m_e/μ.

The calculation of the Dirac expectation values $\langle e^{-xr}/r\rangle_D$ of the Yukawa potential is more complicated, yet the results are similar:

$$\langle e^{-xr}/r\rangle_D = \int(g^2+f^2)e^{-xr}rdr = (2\kappa)^{-2}\int(g^2+f^2)e^{-zx/2\kappa}zdz. \tag{C.31}$$

When V_U has a short range, one needs g^2+f^2 only at small z. An expansion of $F\equiv F(-n_r,b_D,z)$ and $F_-\equiv F(1-n_r,b_D,z)$ to order z^2 is then sufficient:

$$(m_\beta-\kappa_D)^2F^2+n_r^2F_-^2-2n_r(m_\beta-\kappa_D)(\epsilon/\mu)FF_- = c_0+c_1z+c_2z^2. \tag{C.32}$$

In c_0, one approximates ϵ/μ by $1-\alpha_Z^2/2n^2$,

$$c_0 = (m_\beta-\kappa_D-n_r)^2+n_r(m_\beta-\kappa_D)\alpha_Z^2/n^2. \tag{C.33}$$

In c_1 and c_2, one may take $\epsilon/\mu=1$:

$$c_1 = -2(m_\beta-\kappa_D-n_r)(m_\beta-\kappa_D-n_r+1), \tag{C.34}$$

$$\begin{aligned} c_2 = \frac{n_r}{b_D^2(b_D+1)}\big\{&[(m_\beta-\kappa_D)(m_\beta-\kappa_D-2n_r+2)+n_r^2-n_r] \\ &\times[n_r(2b_D+1)-b_D][n_r(2b_D+1)-b_D]-n_r(n_r-1)(2b_D+1)\big\} \end{aligned} \tag{C.35}$$

States with $l=j+\frac{1}{2}$ have $\kappa_D=j+\frac{1}{2}\approx\gamma+\alpha_Z^2/2\gamma$, $m_\beta-\kappa_D=n_r-\alpha_Z^2n_r/n(2j+1)$,

$$c_0(l=j+\tfrac{1}{2})=\alpha_Z^2n_r^2/n^2, \quad c_1(l=j+\tfrac{1}{2})=2\alpha_Z^2n_r/n(2j+1). \tag{C.36}$$

In comparison with the S-states, c_1 and c_2 are suppressed by a factor α_Z^2. This is in fact true for all P-states.

States with $l=j-\frac{1}{2}$ have $\kappa_D=-j-\frac{1}{2}$ and $m_\beta-\kappa_D\approx(n_r+2\gamma)[1+\alpha_Z^2/2n\gamma]$, where α_Z^2/γ serves merely as an abbreviation for $\alpha_Z^2/(j+\frac{1}{2})$. Dropping the argument $l=j-\frac{1}{2}$ of c_i, one obtains from (C.33)–(C.35)

$$c_0 = 4\gamma^2 + \alpha_Z^2(3 + 3\gamma/n - 1/n - \gamma/n^2), \quad c_1 = -4n_r\gamma, \tag{C.37}$$

$$c_2 = [n_r(2b_D - 1) - b_D + 1]n_r/b_D = n_r[2n_r - (n_r + 2\gamma)/(2\gamma + 1)]. \tag{C.38}$$

The index $b_D = 2\gamma + 1 \approx 2j + 2 = 2l + 3$ is then approximately one unit larger than the $b = 2l_\alpha + 2$ of the KG equation. To establish the contact with the nonrelativistic limit, the arguments of the gamma functions in $\Pi_\Gamma^{-1} = \Gamma(b_D + n_r)/\Gamma^2(b_D)$ in (A.24) must be lowered by one, using $\Gamma(2\gamma + 1 + n_r) = (2\gamma + n_r)\Gamma(2\gamma + n_r)$:

$$\tfrac{1}{2}\kappa^{-2}N_D^2 \approx \kappa^2\Gamma(2\gamma + n_r)[\alpha_Z\mu n_r!4\gamma^2\Gamma^2(2\gamma)(1 + \alpha_Z^2/2n\gamma)]^{-1}. \tag{C.39}$$

The integrand of (C.31) contains the combination

$$e^{-xr}zdz(g^2 + f^2) = z^{2\gamma-1}dze^{-\lambda z}(c_0 + c_1z + c_2z^2)N_D^2/2\kappa^2. \tag{C.40}$$

Using now the basic integral (C.9) with $\nu = b_D - 2 = 2\gamma - 1$, $\nu = 2\gamma$ and $\nu = 2\gamma + 1$, one arrives at

$$\langle e^{-xr}/r\rangle_D = \kappa^2\Gamma(2\gamma + n_r)[\alpha_Z\mu n_r!\Gamma(2\gamma)(1 + \alpha_Z^2/2n\gamma)]^{-1}y^{2\gamma}[\,]_y, \tag{C.41}$$

$$[\,]_y = c_0/4\gamma^2 - y(c_0 - c_1)/2\gamma + y^2(1 + 1/2\gamma)(c_0/2 - c_1 + c_2). \tag{C.42}$$

Rewriting the 2γ in (C.41) as $2j + 1 - 2\beta_j = 2l + 2 - 2\beta_j$, one sees that the only difference from $b = 2l + 2 - 2\beta_l$ in (C.15) is the replacement of β_l by $\beta_j \approx \alpha_Z^2/(2j+1)$ (2.146), except for the y^2-terms. In the following, we restrict ourselves again to S-states, where $\gamma = 1 - \alpha_Z^2/2$,$n_r + 1 = n$ and $n_r + 1 = n$:

$$(1 + 1/2\gamma)(c_0/2 - c_1 + c_2) = \tfrac{1}{2}(5n^2 + 1). \tag{C.43}$$

$$\Gamma(2\gamma + n_r)[n_r!\Gamma(2\gamma)n(1 + \alpha_Z^2/2n\gamma)]^{-1} = 1 - \alpha_Z^2[\psi(n + 1) - \psi(2) + 1/2n]. \tag{C.44}$$

The n^{-1}-term of (C.44) cancels that of c_0 (C.37). The only remaining n^{-1}-term arises from the κ^4 of N_D^2,

$$\kappa^4(l = 0) = \kappa_{nr}^4[1 + 2\alpha_Z^2(1/n - 1/n^2)] = \kappa_{nr}^4[1 + 2\alpha_Z^2n_r/n^2]. \tag{C.45}$$

Including a contribution from $I_{U,6} = 6/35$, the total α_Z^2-correction to $\langle V_{U0}\rangle$ is a factor

$$1 + \alpha_Z^2\left[\log\frac{nm_e}{2\alpha_Z\mu} - \Psi(n + 1) + \Psi(2) - \frac{1}{4n^2} + 2\frac{n_r}{n^2} + \frac{326}{105} + \frac{3}{14n^2}\right], \tag{C.46}$$

with $326/105 = 3/2 + 1/3 + 1/5 + 15/14$. The linear α_Z-correction is given by the first term in the bracket of (C.25), as the corresponding integrals differ only at the order α_Z^2.

The relativistic recoil correction in the Uehling energy shift E_U is small. With $r = \rho/\mu$, the dimensionless variable $z = 2\kappa r$ becomes $z = 2\rho\kappa/\mu$, and the Yukawa exponent $-2m_e r\xi$ becomes $-2\rho\xi m_e/\mu$. In summary, the use of

ρ replaces κ by κ/μ, and m_e by m_e/μ. The dimensionless $\langle V_U/\mu\rangle$ depends only on κ/m_e (see (C.28)) and remains unchanged. The only recoil correction for E_U comes from (5.3),

$$E_U = \mu(\epsilon/\mu)_U = \mu\langle V_U/\mu\rangle \approx \frac{m_1 m_2}{m_{12}}\left(1 + \frac{\alpha_Z^2 m_1 m_2}{2n^2 m_{12}^2}\right)\langle V_U/\mu\rangle. \qquad \text{(C.47)}$$

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