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Relativistic effects in bound two-particle systems

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Abstract. The predictions of relativistic Schrödinger theory (RST) for the relativistic effects in helium-like ions with high nuclear charge ($Z \sim 30$–80) are elaborated in the electrostatic approximation (*i.e.* neglection of the magnetic interactions). The corresponding RST results are found to meet with the experimental data and with the predictions of other theoretical approaches, provided an estimate of the (neglected) magnetic effects is taken into account. This suggests to carry through high-precision calculations (including the magnetic forces) in order to further test the physical significance of RST.

PACS. 03.65.Pm Relativistic wave equations – 03.65.Ge Solutions of wave equations: bound states – 03.65.Ud Entanglement and quantum nonlocality (*e.g.* EPR paradox, Bell's inequalities, GHZ states, etc.)

1 Introduction

The present paper is concerned with setting up a general practicable quantum mechanics for relativistic many-particle systems. Indeed, after a century of intense development of quantum physics the relativistic many-particle systems still present a serious challenge for the physicists, perhaps rather for the theorists than for the experimentalists. It is true, there are no theoretical problems with the *non-relativistic* many-particle systems which can be described in an absolutely satisfactory manner by extending Schrödinger's original ideas (about the behavior of a single non-relativistic particle) to the many-particle systems [1]. However, certain problems do emerge when one tries to write down the analogous many-body generalizations for the *relativistic* one-particle systems which are generally described by the well-known Klein-Gordon and Dirac equations, see, *e.g.*, ref. [2]. Following here the generalization process for the non-relativistic systems, one would end up with the *manifestly covariant Hamiltonian formalism with constraints* [3] which, however, seems to have its difficulties when applied to a general particle number N. On the other hand, the well-established quantum field theory [4] is not able to deal directly with the bound states of fixed particle number N, but first it has to be approximated by the notorious Bethe-Salpeter equations [5,6]. However, this type of equations has been found to suffer from various deficiencies [7] and thus is considered as *still difficult to solve and understand* [8].

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1.1 Approximation methods

Thus, in lack of a well-working relativistic N-particle quantum mechanics, one has to resort to approximation and perturbation methods. These become especially important for strong external fields (*e.g.* Coulomb field generated by a large number $z_{\rm ex}$ of charge units located at the force center $r = 0$), since for such ultra-relativistic situations all the non-relativistic approaches become inadequate. (For an overview of the quantum effects in strong fields, see ref. [9]). For instance, the Lamb shift $\Delta_{\rm L}E$ of a one-particle energy level E_n of principal quantum number n amounts to a non-negligible fraction of the rest mass Mc^2 and is of the following general shape [10]:

$$\Delta_{\rm L}E = \frac{\alpha_{\rm s}}{\pi}\frac{(z_{\rm ex}\alpha_{\rm s})^4}{n^3}F(z_{\rm ex}\alpha_{\rm s})Mc^2 \ . \qquad (1.1)$$

Here the function F depends weakly upon the product of nuclear-charge number $z_{\rm ex}$ and fine-structure constant $\alpha_{\rm s}$, so that the Lamb shift $\Delta_{\rm L}E$ essentially varies as $z_{\rm ex}^4$. Thus, for the highly ionized (*i.e.* hydrogen-like) uranium atom with $z_{\rm ex} = 92$ the ground-state Lamb shift is $\Delta_{\rm L}E \approx 458$ eV [11], whereas the corresponding spectral lines can be determined with uncertainties as less as 16 eV [12]. Clearly, such experimental data present a challenge for the theorists to develop adequate approximation methods of comparable uncertainty, *e.g.* the "unified" method of Drake using a relativistic $(1/z_{\rm ex})$ expansion [13], or the multiconfiguration Dirac-Fock method (MCDF) [14,15], the relativistic many-body perturbation theory (MBPT) [16], or finally the all-order technique for relativistic MBPT [17]. For an overview of high-precision

Table 1. Comparison of RST predictions (third column) and experimental values [19] (second column) for the ground-state interaction energy ΔE of the two electrons.

Element ($z_{\rm ex}$)	$\Delta E_{\rm exp}$ (eV)	$\Delta E^{\rm (e)}_{\rm RST}$ (eV)	$\Delta = \dfrac{\Delta E_{\rm exp} - E^{\rm (e)}_{\rm RST}}{\Delta E_{\rm exp}}$ (%)	f_*^2
Ge (32)	562.5 ± 1.6	553.0	1.7	0.296
Xe (54)	1027.2 ± 3.5	974.3	5.1	0.297
Dy (66)	1341.6 ± 4.3	1232	8.2	0.295
W (74)	1568 ± 15	1423	9.3	0.248
Bi (83)	1876 ± 14	1661	11.5	0.222

calculations for helium see also the contribution of G.W.F. Drake in ref. [18]. The predictions of all these theoretical approaches have been tested in a high-precision measurement of the two-electron ground-state interaction energy for helium-like high-$z_{\rm ex}$ ions [19], and it has been found that the observational data fall (up to some residual eV) into the range of values predicted by the theoretical approaches.

1.2 Relativistic Schrödinger theory

These theoretical efforts should sufficiently demonstrate the necessity to have a coherent relativistic quantum mechanics for all the various phenomena occurring with the many-particle systems, especially as a theoretical basis for understanding the relativistic effects occurring in the stationary atomic states. Eventually, those effects due to field quantization (*e.g.* Lamb shift) would not be accounted for by such a theory, but all the relativistic and exchange effects should be truly included in the formalism so that the associated approximation and perturbation methods become obsolete.

A fresh approach to this long-standing problem has recently been put forward in form of the relativistic Schrödinger theory (RST), an alternative approach to relativistic quantum mechanics [20]. After the general mathematical structure of this theory has sufficiently been elaborated in some preceding papers [21–23], one may wish now to see some concrete demonstrations of the practical usefulness of this theory, especially concerning the relativistic effects in the many-electron atoms or ions, as mentioned above. Since it has turned out that the well-known Hartree-Fock approximation of conventional quantum theory is just the non-relativistic limit of RST [24] (or, conversely, RST is the relativistic generalization of the HF approach), the above-mentioned MCDF [14,15] naturally must appear as the direct competitor of RST. Therefore it is now self-suggesting to carry through within RST the high-precision calculations for the two-electron ground-state interaction energy in order to compare the RST results to the experimental and theoretical data reported in ref. [19].

Clearly, such a comparison would then clarify the scientific value of RST; however, merely comparing numbers would yield few insights into the specific way in which these predictions come about on the conceptual background of the new theory and therefore we renounce for the moment numerical precision in favor of a more qualitative line of arguments. This will shed more light upon the structural peculiarities of the new theory.

1.3 Electrostatic approximation

More concretely, we subsequently compute the ground-state interaction energy of the two electrons in the high-$z_{\rm ex}$ ions within the *electrostatic approximation*, where the magnetic contribution to the interaction energy is neglected, but in favor of the transparency of the calculation and insight into the logical architecture of the theoretical framework. Comparing then these approximate RST results to the corresponding collection of experimental and theoretical data of ref. [19] gives us that fraction of the interaction energy ($\lesssim 10\%$, see table 1) which is due to the magnetic forces among the two electrons. On the other hand, this energy contribution due to the magnetic forces may first be estimated by some qualitative arguments being based upon the fundamentals of the new theory; and when one finally finds sufficient agreement between these two results (obtained along rather different routes of reasoning), one may take this as enough motivation in order to undertake the required high-precision calculations for RST (see a separate paper).

1.4 Magnetic interactions

In order to obtain the desired estimate of the magnetic energy contribution, consider first the ground-state energy (M_*c^2, say) of a single Dirac particle of rest mass M in the Coulomb field [2]). This ground-state energy may be split up into two parts (cf. eq. (4.3) below)

$$M_*c^2 = Mc^2\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2} \equiv \frac{Mc^2}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}} - (z_{\rm ex}\alpha_{\rm s})^2\frac{Mc^2}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}}\ . \quad (1.2)$$

Now in RST the one-particle energy eigenvalue (M_*c^2) is always identical to the field energy $E_{\rm T}$ carried by the wave function ψ as the corresponding solution of the energy eigenvalue problem, see ref. [25] or eq. (3.76) below for the case of a spin-0 particle. On the other hand, in RST the single-particle field energy $E_{\rm T}$ is always composed of two contributions, namely the proper matter energy ($E_{\rm M}$)

and the interaction energy $E_{\rm es}$ with respect to the external source, see eq. (2.70) below with omitted interelectronic interaction energies $E_{\rm R}$ and $E_{\rm C}$. Furthermore, one can show [26] that for a Dirac particle these two ground-state energy contributions $E_{\rm M}$ and $E_{\rm es}$ just coincide with the two terms on the right of eq. (1.2):

$$E_{\rm M} \Rightarrow \frac{Mc^2}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}}\,, \tag{1.3a}$$

$$E_{\rm es} \Rightarrow -(z_{\rm ex}\alpha_{\rm s})^2 \frac{Mc^2}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}}\,. \tag{1.3b}$$

Here the matter energy $E_{\rm M}$ (1.3a) is to be interpreted as the rest mass energy of the particle (Mc^2) plus the kinetic energy due to translational motion with a typical ground-state velocity v:

$$E_{\rm M} = \frac{Mc^2}{\sqrt{1-\left(\frac{v}{c}\right)^2}} \tag{1.4}$$

which by comparison to eq. (1.3a) is then estimated as

$$v \approx z_{\rm ex}\alpha_{\rm s}\,. \tag{1.5}$$

However, when a point charge, emitting at rest the electric field $\vec{E}(\vec{r})$, is moving with velocity v it generates a magnetic field $\vec{H}(\vec{r})$ of magnitude

$$|\vec{H}(\vec{r})| \approx \frac{v/c}{\sqrt{1-(v/c)^2}} \cdot |\vec{E}(\vec{r})| = \frac{z_{\rm ex}\alpha_{\rm s}}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}} \cdot |\vec{E}(\vec{r})|\,. \tag{1.6}$$

For moving charge distributions one would modify this relation into

$$|\vec{H}(\vec{r})| \approx f_* \frac{z_{\rm ex}\alpha_{\rm s}}{\sqrt{1-(z_{\rm ex}\alpha_{\rm s})^2}} |\vec{E}(\vec{r})|\,, \tag{1.7}$$

where the constant prefactor f_* reflects the pattern of charge and current distribution of the ground state and is assumed to vary very weakly (or even not at all) with the nuclear charge $z_{\rm ex}$. On the other hand, RST identifies the interelectronic interaction energy as the interaction energy ($E_{\rm R}$, say) of the field modes $\vec{E}_a(\vec{r}) = -\vec{\nabla} A_a(\vec{r})$ ($a = 1 \ldots N$) being emitted by the members of the N-particle system, see the associated energy density ${}^{(\rm R)}T_{00}(\vec{r})$ in eq. (3.58) below. Thus, when the electrostatic and magnetostatic interaction energies of the ground-state configuration are denoted by $\Delta E^{(\rm e)}_{\rm RST}$ and $\Delta E^{(\rm m)}_{\rm RST}$, respectively, one finds the following relationship:

$$\Delta E^{(\rm m)}_{\rm RST} \approx f_*^2 \cdot \frac{(z_{\rm ex}\alpha_{\rm s})^2}{1-(z_{\rm ex}\alpha_{\rm s})^2} \cdot \Delta E^{(\rm e)}_{\rm RST}\,. \tag{1.8}$$

This result is due to the fact that the field strengths $\vec{E}(\vec{r})$ and $\vec{H}(\vec{r})$ do enter the energy functionals quadratically, see the relativistic version hereof given by eq. (2.67) below.

With this estimate of the magnetic energy contribution $\Delta E^{(\rm m)}_{\rm RST}$ being at hand now, one can undertake a first qualitative test of the usefulness of RST in atomic physics; namely by calculating the ground-state interaction energy $\Delta E^{(\rm e)}_{\rm RST}$ of the helium-like high-$z_{\rm ex}$ ions in the electrostatic approximation, then comparing the obtained results to the corresponding experimental and theoretical data $\Delta E_{\rm exp}$ (taken from ref. [19]) and thus identifying the magnetic contribution $\Delta E^{(\rm m)}_{\rm RST}$ (1.8) as

$$\Delta E^{(\rm m)}_{\rm RST} = \Delta E_{\rm exp} - \Delta E^{(\rm e)}_{\rm RST}\,. \tag{1.9}$$

If both results (1.8) and (1.9) for $\Delta E^{(\rm m)}_{\rm RST}$ should agree with respect to the dependence on the nuclear charge $z_{\rm ex}$, one will adopt this as a hint on the usefulness of RST when the corresponding high-precision calculations are actually carried through. The proposed qualitative test (1.8), (1.9) is passed by the subsequent RST calculations in a very satisfying manner. As is clearly demonstrated by table 1, the observed energy difference on the right of eq. (1.9) can satisfactorily be identified with the characteristic form of the magnetic energy $\Delta E^{(\rm m)}_{\rm RST}$ (1.8) since the required weak variability of the prefactor

$$f_*^2 = \frac{1-(z_{\rm ex}\alpha_{\rm s})^2}{(z_{\rm ex}\alpha_{\rm s})^2} \cdot \frac{\Delta E_{\rm exp} - \Delta E^{(\rm e)}_{\rm RST}}{\Delta E^{(\rm e)}_{\rm RST}} \tag{1.10}$$

is realized over the whole range of nuclear-charge numbers from $z_{\rm ex} = 32$ (germanium) up to $z_{\rm ex} = 83$ (bismuth): $0.296 \lesssim f_*^2 \lesssim 0.222$. Observe especially the constancy of f_* for the light nuclei up to $z_{\rm ex} = 66$ (dysprosium).

Thus one arrives at the conclusion that the RST predictions (if calculated exactly) can be expected to approach the observational data with comparable precision as the considered existing theoretical methods [13–18]. Here, it turns out that the main relativistic effects are qualitatively included already in the electrostatic approximation, so that the magnetic effects may be treated as a perturbation hereof.

1.5 Procedure

Our subsequent line of arguments is the following: In sect. 2 we briefly collect the RST fundamentals from various preceding papers in order to have the paper sufficiently self-contained. Since the gravitational (and other gauge) interactions are of minor significance in atomic physics, we simplify the theory and restrict ourselves to working over a flat space-time and considering only the electromagnetic interactions. Furthermore, for the sake of transparency, we are satisfied here with developing the RST formalism for spin-0 particles; and it is only in the last part of the paper (sect. 4.5) that we have to consider spin-$\frac{1}{2}$ particles in order to obtain results which can be compared to the experimental data. The reason why the scalar version of RST (for spin-0 particles) is insufficient in order

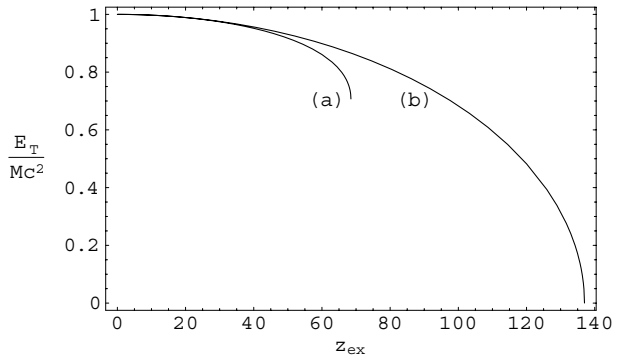

Fig. 1. Breakdown of one-particle ground-state (eq. (4.3)). For weak external fields ($z_{\rm ex} \lesssim 20$, say) the behavior of single fermions and bosons is very similar; however, strong fields induce a qualitatively different behavior: the vacuum breakdown occurs for $z_{\rm ex} \approx 68$ in the *bosonic* case (a), but for $z_{\rm ex} \approx 137$ in the *fermionic* case (b).

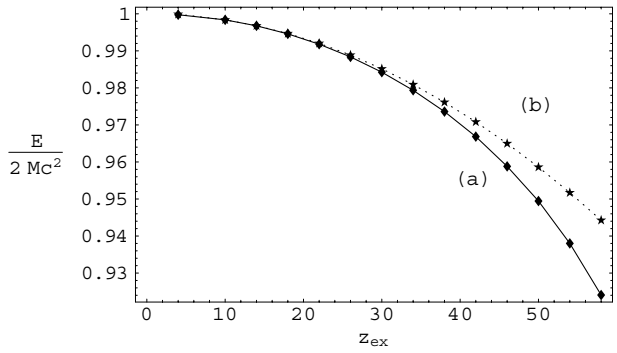

Fig. 2. RST and HF energy. In the non-relativistic regime ($z_{\rm ex} \lesssim 20$) the RST (a) and HF (b) predictions for the $(1s, 2s)$ energy $E_{\rm T}$ (3.68) or (3.69), respectively, are close together as expected; but in the highly relativistic regime ($z_{\rm ex} \gtrsim 60$), the RST curve (a) tends to develop a singularity of the kind known from the one-particle spectrum of fig. 1. This spoils the use of scalar fields in order to approximate the helium spectrum even when the fine structure is neglected (fig. 4).

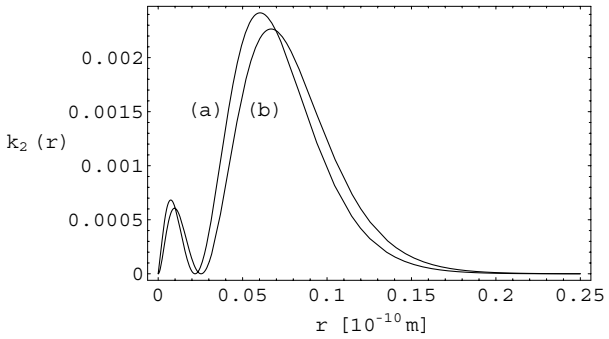

Fig. 3. Shrinking of charge distribution. The RST charge distributions $k_a(\vec{r}), h(\vec{r})$ (3.18a)-(3.19) become shifted towards the origin ($r = 0$) in comparison to their HF counterparts (3.20a)-(3.20c). Curve (a): RST; curve (b): HF. The resulting decrease of the external interaction energy $E_{\rm es}$ (< 0), eqs. (3.51)-(3.52), is responsible for the increase of the binding energy $|E_{\rm T} - 2Mc^2|$; see fig. 2.

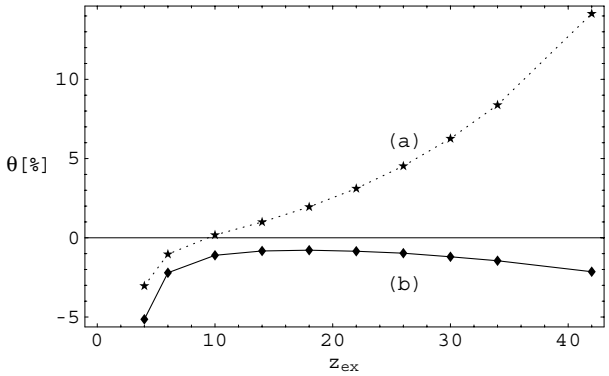

Fig. 4. Frequency deviation Θ (eq. (4.16)) for bosons. The relative deviation $|\Theta|$ (eq. (4.16)) for the transition $(1s, 2s) \to (1s, 1s)$ is smaller for scalar RST (a) than for the HF approach (b) only for moderate external fields ($z_{\rm ex} \lesssim 15$). For strong fields ($z_{\rm ex} \gtrsim 20$), the relativistic one-particle effects of fig. 1 spoil the usefulness of *scalar* RST. The experimental values for $\omega_{\rm ex}$ are taken from ref. [29].

to describe the higher-$z_{\rm ex}$ ions is discussed in detail and illustrated by figs. 1, 2.

In sect. 3 the general RST formalism is cut down to the two-particle systems with electromagnetic interactions and it is demonstrated explicitly how the Hartree-Fock equations do emerge as the non-relativistic limit of RST when one restricts oneself to the treatment of stationary bound states. The concept of relativistic energy functional $E_{\rm T}$ for the stationary states is introduced so that it becomes possible to set up the corresponding energy level systems for the many-electron atoms. As support of the proposed construction of the energy functional $E_{\rm T}$, one applies this to the one-particle systems (sect. 3.7) and finds the coincidence of the proposed field energy $E_{\rm T}$ with the mass eigenvalue as determined from the corresponding energy eigenvalue equation, see eq. (3.76) below.

Finally in sect. 4, the RST mass eigenvalue equations are solved numerically in the electrostatic approximation and the relativistic solutions are compared to their non-relativistic counterparts, *i.e.* the solutions of the Hartree-Fock equations (see fig. 3). Here it is demonstrated that the HF solutions become completely insufficient for describing the high-$z_{\rm ex}$ ions (fig. 4) whereas the spin-$\frac{1}{2}$ RST solutions remain relatively close to the experimental data (fig. 5). This supports the expectation that the RST predictions will come even closer to the experimental data when the (neglected) magnetic part of the gauge field equations is included into the RST calculations, see table 1.

2 Relativistic Schrödinger theory

A natural N-particle generalization of the well-known standard description of one-particle systems (Klein-Gordon theory [2,10]) is the recently established RST [20], an *alternative* form of relativistic quantum mechanics.

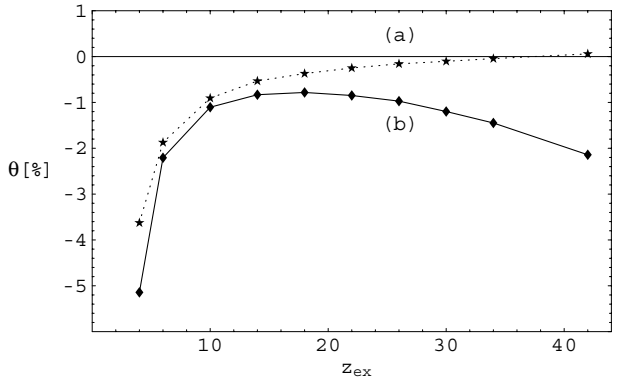

Fig. 5. Frequency deviation Θ (eq. (4.16)) for fermions. The frequency ω (eq. (4.21)) emitted by the fermionic transition $(1s_{1/2}, 2s_{1/2}\ {}^3S_1) \rightarrow (1s_{1/2}, 1s_{1/2}\ {}^1S_0)$ comes closer to the experimental values not only in the weak-field regime ($z_{\rm ex} \lesssim 15$) but also for strong fields $z_{\rm ex} \gtrsim 20$. Thus, the RST predictions (a) are now more precise than the HF predictions (b) for the whole range of field strengths. Compare this to the failure of the bosonic approach in fig. 4.

The most significant distinction with respect to the conventional theory is the circumstance that RST does not resort to the tensor product of Hilbert spaces for the composite systems but rather it is based upon the Whitney sum of the single-particle bundles. Thus, the RST wave functions $\Psi(x)$ for the N-particle systems are sections of a complex vector bundle which take their values in the typical fibre $\mathbb{C}^N$ and, consequently, the RST operators are matrices which take their values in the algebra $\mathcal{GL}(N, \mathbb{C})$ or, respectively, in one of its subalgebras. But apart from this mathematical difference, the RST dynamics has much in common with Schrödinger's original ideas governing non-relativistic quantum mechanics.

2.1 RST dynamics

The basic dynamical equation is the relativistic Schrödinger equation (RSE) for the wave function $\Psi(x)$,

$$i\hbar c \mathcal{D}_\mu \Psi = \mathcal{H}_\mu \Psi, \tag{2.1}$$

respectively the relativistic von Neumann equation (RNE) for the intensity matrix $\mathcal{I}$,

$$\mathcal{D}_\mu \mathcal{I} = \frac{i}{\hbar c} \left[\mathcal{I} \cdot \bar{\mathcal{H}}_\mu - \mathcal{H}_\mu \cdot \mathcal{I} \right] , \tag{2.2}$$

when mixtures are considered in place of pure states Ψ. The latter can be considered as a special kind of mixture, namely when the intensity matrix $\mathcal{I}$ degenerates to the tensor product of a wave function Ψ and its Hermitian conjugate $\bar{\Psi}$:

$$\mathcal{I} \Rightarrow \Psi \otimes \bar{\Psi} . \tag{2.3}$$

In the present paper we restrict ourselves to this special case and we will exclusively make use of pure states (for a treatment of mixtures see, *e.g.*, ref. [27]). In contrast to the conventional non-relativistic theory, the Hamiltonian $\mathcal{H}_\mu$ is not a rigid object but is itself a dynamical variable to be determined from its field equations, *i.e.* the *integrability condition*

$$\mathcal{D}_\mu \mathcal{H}_\nu - \mathcal{D}_\nu \mathcal{H}_\mu + \frac{i}{\hbar c} [\mathcal{H}_\mu, \mathcal{H}_\nu] = i\hbar c \mathcal{F}_{\mu\nu} \tag{2.4}$$

and the *conservation equation*

$$\mathcal{D}^\mu \mathcal{H}_\mu - \frac{i}{\hbar c} \mathcal{H}^\mu \mathcal{H}_\mu = i\hbar c \left(\frac{\mathcal{M} c}{\hbar} \right)^2 . \tag{2.5}$$

The latter equation may be used also in order to deduce the many-particle Klein-Gordon equation (KGE)

$$\mathcal{D}^\mu \mathcal{D}_\mu \Psi + \left(\frac{\mathcal{M} c}{\hbar} \right)^2 \Psi = 0 \tag{2.6}$$

from the RSE (2.1); and this eq. (2.6) is adopted by us as the N-particle generalization of the ordinary one-particle KGE described in the literature [2,10].

2.2 Conservation laws

The conservation equation (2.5) serves to define a conserved current j_μ:

$$\nabla^\mu j_\mu = 0, \tag{2.7}$$

namely through

$$j_\mu = \mathrm{tr}(\mathcal{I} \cdot v_\mu) \Rightarrow \bar{\Psi} \cdot v_\mu \cdot \Psi , \tag{2.8}$$

where the *velocity operator* v_μ reads, in terms of the Hamiltonian $\mathcal{H}_\mu$,

$$v_\mu = \frac{1}{2} \left[\bar{\mathcal{H}}_\mu \cdot \left(\mathcal{M} c^2 \right)^{-1} + \left(\mathcal{M} c^2 \right)^{-1} \cdot \mathcal{H}_\mu \right] . \tag{2.9}$$

For our present purposes, it is sufficient to consider *identical* particles so that the mass operator $\mathcal{M}$ becomes proportional to the identity

$$\mathcal{M} = M \cdot \mathbf{1} . \tag{2.10}$$

Besides the charge conservation law (2.7) the Hamiltonian dynamics (2.4)-(2.5) implies also the source equation for the energy momentum density ${}^{(\mathrm{M})}T_{\mu\nu}$ of matter

$$\nabla^\mu \, {}^{(\mathrm{M})}T_{\mu\nu} = f_\nu . \tag{2.11}$$

Here ${}^{(\mathrm{M})}T_{\mu\nu}$ is defined quite analogously as the current density j_μ (2.8) through

$${}^{(\mathrm{M})}\mathcal{T}_{\mu\nu} = \mathrm{tr} \left(\mathcal{I} \cdot \mathcal{T}_{\mu\nu} \right) \Rightarrow \Psi \cdot \mathcal{T}_{\mu\nu} \cdot \Psi , \tag{2.12}$$

where the *energy momentum operator* $\mathcal{T}_{\mu\nu}$ is given in terms of the Hamiltonian $\mathcal{H}_\mu$ as

$$\mathcal{T}_{\mu\nu} = \frac{1}{2} \Big\{ \bar{\mathcal{H}}_\mu \cdot \left(\mathcal{M} c^2 \right)^{-1} \cdot \mathcal{H}_\nu + \bar{\mathcal{H}}_\nu \cdot \left(\mathcal{M} c^2 \right)^{-1} \cdot \mathcal{H}_\mu - g_{\mu\nu} \left[\bar{\mathcal{H}}^\lambda \cdot \left(\mathcal{M} c^2 \right)^{-1} \cdot \mathcal{H}_\lambda - \mathcal{M} c^2 \right] \Big\} . \tag{2.13}$$

For the pure states (2.3), it is possible to eliminate the Hamiltonian $\mathcal{H}_\mu$ from the matter density ${}^{(\mathrm{M})}T_{\mu\nu}$ (2.12)

by means of the RSE (2.1) in favor of the derivatives of the wave function Ψ:

$$ {}^{(\mathrm{M})}T_{\mu\nu} = \frac{\hbar^2}{2M}\Bigg\{ \left(\mathcal{D}_\mu\bar{\Psi}\right)\left(\mathcal{D}_\nu\Psi\right) + \left(\mathcal{D}_\nu\bar{\Psi}\right)\left(\mathcal{D}_\mu\Psi\right) - g_{\mu\nu}\left[\left(\mathcal{D}_\lambda\bar{\Psi}\right)\left(\mathcal{D}^\lambda\Psi\right) - \left(\frac{\mathcal{M}c}{\hbar}\right)^2\bar{\Psi}\cdot\Psi\right]\Bigg\}, \tag{2.14} $$

which is the N-particle generalization of the well-known one-particle tensor [2,25]. Moreover, the force density f_ν (2.11) is found as the product of the field strength $\mathcal{F}_{\mu\nu}$ and Hamiltonian $\mathcal{H}_\mu$

$$ f_\nu = \mathrm{tr}(\mathcal{I}\cdot\mathfrak{f}_\nu) \Rightarrow \bar{\Psi}\cdot\mathfrak{f}_\nu\cdot\Psi \tag{2.15} $$

with the *force operator* $\mathfrak{f}_\nu$ being given by

$$ \mathfrak{f}_\nu = \frac{i\hbar c}{2}\left[\bar{\mathcal{H}}^\mu\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\mathcal{F}_{\mu\nu} + \mathcal{F}_{\mu\nu}\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\mathcal{H}^\mu\right]. \tag{2.16} $$

Clearly, this force density f_ν (2.15) must again be regarded as the N-particle generalization of the one-particle case being usually treated in the textbooks (*Lorentz force* [28]) which readily will become more obvious.

2.3 Abelian symmetry breaking

The force density f_ν (2.15) plays an important part for the construction of the total energy momentum density ${}^{(\mathrm{T})}T_{\mu\nu}$ of the N-particle system and must therefore be considered in some detail. Splitting up the field strength $\mathcal{F}_{\mu\nu}$ into its external and internal parts:

$$ \mathcal{F}_{\mu\nu} = {}^{(\mathrm{ex})}\mathcal{F}_{\mu\nu} + {}^{(\mathrm{s})}\mathcal{F}_{\mu\nu}\ , \tag{2.17} $$

it is clear that the external part (being generated by some external source, *e.g.* the atomic nucleus) acts upon every particle in the same way and therefore must be proportional to the identity

$$ {}^{(\mathrm{ex})}\mathcal{F}_{\mu\nu} = -i\,{}^{(\mathrm{ex})}F_{\mu\nu}\cdot\mathbf{1}\ . \tag{2.18} $$

On the other hand, the internal part ${}^{(\mathrm{s})}\mathcal{F}_{\mu\nu}$ is generated by the system's particles and therefore incorporates both the electromagnetic and the exchange interactions which become unified here into a $U(N)$ gauge theory. However, this gauge symmetry undergoes *Abelian symmetry breaking* $U(N) \Rightarrow U(1)\times U(1)\ldots\times U(1)$ so that the N-dimensional Abelian product $U(1)\times U(1)\ldots\times U(1)$ constitutes the residual gauge symmetry due to the ordinary electromagnetic interactions. Thus, selecting N anti-Hermitian generators τ_a $(a = 1\ldots N)$ for the residual gauge group $U(1)\times U(1)\ldots U(1)$, and $(N^2-N)/2$ generators χ_A $(A = 1\ldots N(N-1)/2)$ for the broken gauge degrees of freedom, the internal-field strength ${}^{(\mathrm{s})}\mathcal{F}_{\mu\nu} = -{}^{(\mathrm{s})}\bar{\mathcal{F}}_{\mu\nu}$ decomposes as

$$ {}^{(\mathrm{s})}\mathcal{F}_{\mu\nu} = F^a{}_{\mu\nu}\tau_a + G^A{}_{\mu\nu}\chi_A - \overset{*}{G}{}^A{}_{\mu\nu}\bar{\chi}_A\ . \tag{2.19} $$

Since the Abelian generators τ_a are adopted to be anti-Hermitian ($\bar{\tau}_a = -\tau_a$), the *electromagnetic field strengths* $F^a{}_{\mu\nu}$ $(a = 1\ldots N)$ are real ($\overset{*}{F}{}^a{}_{\mu\nu} = F^a{}_{\mu\nu}$), whereas the *exchange field strengths* $G^A{}_{\mu\nu}$ $(A = 1\ldots N(N-1)/2)$ are complex 2-forms.

With such an arrangement for the $\mathcal{U}(N)$-valued field strength $\mathcal{F}_{\mu\nu}$, the Lorentz force operator $\mathfrak{f}_\nu$ (2.16) is also split up into two parts

$$ \mathfrak{f}_\nu = {}^{(\mathrm{ex})}\mathfrak{f}_\nu + {}^{(\mathrm{s})}\mathfrak{f}_\nu\,, \tag{2.20} $$

where the external part is built up by the total velocity operator v_μ (2.9) and the external-field strength ${}^{(\mathrm{ex})}F_{\mu\nu}$ (2.18):

$$ {}^{(\mathrm{ex})}\mathfrak{f}_\nu = \hbar c\,{}^{(\mathrm{ex})}F_{\mu\nu}\cdot v^\mu, \tag{2.21} $$

and similarly the "internal part" appears in the following form:

$$ {}^{(\mathrm{s})}\mathfrak{f}_\nu = \hbar c\left(F^a{}_{\mu\nu}v_a{}^\mu + G^A{}_{\mu\nu}w_A{}^\mu + \overset{*}{G}{}^A{}_{\mu\nu}\bar{w}_A{}^\mu\right), \tag{2.22} $$

provided one introduces the *electromagnetic velocity operators* $v_{a\mu}$ $(a = 1\ldots N)$ through

$$ v_{\alpha\mu} = \frac{i}{2}\left[\bar{\mathcal{H}}_\mu\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\tau_\alpha + \tau_\alpha\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\mathcal{H}_\mu\right] \tag{2.23} $$

and the *exchange velocity operators* $w_{A\mu}$ $(A = 1\ldots N(N-1)/2)$ through

$$ w_{A\mu} = \frac{i}{2}\left[\bar{\mathcal{H}}_\mu\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\chi_A + \chi_A\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\mathcal{H}_\mu\right], \tag{2.24a} $$

$$ \bar{w}_{A\mu} = -\frac{i}{2}\left[\bar{\mathcal{H}}_\mu\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\bar{\chi}_A + \bar{\chi}_A\cdot\left(\mathcal{M}c^2\right)^{-1}\cdot\mathcal{H}_\mu\right]. \tag{2.24b} $$

This construction then implies the corresponding splitting of the Lorentz force density f_ν (2.15) into an external and internal part:

$$ f_\nu = {}^{(\mathrm{ex})}f_\nu + {}^{(\mathrm{s})}f_\nu \tag{2.25} $$

with the external contribution being given by

$$ {}^{(\mathrm{ex})}f_\nu = \mathrm{tr}\left(\mathcal{I}\cdot{}^{(\mathrm{ex})}\mathfrak{f}_\nu\right) = \hbar c\,{}^{(\mathrm{ex})}F_{\mu\nu}j^\mu\ , \tag{2.26} $$

and similarly for the internal part

$$ {}^{(\mathrm{s})}f_\nu = \mathrm{tr}(\mathcal{I}\cdot{}^{(\mathrm{s})}\mathfrak{f}_\nu) = \hbar c\left(F^a{}_{\mu\nu}j_a{}^\mu + G^A{}_{\mu\nu}h_A{}^\mu + \overset{*}{G}{}^A{}_{\mu\nu}\overset{*}{h}{}_A{}^\mu\right). \tag{2.27} $$

Here, the definitions of the *electromagnetic currents* $j_{a\mu}$ and *exchange currents* $h_{A\mu}$ proceed along the same line of arguments as for the total current j_μ (2.8), *i.e.*

$$ j_{a\mu} = \mathrm{tr}(\mathcal{I}\cdot v_{a\mu})\,, \tag{2.28a} $$

$$ h_{A\mu} = \mathrm{tr}(\mathcal{I}\cdot w_{A\mu})\,, \tag{2.28b} $$

$$ \overset{*}{h}{}_{A\mu} = \mathrm{tr}(\mathcal{I}\cdot\bar{w}_{a\mu}). \tag{2.28c} $$

2.4 Maxwell equations

Since the field strength $\mathcal{F}_{\mu\nu}$ belongs to the set of dynamical variables of RST, it becomes now necessary to specify some field equation for this object in order to close the whole dynamical system. Here it seems immediately plausible that the N-particle generalization of the well-known Abelian Maxwell equations will be their non-Abelian version:

$$\mathcal{D}^\mu \mathcal{F}_{\mu\nu} = -4\pi i \alpha_{\rm s} \mathcal{J}_\nu \qquad \left(\alpha_{\rm s} = \frac{e^2}{\hbar c}\right). \tag{2.29}$$

The $\mathcal{U}(2)$-valued field strength $\mathcal{F}_{\mu\nu}$ (*i.e.* bundle curvature) is generated in the usual way by the gauge potential $\mathcal{A}_\mu$ (*i.e.* bundle connection)

$$\mathcal{F}_{\mu\nu} = \nabla_\mu \mathcal{A}_\nu - \nabla_\nu \mathcal{A}_\mu + [\mathcal{A}_\mu, \mathcal{A}_\nu] \tag{2.30}$$

so that the Bianchi identity holds,

$$\mathcal{D}_\lambda \mathcal{F}_{\mu\nu} + \mathcal{D}_\mu \mathcal{F}_{\nu\lambda} + \mathcal{D}_\nu \mathcal{F}_{\lambda\mu} \equiv 0 \qquad \big(\mathcal{D}_\lambda \mathcal{F}_{\mu\nu} \doteqdot \nabla_\lambda \mathcal{F}_{\mu\nu} + [\mathcal{A}_\lambda, \mathcal{F}_{\mu\nu}]\,\big). \tag{2.31}$$

Indeed, if the current operator $\mathcal{J}_\nu$ on the right of the Maxwell equations (2.29) can be specified in terms of the wave function Ψ and potential $\mathcal{A}_\mu$, one has a closed dynamical system of matter and gauge fields.

However, it is exactly this problem of specifying the current operator $\mathcal{J}_\mu$ in terms of the RST currents $j_{a\mu}$ and $h_{A\mu}$ (2.28a)-(2.28c) which is a somewhat delicate point with respect to the emergence of unwanted self-interactions. In order to see this problem more clearly, first split off the external part of the Maxwell equation by putting

$$\mathcal{J}_\mu = {}^{(\rm ex)}\mathcal{J}_\mu + {}^{(\rm s)}\mathcal{J}_\mu\,, \tag{2.32}$$

with the external part consisting of the external current ${}^{(\rm ex)}j_\mu$ in a self-evident way:

$${}^{(\rm ex)}\mathcal{J}_\mu = {}^{(\rm ex)}j_\mu \cdot \mathbf{1}\ . \tag{2.33}$$

Thus, the external part of the Maxwell equation (2.29) reads

$$\mathcal{D}^\mu\, {}^{(\rm ex)}\mathcal{F}_{\mu\nu} = -4\pi i \alpha_{\rm s}\, {}^{(\rm ex)}\mathcal{J}_\nu \qquad \left(\nabla^\mu\, {}^{(\rm ex)}F_{\mu\nu} = 4\pi\alpha_{\rm s}\, {}^{(\rm ex)}j_\nu\right) \tag{2.34}$$

and is essentially the same as in classical electrodynamics [28]. The physical reason for this is that the N particles of the considered system do not become entangled with the external source. What then remains to be considered is the internal part of Maxwell's equations:

$${}^{(\rm s)}\mathcal{D}^\mu\, {}^{(\rm s)}\mathcal{F}_{\mu\nu} = -4\pi i \alpha_{\rm s}\, {}^{(\rm s)}\mathcal{J}_\nu\ , \tag{2.35}$$

where the covariant derivative ${}^{(\rm s)}\mathcal{D}^\mu$ refers to the internal gauge potential ${}^{(\rm s)}\mathcal{A}_\mu$:

$${}^{(\rm s)}\mathcal{A}_\mu = \mathcal{A}_\mu - {}^{(\rm ex)}\mathcal{A}_\mu = \mathcal{A}_\mu + i\, {}^{(\rm s)}A_\mu \cdot \mathbf{1} = A^a{}_\mu \tau_a + B^A{}_\mu \chi_A - \overset{*}{B}{}^A{}_\mu \bar{\chi}_A\ . \tag{2.36}$$

Moreover, the internal current operator ${}^{(\rm s)}\mathcal{J}_\mu$, occurring on the right-hand side of Maxwell's equations (2.35), may be decomposed in a similar way as

$${}^{(\rm s)}\mathcal{J}_\mu = i\left(\,'j^a{}_\mu \tau_a + {}'h^A{}_\mu \chi_A + \overset{*}{{}'h}{}^A{}_\mu \bar{\chi}_A\right). \tag{2.37}$$

Thus, we arrive at the crucial point, namely to determine the *Maxwell currents* $\{\,'j^\alpha{}_\mu\} \equiv \{\,'j^a{}_\mu;\, {}'h^A{}_\mu, \overset{*}{{}'h}{}^A{}_\mu\}$ in terms of the *RST currents* $\{j_{\alpha\mu}\} \equiv \{j_{a\mu}; h_{A\mu}, \overset{*}{h}_{A\mu}\}$, $\alpha = 1 \ldots N^2$, which have been defined through eqs. (2.28a)-(2.28c).

It must be stressed here that one cannot solve this problem by simply identifying both kinds of currents (*e.g.* $'j^\alpha{}_\mu = \delta^{\alpha\beta} j_{\beta\mu}$, etc.), because in this case the electromagnetic field strengths $F^a{}_{\mu\nu}$, being generated by the Maxwell currents $'j^a{}_\mu$ via the Maxwell equations (2.35), would act back to their own sources $j_{a\mu} \equiv (\,'j^a{}_\mu)$ via the Lorentz force density ${}^{(\rm s)}f_\nu$ (2.27). Obviously, one has to think of a more intelligent link of both kinds of currents in order to avoid these notorious *self-interactions*!

2.5 Compatibility condition

The desired link between the Maxwell and RST currents actually emerges as a condition for the compatibility of the Maxwell and RST subdynamics [23]. Observe here that the Maxwell equations imply the following conservation law in operator form:

$$\mathcal{D}^\mu \mathcal{J}_\mu \equiv 0, \tag{2.38}$$

namely as a consequence of the generally valid bundle identity for the curvature $\mathcal{F}_{\mu\nu}$,

$$\mathcal{D}^\mu \mathcal{D}^\nu \mathcal{F}_{\mu\nu} \equiv 0. \tag{2.39}$$

Putting both the connection ${}^{(\rm s)}\mathcal{A}_\mu$ (2.36) and the current operator ${}^{(\rm s)}\mathcal{J}_\mu$ (2.37) into the self-evident short-hand notation

$${}^{(\rm s)}\mathcal{A}_\mu = A^\alpha{}_\mu \tau_\alpha\,, \tag{2.40a}$$

$${}^{(\rm s)}\mathcal{J}_\mu = i\,'j^\alpha{}_\mu \tau_\alpha\,, \tag{2.40b}$$

with the N^2 generators τ_α obeying the commutation relations

$$[\tau_\alpha, \tau_\beta] = C^\gamma{}_{\alpha\beta}\tau_\gamma, \tag{2.41}$$

the operator identity (2.38) reads, in components,

$$\nabla^\mu\, 'j^\alpha{}_\mu = -C^\alpha{}_{\beta\gamma} A^{\beta\mu}\, 'j^\gamma{}_\mu\ . \tag{2.42}$$

But, on the other hand, such source relations also exist for the RST currents $j_{\alpha\mu}$ (2.28a)-(2.28c), which is easily seen by explicitly carrying through the required differentiation process with the help of the RSE (2.1), or of the KGE (2.6), respectively, which then yields

$$\nabla^\mu j_{\alpha\mu} = C^\gamma{}_{\beta\alpha} A^{\beta\mu} j_{\gamma\mu}\ . \tag{2.43}$$

Now when both currents ${}'j^{\alpha}{}_{\mu}$ and $j_{\alpha\mu}$ are related by some linear transformation $\mathcal{K} = \{K^{\alpha}{}_{\beta}\}$, *i.e.*

$$j_{\alpha\mu} = K_{\alpha\beta}\, {}'j^{\beta}{}_{\mu} \qquad (2.44)$$
$$\big(K_{\alpha\beta} \doteqdot \delta_{\alpha\gamma} K^{\gamma}{}_{\beta}\,,\ \text{etc.}\big),$$

then the simultaneous validity of both source relations (2.42) and (2.43) requires that the *compatibility tensor* $\mathcal{K}$ anti-commutes with the adjoint representations $\mathfrak{C}_{\alpha} = \{C^{\beta}{}_{\alpha\gamma}\}$ of the generators τ_{α} (2.41):

$$\mathfrak{C}_{\alpha}^{\mathrm{T}} \cdot \mathcal{K} + \mathcal{K} \cdot \mathfrak{C}_{\alpha} = 0\ . \qquad (2.45)$$

Thus, the crucial point with the avoidance of self-interactions is to select the generators $\{\tau_{\alpha}\} = \{\tau_a; \chi_A, \bar{\chi}_A\}$ in such a way that all diagonal elements $(K^{\alpha}{}_{\alpha})$ of the associated compatibility tensor $\mathcal{K}$ (2.44) are zero. The subsequent treatment of the two-particle systems suggests that this requirement can actually be satisfied for the general N-particle situation (for the three-particle systems see ref. [23]).

2.6 Energy momentum densities

With a consistent framework for the N-particle systems being at hand now, one can return to our original problem of determining the corresponding N-particle energy functional E_{T}. In the true spirit of a relativistic field theory, one wishes to identify this energy E_{T}, measured relative to some inertial frame, as an integral of the time component ${}^{(\mathrm{T})}T_{00}$ of some energy momentum tensor ${}^{(\mathrm{T})}T_{\mu\nu}$ over the whole three-space:

$$E_{\mathrm{T}} = \int \mathrm{d}^3\vec{r}\ {}^{(\mathrm{T})}T_{00}(\vec{r})\ . \qquad (2.46)$$

Consequently, the first task is to find the energy momentum density ${}^{(\mathrm{T})}T_{\mu\nu}$ carried by the coupled system of wave functions and gauge fields. Intuitively, one will expect the desired energy momentum density ${}^{(\mathrm{T})}T_{\mu\nu}$ to be composed of three contributions, namely the matter part ${}^{(\mathrm{M})}T_{\mu\nu}$ and the contributions due to the internal (${}^{(\mathrm{G})}T_{\mu\nu}$) and external (${}^{(\mathrm{es})}T_{\mu\nu}$) interactions:

$${}^{(\mathrm{T})}T_{\mu\nu} = {}^{(\mathrm{M})}T_{\mu\nu} + {}^{(\mathrm{G})}T_{\mu\nu} + {}^{(\mathrm{es})}T_{\mu\nu}\ . \qquad (2.47)$$

Clearly, for the one-particle systems the internal interaction part ${}^{(\mathrm{G})}T_{\mu\nu}$ is missing [25]. Concerning their source relations, from which the partial tensors $\{{}^{(\mathrm{M})}T_{\mu\nu}, {}^{(\mathrm{G})}T_{\mu\nu}, {}^{(\mathrm{es})}T_{\mu\nu}\}$ have to be determined, it is plausible to assume that the interaction between the N-particle system and an external source occurs along some overall field to which every particle contributes in the same way. The first one of these overall objects is the *total current* j_{μ} (2.8) which we may conceive as the sum of all the Maxwell currents ${}'j^{a}{}_{\mu}$ (2.28a):

$$j_{\mu} = -\frac{1}{N-1}\sum_{a=1}^{N} {}'j^{a}{}_{\mu} = -\frac{1}{N-1}\,\mathrm{tr}\ {}^{(\mathrm{s})}\mathcal{J}_{\mu}\ . \qquad (2.48)$$

This can be realized by choosing the Abelian generators τ_a $(a = 1 \ldots N)$ to be proportional to $(N-1)$-dimensional projectors

$$\tau_a = -i\,(\mathbf{1} - \mathcal{P}_a)\ , \qquad (2.49a)$$
$$\mathcal{P}_a \cdot \mathcal{P}_b = \delta_{ab} \cdot \mathcal{P}_a\,, \qquad (2.49b)$$
$$\sum_{a=1}^{N} \mathcal{P}_a = \mathbf{1}\,, \qquad (2.49c)$$
$$\mathrm{tr}\,\mathcal{P}_a = 1\ , \qquad (2.49d)$$

and by taking traceless exchange generators χ_A:

$$\mathrm{tr}\,\chi_a = 0\ . \qquad (2.50)$$

In a similar way, one introduces the *total field strength* $F_{\mu\nu}$ as the coherent superposition of all the electromagnetic fields $F^{a}{}_{\mu\nu}$ through

$$F_{\mu\nu} = \sum_{a=1}^{N} F^{a}{}_{\mu\nu} = \frac{i}{N-1}\,\mathrm{tr}\ {}^{(\mathrm{s})}\mathcal{F}_{\mu\nu}\,, \qquad (2.51)$$

which, according to the (non-Abelian) Maxwell equation (2.35), is linked to the total current j_{μ} (2.48) via the ordinary Maxwell equation

$$\nabla^{\mu} F_{\mu\nu} = -4\pi\alpha_{\mathrm{s}} j_{\nu}\ . \qquad (2.52)$$

Observe here that the total current j_{μ} enters the Maxwell equations (2.52) with a minus sign because the system's particles are thought to be negatively charged, in contrast to the positive charge of the external source (2.34).

These global objects of the N-particle system become now relevant for the source equations of the energy momentum densities in the following sense: presuming that the total arrangement of N-particle system plus external source (with energy momentum density ${}^{(\mathrm{ex})}T_{\mu\nu}$) is closed

$$\nabla^{\mu}\Big({}^{(\mathrm{T})}T_{\mu\nu} + {}^{(\mathrm{ex})}T_{\mu\nu}\Big) = 0\ , \qquad (2.53)$$

and adopting also the following nearby guess for the source (${}^{(\mathrm{xe})}f_{\nu}$, say) of the external density ${}^{(\mathrm{ex})}T_{\mu\nu}$

$$\nabla^{\mu}\,{}^{(\mathrm{ex})}T_{\mu\nu} = {}^{(\mathrm{xe})}f_{\nu} = -\hbar c F_{\mu\nu}\,{}^{(\mathrm{ex})}j^{\mu}\,, \qquad (2.54)$$

one concludes, from the closedness condition (2.53),

$$\nabla^{\mu}\,{}^{(\mathrm{T})}T_{\mu\nu} = -\,{}^{(\mathrm{xe})}f_{\nu} = \hbar c F_{\mu\nu}\,{}^{(\mathrm{ex})}j^{\mu}\ . \qquad (2.55)$$

On the other hand, the total density ${}^{(\mathrm{T})}T_{\mu\nu}$ (2.47) consists of three parts, ${}^{(\mathrm{M})}T_{\mu\nu}$, ${}^{(\mathrm{G})}T_{\mu\nu}$ and ${}^{(\mathrm{es})}T_{\mu\nu}$, where the source ${}^{(\mathrm{s})}f_{\nu}$ of the matter part ${}^{(\mathrm{M})}T_{\mu\nu}$ has already been specified by eqs. (2.27). Therefore, we are left with the source equations for the sum of external and internal energy momentum tensors ${}^{(\mathrm{G})}T_{\mu\nu}$ and ${}^{(\mathrm{es})}T_{\mu\nu}$:

$$\nabla^{\mu}\Big({}^{(\mathrm{G})}T_{\mu\nu} + {}^{(\mathrm{es})}T_{\mu\nu}\Big) = -\,{}^{(\mathrm{ex})}f_{\nu} - {}^{(\mathrm{s})}f_{\nu} - {}^{(\mathrm{xe})}f_{\nu}\ . \qquad (2.56)$$

But here we presume that when the internal gauge fields pull at the matter system with the force density ${}^{(\mathrm{s})}f_\nu$ (2.27), then the matter system acts back upon the internal gauge field system with the negative force $(-{}^{(\mathrm{s})}f_\nu)$, *i.e.* we put

$$\nabla^\mu\,{}^{(\mathrm{G})}T_{\mu\nu} = -\,{}^{(\mathrm{s})}f_\nu\ . \tag{2.57}$$

Combining this assumption with the preceding source relation (2.56), let us find the remaining source equation for the external interaction as

$$\nabla^\mu\,{}^{(\mathrm{es})}T_{\mu\nu} = -\left({}^{(\mathrm{ex})}f_\nu + {}^{(\mathrm{xe})}f_\nu\right) = \hbar c\left(F_{\mu\nu}\,{}^{(\mathrm{ex})}j^\mu - {}^{(\mathrm{ex})}F_{\mu\nu}j^\mu\right)\ . \tag{2.58}$$

However, once the source relations (2.57)-(2.58) for the internal and external gauge interactions have been established, it is a straightforward matter to elaborate the corresponding solutions ${}^{(\mathrm{G})}T_{\mu\nu}$ and ${}^{(\mathrm{es})}T_{\mu\nu}$. For the latter case, one tries the self-suggesting bilinear form

$${}^{(\mathrm{es})}T_{\mu\nu} = -\frac{\hbar c}{4\pi\alpha_\mathrm{s}}\Bigg({}^{(\mathrm{ex})}F_{\mu\nu}\cdot F_\nu{}^\lambda + F_{\mu\lambda}\cdot\,{}^{(\mathrm{ex})}F_\nu{}^\lambda - \frac{1}{2}\,g_{\mu\nu}\,{}^{(\mathrm{ex})}F_{\sigma\lambda}\cdot F^{\sigma\lambda}\Bigg) \tag{2.59}$$

and verifies that this is actually a solution of (2.58) by means of the "total" Maxwell equation (2.52), together with its "exterior" counterpart (2.34), and by use of the Bianchi identities

$$\nabla_\lambda F_{\mu\nu} + \nabla_\mu F_{\nu\lambda} + \nabla_\nu F_{\lambda\mu} \equiv 0\,, \tag{2.60a}$$

$$\nabla_\lambda\,{}^{(\mathrm{ex})}F_{\mu\nu} + \nabla_\mu\,{}^{(\mathrm{ex})}F_{\nu\lambda} + \nabla_\nu\,{}^{(\mathrm{ex})}F_{\lambda\mu} \equiv 0\ . \tag{2.60b}$$

These identities are implied by the fact that both two-forms $F_{\mu\nu}$ and ${}^{(\mathrm{ex})}F_{\mu\nu}$ are the exterior differentials of the corresponding vector potentials:

$$F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu\,, \tag{2.61a}$$

$${}^{(\mathrm{ex})}F_{\mu\nu} = \nabla_\mu\,{}^{(\mathrm{ex})}A_\nu - \nabla_\nu\,{}^{(\mathrm{ex})}A_\mu\,, \tag{2.61b}$$

where the second one (2.61b) is implied by the general curl relation (2.30) and the first one (2.61a) is nothing else than the remaining internal trace part of that link between bundle curvature $\mathcal{F}_{\mu\nu}$ and connection $\mathcal{A}_\mu$,

$$A_\mu = \frac{i}{N-1}\,\mathrm{tr}\,{}^{(\mathrm{s})}\mathcal{A}_\mu = \frac{1}{N-1}\sum_{a=1}^{N} A^a{}_\mu\ . \tag{2.62}$$

The analogous situation with the internal density ${}^{(\mathrm{G})}T_{\mu\nu}$ (2.57) is somewhat more complicated because it appears as the difference of the contributions of real and complex field modes [23]:

$${}^{(\mathrm{G})}T_{\mu\nu} = {}^{(\mathrm{R})}T_{\mu\nu} - {}^{(\mathrm{C})}T_{\mu\nu}. \tag{2.63}$$

Here the contribution ${}^{(\mathrm{R})}T_{\mu\nu}$ of the real field modes $F^a{}_{\mu\nu}$ (*electromagnetic fields*) is given by

$${}^{(\mathrm{R})}T_{\mu\nu} = \frac{1}{2}\left({}^{(\mathrm{F})}T_{\mu\nu} - \sum_{a=1}^{N}{}^{(\mathrm{a})}T_{\mu\nu}\right)\ , \tag{2.64}$$

where ${}^{(\mathrm{F})}T_{\mu\nu}$ is due to the coherent field $F_{\mu\nu}$ (2.51)

$${}^{(\mathrm{F})}T_{\mu\nu} = -\frac{\hbar c}{2\pi\alpha_\mathrm{s}}\left(F_{\mu\lambda}F_\nu{}^\lambda - \frac{1}{4}\,g_{\mu\nu}F_{\lambda\sigma}F^{\lambda\sigma}\right) \tag{2.65}$$

and the individual mode densities ${}^{(a)}T_{\mu\nu}$ are given by

$${}^{(a)}T_{\mu\nu} = -\frac{\hbar c}{2\pi\alpha_\mathrm{s}}\left(F^a{}_{\mu\lambda}F^a{}_\nu{}^\lambda - \frac{1}{4}\,g_{\mu\nu}F^a{}_{\lambda\sigma}F^{a\lambda\sigma}\right). \tag{2.66}$$

Thus the contribution ${}^{(\mathrm{R})}T_{\mu\nu}$ of the real field modes actually consists in their mutual interaction energy, with omission of the self-energies:

$${}^{(\mathrm{R})}T_{\mu\nu} = -\frac{\hbar c}{4\pi\alpha_\mathrm{s}} \cdot\sum_{a<b}^{N}\left(F^a{}_{\mu\lambda}F^b{}_\nu{}^\lambda + F^b{}_{\mu\lambda}F^a{}_\nu{}^\lambda - \frac{1}{2}\,g_{\mu\nu}F^a{}_{\sigma\lambda}F^{b\sigma\lambda}\right). \tag{2.67}$$

A similar effect occurs also with the exchange density ${}^{(\mathrm{C})}T_{\mu\nu}$ due to the complex modes whose field strengths $G^A{}_{\mu\nu}$ combine with their complex conjugate:

$${}^{(\mathrm{C})}T_{\mu\nu} = -\frac{\hbar c}{4\pi\alpha_\mathrm{s}}\sum_A\left(\overset{*}{G}{}^A{}_{\mu\lambda}G^A{}_\nu{}^\lambda + \overset{*}{G}{}^A{}_{\nu\lambda}G^A{}_\mu{}^\lambda - \frac{1}{2}\,g_{\mu\nu}\overset{*}{G}{}^A{}_{\sigma\lambda}G^{A\sigma\lambda}\right). \tag{2.68}$$

Summarizing, after the internal gauge field contribution ${}^{(\mathrm{G})}T_{\mu\nu}$ has turned out to consist of two parts ${}^{(\mathrm{R})}T_{\mu\nu}$ and ${}^{(\mathrm{C})}T_{\mu\nu}$, the total energy momentum density ${}^{(\mathrm{T})}T_{\mu\nu}$ (2.47) reads, in more detail,

$${}^{(\mathrm{T})}T_{\mu\nu} = {}^{(\mathrm{M})}T_{\mu\nu} + {}^{(\mathrm{R})}T_{\mu\nu} - {}^{(\mathrm{C})}T_{\mu\nu} + {}^{(\mathrm{es})}T_{\mu\nu}\ . \tag{2.69}$$

Correspondingly, one expects the total energy functional E_T (2.46) to be of an analogous form,

$$E_\mathrm{T} = E_\mathrm{M} + E_\mathrm{R} - E_\mathrm{C} + E_\mathrm{es}\,, \tag{2.70}$$

with the obvious definitions of the corresponding energy contributions

$$E_\mathrm{M} = \int \mathrm{d}^3\vec{r}\ {}^{(\mathrm{M})}T_{00}(\vec{r}) \tag{2.71a}$$

$$E_\mathrm{R} = \int \mathrm{d}^3\vec{r}\ {}^{(\mathrm{R})}T_{00}(\vec{r}) \tag{2.71b}$$

$$E_\mathrm{C} = \int \mathrm{d}^3\vec{r}\ {}^{(\mathrm{C})}T_{00}(\vec{r}) \tag{2.71c}$$

$$E_\mathrm{es} = \int \mathrm{d}^3\vec{r}\ {}^{(\mathrm{es})}T_{00}(\vec{r}). \tag{2.71d}$$

A certain check for the correctness of the proposed energy functional E_T (2.70) can be performed for the one-particle systems ($N = 1$), where exact solutions of the mass eigenvalue problem are available (see the discussion below).

However, in order to get a more detailed picture of the interparticle interactions which are of course missing for the one-particle systems, it is helpful to consider a higher particle number N, preferably the most simple but nontrivial one (*i.e.* $N = 2$).

3 Two-particle systems

Concerning a test of the *many-particle* functional $E_{\rm T}$ (2.70) upon some exact N-particle solution, the situation is not so favorable as with the one-particle systems. The reason for this is twofold: first, exact solutions in analytic form are not known for the relativistic many-particle systems ($N \geq 2$) and second, even if they were known, the corresponding field energy $E_{\rm T}$ would not be directly related to the mass eigenvalues, as was the case with the one-particle systems [23]. Indeed, since each of the mass eigenvalues ($M_a;\ a = 1, \dots N$) takes account of the internal interactions of the a-th particle with all the other particles $b\,(\neq a)$, the sum of the eigenvalues $\sum M_a$ would count the interparticle interactions twice! Thus, for the N-particle systems it is even more urgent to have an energy functional than for the one-particle systems, where one could be satisfied with determining the energy directly from the eigenvalue equation in form of the mass eigenvalue. However, what can be checked also for the N-particle systems is the non-relativistic limit which must agree with the well-established non-relativistic many-particle theory. In this sense, it will readily be demonstrated that the non-relativistic limit of RST just coincides with the well-known Hartree-Fock approach, so that RST in turn may be conceived as the relativistic generalization of the latter approximation method.

3.1 Selection of the generators

As mentioned in connection with the compatibility theorem (2.44)-(2.45), the generators τ_α of the original gauge group $U(\,N\,)$ must be chosen in such a way that all the diagonal elements of the compatibility tensor $\mathcal{K}$ are zero. Therefore, we choose the $N^2 = 4$ generators $\{\tau_\alpha\} = \{\tau_a, \chi, \bar{\chi}\}$ of the two-particle group $U(2)$ in the following way:

$$\tau_1 = \begin{pmatrix} 0 & 0 \\ 0 & -i \end{pmatrix}, \qquad \tau_2 = \begin{pmatrix} -i & 0 \\ 0 & 0 \end{pmatrix}, \qquad \chi = \begin{pmatrix} 0 & -i \\ 0 & 0 \end{pmatrix}, \qquad \bar{\chi} = \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}. \tag{3.1}$$

Their adjoint representatives $\{\mathfrak{C}_\alpha\} = \{\mathcal{T}_a, \mathcal{X}, \bar{\mathcal{X}}\}$ obey the same commutation relations as the original τ_α:

$$[\tau_1, \tau_2] = 0\,, \tag{3.2a}$$
$$[\tau_1, \chi] = i\chi\,, \tag{3.2b}$$
$$[\tau_2, \chi] = -i\chi\,, \tag{3.2c}$$
$$[\chi, \bar{\chi}] = -i(\,\tau_1 - \tau_2\,)\,, \tag{3.2d}$$

and therefore they can easily be written down in terms of the structure constants $C^\gamma{}_{\alpha\beta}$ (2.41) through the well-known recipe

$$(\mathfrak{C}_\alpha)^\beta{}_\gamma = C^\gamma{}_{\alpha\beta}\ . \tag{3.3}$$

But once the (4×4)-matrices $\mathfrak{C}_\alpha$ have been specified in this way, the compatibility condition (2.45) is easily seen to admit the following solution:

$$\mathcal{K} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{3.4}$$

3.2 Currents

However, with the compatibility tensor $\mathcal{K}$ being known, the relationship between the RST and the Maxwell currents (2.44) is also fixed and reads, for the present two-particle case,

$$j_{1\mu} = -\,{}'j^2_\mu\,, \tag{3.5a}$$
$$j_{2\mu} = -\,{}'j^1_\mu\,, \tag{3.5b}$$
$$j_{3\mu} \doteq h_\mu = -\,{}'j^4_\mu\,, \tag{3.5c}$$
$$j_{4\mu} \doteq -\overset{*}{h}_\mu = -\,{}'j^3_\mu\ . \tag{3.5d}$$

Consequently, the current operator ${}^{(\rm s)}\mathcal{J}_\mu$ (2.37) adopts the following form in terms of the RST currents $\{j_{a\mu}, h_\mu, \overset{*}{h}_\mu\}$:

$$\begin{aligned} {}^{(\rm s)}\mathcal{J}_\mu &= i\big\{ -j_{2\mu}\tau_1 - j_{1\mu}\tau_2 + \overset{*}{h}_\mu\chi - h_\mu\bar{\chi}\big\} \\ &\equiv i\big\{ -k_{1\mu}\tau_1 - k_{2\mu}\tau_2 + \overset{*}{h}_\mu\chi - h_\mu\bar{\chi}\big\}\,, \end{aligned} \tag{3.6}$$

where the *single-particle currents* $k_{a\mu}$ are deduced from the general definition of the RST currents $j_{a\mu}$ (2.28a) in the following way:

$$k_{1\mu} \doteq j_{2\mu} = \frac{i\hbar}{2Mc}\big\{\psi_1^*\,(D_\mu\psi_1) - \psi_1\,(D_\mu\psi_1^*)\,\big\}\,, \tag{3.7a}$$
$$k_{2\mu} \doteq j_{1\mu} = \frac{i\hbar}{2Mc}\big\{\psi_2^*\,(D_\mu\psi_2) - \psi_2\,(D_\mu\psi_2^*)\,\big\}\,. \tag{3.7b}$$

Similarly, the *exchange current* h_μ appears here as the two-particle realization of the general definition (2.28b):

$$h_\mu = \frac{i\hbar}{2Mc}\big\{\psi_1^*\,(D_\mu\psi_2) - \psi_2\,(D_\mu\psi_1^*)\,\big\}\ . \tag{3.8}$$

After the generators have been fixed, the covariant derivatives of the components ψ_a $(a = 1, 2)$ of the wave function Ψ are defined here in a self-evident manner, *i.e.* one puts

$$\mathcal{D}_\mu\Psi = \begin{pmatrix} D_\mu\psi_1 \\ D_\mu\psi_2 \end{pmatrix}\ . \tag{3.9}$$

Furthermore, when the two-particle version of the general connection ${}^{(\rm s)}\mathcal{A}_\mu$ (2.36) is decomposed with respect to the chosen basis set of generators (3.1) as

$${}^{(\rm s)}\mathcal{A}_\mu = A_{1\mu}\tau_1 + A_{2\mu}\tau_2 + B_\mu\chi - \overset{*}{B}{}_\mu\bar{\chi}\ , \tag{3.10}$$

the covariant derivatives of the single-particle wave functions (3.9) read

$$D_\mu\psi_1 = \partial_\mu\psi_1 - i\left({}^{(\rm ex)}A_\mu + A_{2\mu}\right)\psi_1 - iB_\mu\psi_2\,, \tag{3.11a}$$
$$D_\mu\psi_2 = \partial_\mu\psi_2 - i\left({}^{(\rm ex)}A_\mu + A_{1\mu}\right)\psi_2 - i\overset{*}{B}_\mu\psi_1\ . \tag{3.11b}$$

Naturally, the crucial point with the currents must refer to the charge conservation laws. Consider first the conservation law in operator form (2.38) which by the splitting of $\mathcal{J}_\mu$ (2.32) into an external and internal part also splits up into the separate conservation of those parts:

$$\mathcal{D}^{\mu\,(\mathrm{ex})}\mathcal{J}_\mu = 0 \Rightarrow \nabla^{\mu\,(\mathrm{ex})} j_\mu = 0\,, \tag{3.12a}$$

$$\mathcal{D}^{\mu\,(\mathrm{s})}\mathcal{J}_\mu = 0\ . \tag{3.12b}$$

Concerning the internal part ${}^{(\mathrm{s})}\mathcal{J}_\mu$ (3.6), one transcribes the operator equation (3.12b) to the current components and finds

$$\nabla^\mu k_{1\mu} = i\left(h^\mu B_\mu - \overset{*}{h}{}^\mu \overset{*}{B}_\mu\right)\,, \tag{3.13a}$$

$$\nabla^\mu k_{2\mu} = -i\left(h^\mu B_\mu - \overset{*}{h}{}^\mu \overset{*}{B}_\mu\right)\,, \tag{3.13b}$$

$$\nabla^\mu h_\mu - i\left[A_{1\mu} - A_{2\mu}\right] h^\mu = i\overset{*}{B}{}^\mu \left[k_{1\mu} - k_{2\mu}\right]\,, \tag{3.13c}$$

$$\nabla^\mu \overset{*}{h}{}_\mu + i\left[A_{1\mu} - A_{2\mu}\right] \overset{*}{h}{}^\mu = -iB^\mu \left[k_{1\mu} - k_{2\mu}\right]\ . \tag{3.13d}$$

These source equations own a very pleasant property, namely adding up both eqs. (3.13a) and (3.13b) yields the conservation law (2.7) with the total current j_μ of the two-particle system being defined by

$$j_\mu \doteq k_{1\mu} + k_{2\mu} = -\mathrm{tr}^{(\mathrm{s})}\mathcal{J}_\mu\ , \tag{3.14}$$

cf. (2.48). The differential law (2.7) may be converted also into global form:

$$\int\limits_{(S)} j_\mu \,\mathrm{d}S^\mu = z\ , \tag{3.15}$$

which says that the *particle number* z (here $z = 2$) is independent of the choice of the hypersurface (S) in spacetime. Observe, however, that the single conservation law (2.7) is not sufficient to fix the absolute magnitude of both wave functions $\psi_a(x)$ $(a = 1, 2)$, so that one has to look for further conservation laws of the kind (2.7); see the discussion below in connection with the Maxwell equations.

3.3 Bound states

For the stationary (bound) states, one tries the ansatz:

$$\psi_a(\vec{r},t) = \exp\left[-i\frac{M_a c^2}{\hbar}t\right]\cdot\psi_a(\vec{r})\,, \tag{3.16a}$$

$${}^{(\mathrm{ex})}A_\mu(\vec{r},t) = A_{\mathrm{ex}}(\vec{r})\,\hat{t}_\mu\,, \tag{3.16b}$$

$$A^a{}_\mu(\vec{r},t) = A_a(\vec{r})\,\hat{t}_\mu\,, \tag{3.16c}$$

$$B_\mu(\vec{r},t) = \exp\left[-i\frac{M_1 - M_2}{\hbar}c^2 t\right]\cdot B(\vec{r})\,\hat{t}_\mu\ , \tag{3.16d}$$

with the unit vector $\hat{t}_\mu$ $(= \partial_\mu t)$ pointing into the time direction $(\hat{t}^\mu\hat{t}_\mu = 1)$. Indeed with such an ansatz one finds the current densities to be actually of the required stationary form:

$$k_{a\mu} = k_a(\vec{r})\,\hat{t}_\mu\,, \tag{3.17a}$$

$$h_\mu(\vec{r},t) = \exp\left[i\frac{M_1 - M_2}{\hbar}c^2 t\right]\cdot h(\vec{r})\,\hat{t}_\mu\ , \tag{3.17b}$$

provided one neglects the magnetic interactions between the particles (which would require non-zero spatial components of the vector potentials and current densities). For the subsequent discussion of the stationary states, we restrict ourselves to this *electrostatic approximation* where we need to take into account exclusively the *electrostatic charge densities* $k_a(\vec{r})$:

$$\begin{aligned} k_1(\vec{r}) =& \frac{\hbar}{Mc}\left\{\frac{M_1 c}{\hbar} + A_{\mathrm{ex}}(\vec{r}) + A_2(\vec{r})\right\}\overset{*}{\psi}_1(\vec{r})\psi_1(\vec{r}) \\ &+ \frac{\hbar}{2Mc}\left\{B(\vec{r})\overset{*}{\psi}_1(\vec{r})\psi_2(\vec{r}) + \overset{*}{B}(\vec{r})\overset{*}{\psi}_2(\vec{r})\psi_1(\vec{r})\right\}\,, \end{aligned} \tag{3.18a}$$

$$\begin{aligned} k_2(\vec{r}) =& \frac{\hbar}{Mc}\left\{\frac{M_2 c}{\hbar} + A_{\mathrm{ex}}(\vec{r}) + A_1(\vec{r})\right\}\overset{*}{\psi}_2(\vec{r})\psi_2(\vec{r}) \\ &+ \frac{\hbar}{2Mc}\left\{\overset{*}{B}(\vec{r})\overset{*}{\psi}_2(\vec{r})\psi_1(\vec{r}) + B(\vec{r})\overset{*}{\psi}_1(\vec{r})\psi_2(\vec{r})\right\}, \end{aligned} \tag{3.18b}$$

and the *exchange density* $h(\vec{r})$:

$$\begin{aligned} h(\vec{r}) =& \left\{\frac{M_1 + M_2}{2M} + \frac{\hbar}{2M}\Big[2A_{\mathrm{ex}}(\vec{r}) + A_1(\vec{r}) + A_2(\vec{r})\Big]\right\} \\ &\cdot\overset{*}{\psi}_1(\vec{r})\psi_2(\vec{r}) + \frac{\hbar}{2Mc}\overset{*}{B}(\vec{r}) \\ &\cdot\Big[\overset{*}{\psi}_1(\vec{r})\psi_1(\vec{r}) + \overset{*}{\psi}_2(\vec{r})\psi_2(\vec{r})\Big]. \end{aligned} \tag{3.19}$$

For the non-relativistic limit, to be discussed below, one neglects all the potentials and approximates the *mass eigenvalues* M_a $(a = 1, 2)$ simply by the rest mass M of the particles which then yields for the densities

$$k_1(\vec{r}) \Rightarrow \overset{*}{\psi}_1(\vec{r})\psi_1(\vec{r})\,, \tag{3.20a}$$

$$k_2(\vec{r}) \Rightarrow \overset{*}{\psi}_2(\vec{r})\psi_2(\vec{r})\,, \tag{3.20b}$$

$$h(\vec{r}) \Rightarrow \overset{*}{\psi}_1(\vec{r})\psi_2(\vec{r})\ . \tag{3.20c}$$

In this limit, one usually imposes the following orthonormality conditions upon the non-relativistic wave functions:

$$\int \mathrm{d}^3\vec{r}\,\overset{*}{\psi}_1(\vec{r})\psi_1(\vec{r}) = \int \mathrm{d}^3\vec{r}\,\overset{*}{\psi}_2(\vec{r})\psi_2(\vec{r}) = 1\,, \tag{3.21a}$$

$$\int \mathrm{d}^3\vec{r}\,\overset{*}{\psi}_1(\vec{r})\psi_2(\vec{r}) = 0\ . \tag{3.21b}$$

This suggests that one has for the fully relativistic case the analogous conditions

$$\int \mathrm{d}^3\vec{r}\, k_1(\vec{r}) = \int \mathrm{d}^3\vec{r}\, k_2(\vec{r}) = 1\,, \tag{3.22a}$$

$$\int \mathrm{d}^3\vec{r}\, h(\vec{r}) = 0\,. \tag{3.22b}$$

Indeed this suggestion can readily be verified now by a closer inspection of the gauge field dynamics.

3.4 Maxwell equations

Quite similarly as for the two-particle objects ${}^{(\mathrm{s})}\mathcal{J}_\mu$ (3.6) and ${}^{(\mathrm{s})}\mathcal{A}_\mu$ (3.10), one puts for the two-particle field strength ${}^{(\mathrm{s})}\mathcal{F}_{\mu\nu}$ (2.19)

$${}^{(\mathrm{s})}\mathcal{F}_{\mu\nu} = F_{1\mu\nu}\tau_1 + F_{2\mu\nu}\tau_2 + G_{\mu\nu}\chi - \overset{*}{G}{}_{\mu\nu}\bar{\chi}, \tag{3.23}$$

where the curvature components are found to read, in terms of the potentials, as follows:

$$F_{1\mu\nu} = \nabla_\mu A_{1\nu} - \nabla_\nu A_{1\mu} - i\Big[\overset{*}{B}{}_\mu B_\nu - \overset{*}{B}{}_\nu B_\mu\Big]\,, \tag{3.24a}$$

$$F_{2\mu\nu} = \nabla_\mu A_{2\nu} - \nabla_\nu A_{2\mu} + i\Big[\overset{*}{B}{}_\mu B_\nu - \overset{*}{B}{}_\nu B_\mu\Big]\,, \tag{3.24b}$$

$$G_{\mu\nu} = \nabla_\mu B_\nu - \nabla_\nu B_\mu + i\,(A_{1\mu} - A_{2\mu})\,B_\nu - i\,(A_{1\nu} - A_{2\nu})\,B_\mu\,, \tag{3.24c}$$

$$\overset{*}{G}{}_{\mu\nu} = \nabla_\mu \overset{*}{B}{}_\nu - \nabla_\nu \overset{*}{B}{}_\mu - i\,(A_{1\mu} - A_{2\mu})\,\overset{*}{B}{}_\nu + i\,(A_{1\nu} - A_{2\nu})\,\overset{*}{B}{}_\mu. \tag{3.24d}$$

With this decomposition, the abstract Maxwell equations (2.35) read, in component form,

$$\nabla^\mu F_{1\mu\nu} - i\left[\overset{*}{B}{}^\mu G_{\mu\nu} - B^\mu \overset{*}{G}{}_{\mu\nu}\right] = -4\pi\alpha_s k_{1\nu}\,, \tag{3.25a}$$

$$\nabla^\mu F_{2\mu\nu} + i\left[\overset{*}{B}{}^\mu G_{\mu\nu} - B^\mu \overset{*}{G}{}_{\mu\nu}\right] = -4\pi\alpha_s k_{2\nu}\,, \tag{3.25b}$$

$$\nabla^\mu G_{\mu\nu} + i\,(A_1^\mu - A_2^\mu)\,G_{\mu\nu} - iB^\mu\,[F_{1\mu\nu} - F_{2\mu\nu}] = 4\pi\alpha_s \overset{*}{h}_\nu\,, \tag{3.25c}$$

$$\nabla^\mu \overset{*}{G}{}_{\mu\nu} - i\,(A_1^\mu - A_2^\mu)\,\overset{*}{G}{}_{\mu\nu} + i\overset{*}{B}{}^\mu\,[F_{1\mu\nu} - F_{2\mu\nu}] = 4\pi\alpha_s h_\nu\,. \tag{3.25d}$$

This gauge field dynamics has some very pleasant properties to be discussed now in more detail.

First, add up both eqs. (3.24a) and (3.24b) in order to see that the total field strength $F_{\mu\nu}$ (2.51),

$$F_{\mu\nu} = F_{1\mu\nu} + F_{2\mu\nu} = i\,\mathrm{tr}\;{}^{(\mathrm{s})}\mathcal{F}_{\mu\nu}\,, \tag{3.26}$$

is actually generated by the total potential A_μ (2.62):

$$A_\mu = A_{1\mu} + A_{2\mu} = i\,\mathrm{tr}\;{}^{(\mathrm{s})}\mathcal{A}_\mu\,, \tag{3.27}$$

according to the curl relation (2.61a) and therefore it obeys the Bianchi identity (2.60a). Furthermore, adding up both Maxwell equations (3.25a) and (3.25b) says that the total field $F_{\mu\nu}$ (3.26) is actually generated by the total current j_μ (3.14) in agreement with the former Maxwell equation (2.52). Obviously, these total objects $F_{\mu\nu}$ and j_μ describe the overall properties of the two-particle system when its internal structure is neglected. For this reason, the present two-particle equations (2.52), (2.60a) and (2.61a) are formally the same as for the one-particle systems [25]. This circumstance is then transferred also to the force densities ${}^{(\mathrm{ex})}f_\nu$ (2.26) and ${}^{(\mathrm{xe})}f_\nu$ (2.54) which thus look identical for all particle numbers N. This may be interpreted in the sense that the handle of the two-particle system for being acted upon by the external-field strength ${}^{(\mathrm{ex})}F_{\mu\nu}$ is just its total current j_μ (3.14); and conversely the two-particle system acts back upon the external source via its total field strength $F_{\mu\nu}$ (3.26) entering the force density ${}^{(\mathrm{xe})}f_\nu$ (2.54). Naturally, the energy momentum content due to this interactive system is described by the two-particle tensor ${}^{(\mathrm{es})}T_{\mu\nu}$ (2.59) which thus looks identical for all particle numbers N.

Next, consider the problem of fixing the "absolute magnitude" of the wave functions $\psi_a(x)$, $(a = 1, 2)$, *i.e.* the problem of the normalization conditions. In the relativistic context, one would like to have two four-vector fields $l_{a\mu}$ ($a = 1, 2$), as functionals of the wave functions ψ_a, obeying the conservation laws

$$\nabla^\mu l_{a\mu} = 0\,. \tag{3.28}$$

Indeed, this then would allow us to impose the normalization conditions ($a = 1, 2$)

$$\int\limits_{(S)} l_{a\mu}\,\mathrm{d}S^\mu = 1\,, \tag{3.29}$$

independently of the chosen hypersurface (S). However, such vector fields $l_{a\mu}$ are actually obtainable, namely by means of the observation that the right-hand sides of the source equations (3.13a) and (3.13b) can be recast into the form of a divergence of some vector field G_μ:

$$\overset{*}{h}{}^\mu \overset{*}{B}{}_\mu - h^\mu B_\mu = -i\nabla^\mu G_\mu\,. \tag{3.30}$$

The solution of this equation for G_μ is

$$G_\mu = \frac{i}{4\pi\alpha_s}\left(\overset{*}{B}{}^\nu G_{\mu\nu} - B^\nu \overset{*}{G}{}_{\mu\nu}\right), \tag{3.31}$$

which can easily be verified by straightforward differentiation and use of eqs. (3.24c)-(3.24d) and (3.25c)-(3.25d). Consequently, the substitution of the result (3.30) into the source equations (3.13a)-(3.13b) yields just the two desired conservation laws, necessary for the normalization of the wave functions via (3.29), namely:

$$\nabla^\mu l_{1\mu} \equiv \nabla^\mu\,(k_{1\mu} + G_\mu) = 0\,, \tag{3.32a}$$

$$\nabla^\mu l_{2\mu} \equiv \nabla^\mu\,(k_{2\mu} - G_\mu) = 0\,. \tag{3.32b}$$

For the stationary states, one will resort again to the electrostatic approximation (3.16b)-(3.16d) which implies the vanishing of the time component of the "entanglement vector" G_μ (3.31). Therefore, the general normalization conditions (3.29) degenerate into their static form (3.22a) which thus receives its legitimation. Moreover, the relativistic orthogonality condition (3.22b) can also be validated for the electrostatic approach. In order to demonstrate this, observe that the Maxwell equations (3.25a)-(3.25d) for the curvature components $F_{a\mu\nu}$, $G_{\mu\nu}$ transcribe to the static potentials $A_a(\vec{r})$, $B(\vec{r})$ (3.16c)-(3.16d) in form of the Poisson equations:

$$\Delta A_a(\vec{r}) = 4\pi\alpha_s k_a(\vec{r})\,, \tag{3.33a}$$

$$\Delta B(\vec{r}) = -4\pi\alpha_s \overset{*}{h}(\vec{r})\,, \tag{3.33b}$$

with the corresponding solutions:

$$A_a(\vec{r}) = -\alpha_s \int \mathrm{d}^3\vec{r}\,' \, \frac{k_a(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,, \tag{3.34a}$$

$$B(\vec{r}) = \quad \alpha_s \int \mathrm{d}^3\vec{r}\,' \, \frac{\overset{*}{h}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}. \tag{3.34b}$$

On the other hand, the stationary form of the source eq. (3.13c) for the exchange current h_μ reads:

$$\frac{M_1-M_2}{\hbar}\, c\cdot h(\vec{r}) = \Big[A_1(\vec{r}) - A_2(\vec{r})\Big] h(\vec{r}) + \overset{*}{B}(\vec{r})\Big[k_1(\vec{r}) - k_2(\vec{r})\Big]\,. \tag{3.35}$$

Now, integrating this equation over the whole three-space with use of the potentials $A_a(\vec{r})$ (3.34a) and $B(\vec{r})$ (3.34b) directly leads to the relativistic orthogonality claim (3.22b) which thus receives its rigorous proof.

3.5 Hartree-Fock equations

With the stationary form of the gauge field configurations being at hand now, it is a rather straightforward matter to deduce the well-known Hartree-Fock equations from the Klein-Gordon equation (2.6). This equation reads, for the present two-particle systems in component form ($a = 1, 2$),

$$D^\mu D_\mu \psi_a + \left(\frac{Mc}{\hbar}\right)^2 \psi_a = 0\,, \tag{3.36}$$

with the covariant derivatives of the wave functions ψ_a being specified by the former equations (3.11a)-(3.11b). For the stationary field configurations (3.16a)-(3.16d), the KGEs (3.36) adopt the following form:

$$\frac{-\hbar^2}{2M}\Delta\psi_1(\vec{r}) + V_{11}\cdot\psi_1(\vec{r}) + V_{12}\cdot\psi_2(\vec{r}) = \frac{M_1^2-M^2}{2M}c^2\cdot\psi_1(\vec{r})\,, \tag{3.37a}$$

$$\frac{-\hbar^2}{2M}\Delta\psi_2(\vec{r}) + V_{21}\cdot\psi_1(\vec{r}) + V_{22}\cdot\psi_2(\vec{r}) = \frac{M_2^2-M^2}{2M}c^2\cdot\psi_2(\vec{r})\,. \tag{3.37b}$$

Here the Hermitian potential matrix $V_{ab}(=V_{ba}^*)$ is given in terms of the static gauge potentials $A_a(\vec{r})$ and $B(\vec{r})$ through

$$V_{11}(\vec{r}) = -\frac{\hbar^2}{2M}\left[\left(\frac{M_1 c}{\hbar} + A_{\mathrm{ex}}(\vec{r}) + A_2(\vec{r})\right)^2 - \left(\frac{M_1 c}{\hbar}\right)^2 + \overset{*}{B}(\vec{r})B(\vec{r})\right], \tag{3.38a}$$

$$V_{12}(\vec{r}) = -\frac{\hbar^2}{2M}B(\vec{r})\left[\frac{M_1+M_2}{\hbar}c + 2A_{\mathrm{ex}}(\vec{r}) + A_1(\vec{r}) + A_2(\vec{r})\right], \tag{3.38b}$$

$$V_{21}(\vec{r}) = -\frac{\hbar^2}{2M}\overset{*}{B}(\vec{r})\left[\frac{M_1+M_2}{\hbar}c + 2A_{\mathrm{ex}}(\vec{r}) + A_1(\vec{r}) + A_2(\vec{r})\right], \tag{3.38c}$$

$$V_{22}(\vec{r}) = -\frac{\hbar^2}{2M}\left[\left(\frac{M_2 c}{\hbar} + A_{\mathrm{ex}}(\vec{r}) + A_1(\vec{r})\right)^2 - \left(\frac{M_2 c}{\hbar}\right)^2 + \overset{*}{B}(\vec{r})B(\vec{r})\right]. \tag{3.38d}$$

The non-linearly coupled Klein-Gordon system (3.37a)-(3.37b) represents the relativistic eigenvalue problem which is to be solved for the mass eigenvalues M_a ($a = 1, 2$) and thus is to be considered as the most immediate two-particle generalization of the one-particle case [25]. In contrast to the one-particle situation, the present two-particle system is highly non-linear, cf. the RST potentials $A_a(\vec{r})$ and $B(\vec{r})$ (3.34a)-(3.34b), and therefore one must impose the normalization conditions (3.22a) in order to make the solutions unique.

The Hartree-Fock equations, as the non-relativistic limit of the RST system (3.37a)-(3.37b), do emerge now quite similarly as the one-particle Schrödinger equation arises from the stationary Klein-Gordon equation [2]: namely by neglecting all squares of potentials A_{ex}, A_a, B for the potential matrix V_{ab} (3.38a)-(3.38d) and furthermore by replacing the mass eigenvalues M_a by the rest mass M of the particles which yields then ultimately

$$V_{11} \Rightarrow -\hbar c A_{\mathrm{ex}}(\vec{r}) + e^2 \int \mathrm{d}^3\vec{r}\,' \, \frac{|\psi_2(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\,, \tag{3.39a}$$

$$V_{12} \Rightarrow -e^2 \int \mathrm{d}^3\vec{r}\,' \, \frac{\overset{*}{\psi}_2(\vec{r}\,')\psi_1(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,, \tag{3.39b}$$

$$V_{21} \Rightarrow -e^2 \int \mathrm{d}^3\vec{r}\,' \, \frac{\overset{*}{\psi}_1(\vec{r}\,')\psi_2(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,, \tag{3.39c}$$

$$V_{22} \Rightarrow -\hbar c A_{\mathrm{ex}}(\vec{r}) + e^2 \int \mathrm{d}^3\vec{r}\,' \, \frac{|\psi_1(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\,. \tag{3.39d}$$

Here we have retained only the terms linear in the potentials A_a, B (3.34a)-(3.34b) and simultaneously we have

replaced the relativistic densities $k_a(\vec{r})$ by their non-relativistic limits (3.20a)-(3.20c). When we now introduce the non-relativistic energy eigenvalues E_a in the same way as for the one-particle systems [24], *i.e.* when we approximate the right-hand sides of the relativistic eigenvalue equations (3.37a)-(3.37b) by

$$\frac{M_a^2 - M^2}{2M} \Rightarrow E_a \,, \tag{3.40}$$

then the relativistic system reappears in the form of the well-known Hartree-Fock equations:

$$\begin{aligned} &-\frac{\hbar^2}{2M}\Delta\psi_1(\vec{r}) - \hbar c A_{\rm ex}(\vec{r})\cdot\psi_1(\vec{r}) \\ &+e^2\int \mathrm{d}^3\vec{r}\,'\frac{|\psi_2(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\cdot\psi_1(\vec{r}) \\ &-e^2\int \mathrm{d}^3\vec{r}\,'\frac{\overset{*}{\psi}_2(\vec{r}\,')\psi_1(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\cdot\psi_2(\vec{r}) = E_1\psi_1(\vec{r})\,, \end{aligned} \tag{3.41a}$$

$$\begin{aligned} &-\frac{\hbar^2}{2M}\Delta\psi_2(\vec{r}) - \hbar c A_{\rm ex}(\vec{r})\cdot\psi_2(\vec{r}) \\ &+e^2\int \mathrm{d}^3\vec{r}\,'\frac{|\psi_1(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\cdot\psi_2(\vec{r}) \\ &-e^2\int \mathrm{d}^3\vec{r}\,'\frac{\overset{*}{\psi}_1(\vec{r}\,')\psi_2(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\cdot\psi_1(\vec{r}) = E_2\psi_2(\vec{r})\,. \end{aligned} \tag{3.41b}$$

Clearly, for solving the latter non-relativistic system (3.41a)-(3.41b), one will apply the *non-relativistic* orthonormalization conditions (3.21a)-(3.21b), whereas the solution of the fully relativistic system (3.37a)-(3.37b) requires application of the *relativistic* orthonormalization conditions (3.22a)-(3.22b)!

3.6 Energy functional

The scientific value of a theory is always measured by the truth of its experimental predictions, and thus one has to inspect now the energy levels $E_{\rm T}$ (2.70) predicted by the present two-particle theory. Since this total energy $E_{\rm T}$ consists of four contributions, we will consider now each part separately.

First, let us turn to the matter part $E_{\rm M}$ which is present already for the one-particle systems, but whose energy density ${}^{(\rm M)}T_{00}(\vec{r})$ must now be deduced from the general tensor ${}^{(\rm M)}T_{\mu\nu}$ (2.14):

$${}^{(\rm M)}T_{00} = \frac{\hbar^2}{2M}\Bigg\{(\mathcal{D}_0\bar{\Psi})(\mathcal{D}_0\Psi) + \sum_{j=1}^{3}(\mathcal{D}_j\bar{\Psi})(\mathcal{D}_j\Psi) + \left(\frac{Mc}{\hbar}\right)^2\bar{\Psi}\Psi\Bigg\}. \tag{3.42}$$

For the stationary configurations (3.16a)- (3.16d), one can easily verify that the covariant time derivatives obey the relation

$$(\mathcal{D}_0\bar{\Psi})(\mathcal{D}_0\Psi) = -\bar{\Psi}(\mathcal{D}_0\mathcal{D}_0\Psi)\,, \tag{3.43}$$

and this provides us with the possibility to eliminate the time derivatives completely from the matter energy $E_{\rm M}$ (2.71a); namely by multiplying through the Klein-Gordon equation (2.6)

$$\mathcal{D}_0\mathcal{D}_0\Psi - \Delta\Psi + \left(\frac{Mc}{\hbar}\right)^2\Psi = 0 \tag{3.44}$$

with the Hermitian conjugate $\bar{\Psi}$ and by subsequent partial integration which ultimately yields

$$E_{\rm M} = Mc^2\int \mathrm{d}^3\vec{r}\,\bar{\Psi}\Psi + 2\frac{\hbar^2}{2M}\int \mathrm{d}^3\vec{r}\,\vec{\nabla}\bar{\Psi}\cdot\vec{\nabla}\Psi\,. \tag{3.45}$$

Obviously, this two-particle matter energy $E_{\rm M}$ is the sum of the two single-particle contributions $E_{\rm M}(a)$:

$$E_{\rm M} = \sum_{a=1}^{2} E_{\rm M}(a)\,, \tag{3.46a}$$

$$\begin{aligned} E_{\rm M}(a) = {}& Mc^2\int \mathrm{d}^3\vec{r}\,\overset{*}{\psi}_a(\vec{r})\psi_a(\vec{r}) \\ &+2\frac{\hbar^2}{2M}\int \mathrm{d}^3\vec{r}\,\vec{\nabla}\overset{*}{\psi}_a(\vec{r})\cdot\vec{\nabla}\psi_a(\vec{r})\,. \end{aligned} \tag{3.46b}$$

Comparing this result to the corresponding one-particle case [25], one realizes that there emerges again the same "pseudo-problem" of an additional factor of two in front of the kinetic energies $\langle T_a\rangle$:

$$E_{\rm M}(a) = Mc^2\cdot Z_a^2 + 2\langle T_a\rangle\,, \tag{3.47}$$

where some self-evident definitions have been used:

$$Z_a^2 \doteq \int \mathrm{d}^3\vec{r}\,\overset{*}{\psi}_a(\vec{r})\psi_a(\vec{r})\,, \tag{3.48a}$$

$$\langle T_a\rangle \doteq \frac{\hbar^2}{2M}\int \mathrm{d}^3\vec{r}\,\vec{\nabla}\overset{*}{\psi}_a(\vec{r})\cdot\vec{\nabla}\psi_a(\vec{r})\,. \tag{3.48b}$$

However, it should be a matter of course that this "problem" for the two-particle systems is resolved in the same way as for the one-particle systems, see ref. [25]. Indeed, if the correct relativistic normalization conditions (3.22a) are applied, the higher-order approximations for the *renormalization constants* Z_a (3.48a) read, in analogy to the one-particle case,

$$Z_a^2 \simeq 1 - \frac{\langle T_a\rangle}{Mc^2}\quad,\quad a = 1,2 \tag{3.49}$$

and this yields again the correct non-relativistic limit of the matter energies $E_{\rm M}(a)$ (3.47):

$$E_{\rm M}(a) \Rightarrow Mc^2\left(1 - \frac{\langle T_a\rangle}{Mc^2}\right) + 2\langle T_a\rangle = Mc^2 + \langle T_a\rangle. \tag{3.50}$$

Thus, one obtains the relativistic matter energy $E_{\rm M}$ by substituting the solutions ψ_a of the RST system (3.37a)-(3.37b) into the relativistic energy functional $E_{\rm M}$ (3.46a)-(3.46b); but when one is satisfied with the non-relativistic approximation, one takes the values of the non-relativistic

functionals (3.50) upon the solutions of the Hartree-Fock equations (3.41a)-(3.41b).

Next, consider the contribution $E_{\rm es}$ (2.71d) to the total energy $E_{\rm T}$ (2.70) which is due to the interaction of the two-particle system with the external source ${}^{(\rm ex)}j_\mu$ and which therefore is also present already for the one-particle systems. Transferring this kind of energy content $E_{\rm es}$ to the two-particle systems, one has to deduce the corresponding energy density ${}^{(\rm es)}T_{00}(\vec{r})$ from the energy momentum tensor ${}^{(\rm es)}T_{\mu\nu}$ (2.59) which however looks formally identical to its one-particle analogue because it is built up exclusively by the overall objects $F_{\mu\nu}$ and ${}^{(\rm ex)}F_{\mu\nu}$. The difference of both cases is simply that the system's total field $F_{\mu\nu}$ (2.51) is generated by only one particle in the first case according to the Maxwell equation (2.52), whereas for the second case it is the sum of two single-particle contributions ${F^a}_{\mu\nu}$ (3.26), which, according to the Maxwell equation (2.52), has as its source just the sum j_μ (3.14) of the two single-particle currents $k_{a\mu}$. Therefore, the one-particle result for $E_{\rm es}$ can be immediately transcribed to the two-particle situation and thus looks as follows:

$$\begin{aligned} E_{\rm es} &= -\hbar c \int {\rm d}^3\vec{r}\, A_{\rm ex}(\vec{r})\,\{k_1(\vec{r}) + k_2(\vec{r})\} \qquad (3.51)\\ &\equiv E_{\rm es}(1) + E_{\rm es}(2)\ . \end{aligned}$$

This external energy functional $E_{\rm es}$ applies again to the solutions of the RST system (3.37a)-(3.37b); but when one is satisfied with the non-relativistic case of the Hartree-Fock equations (3.41a)-(3.41b), one can resort to the non-relativistic limit of the charge densities $k_a(\vec{r})$ (3.20a)-(3.20b) and thus one obtains the non-relativistic limit of the external interaction energy $E_{\rm es}$ (3.51) as

$$E_{\rm es} \Rightarrow -\hbar c \int {\rm d}^3\vec{r}\, A_{\rm ex}(\vec{r})\,\left\{|\psi_1(\vec{r})|^2 + |\psi_2(\vec{r})|^2\right\}. \quad (3.52)$$

For instance, for the binding Coulomb potential

$$A_{\rm ex}(\vec{r}) \Rightarrow z_{\rm ex}\frac{\alpha_{\rm s}}{r}\ , \qquad (3.53)$$

one obtains the sum of its expectation values relative to both quantum states ψ_1 and ψ_2:

$$E_{\rm es} \Rightarrow -z_{\rm ex}e^2 \int {\rm d}^3\vec{r}\,\frac{|\psi_1(\vec{r})|^2 + |\psi_2(\vec{r})|^2}{r}\ . \qquad (3.54)$$

Finally, the internal gauge field energy $E_{\rm G}$, due to ${}^{(G)}T_{\mu\nu}$ (2.63), must be considered. Since this kind of energy describes the internal interactions of the system's particles, it has no analogue for the one-particle systems. The reason is that in RST the self-interactions of the particles are avoided and therefore there must be present at least two particles in order that a non-trivial energy contribution can arise. The energy $E_{\rm G}$ itself consists of two parts:

$$E_{\rm G} = E_{\rm R} - E_{\rm C} \qquad (3.55)$$

with the energy content $E_{\rm R}$ of the real gauge field modes being given by eq. (2.71b) and that of the complex modes $E_{\rm C}$ by (2.71c). First, consider the real modes whose energy density ${}^{(\rm R)}T_{00}(\vec{r})$ is to be deduced from the general tensor ${}^{(\rm R)}T_{\mu\nu}(\vec{r})$ (2.67) which yields, in the electrostatic approximation,

$${}^{(\rm R)}T_{00} = -\frac{\hbar c}{4\pi\alpha_{\rm s}}F_{10\lambda}F_{20}{}^{\lambda}\ . \qquad (3.56)$$

Now, remember here the link of the electromagnetic field strengths $F_{a\mu\nu}$ to the potentials $A_{a\mu}$ (3.24a)-(3.24b) which, under neglection of the magnetic forces, simplifies to

$$F_{a0j} = -\partial_j A_a(\vec{r})\ , \qquad (3.57)$$

so that the energy density ${}^{(\rm R)}T_{00}$ (3.56) reads, in terms of the electrostatic potentials $A_a(\vec{r})$,

$${}^{(\rm R)}T_{00} = \frac{\hbar c}{4\pi\alpha_{\rm s}}\vec{\nabla}A_1(\vec{r})\cdot\vec{\nabla}A_2(\vec{r})\ . \qquad (3.58)$$

Consequently, the energy $E_{\rm R}$ (2.71b) located in the real modes of the internal gauge field becomes, by partial integration and use of the Poisson equations (3.33a),

$$E_{\rm R} = -\hbar c \int {\rm d}^3\vec{r}\, A_1(\vec{r})\cdot k_2(\vec{r})\ , \qquad (3.59)$$

or, when the solutions (3.34a) for the static potentials $A_a(\vec{r})$ are inserted,

$$E_{\rm R} = e^2 \iint {\rm d}^3\vec{r}\,{\rm d}^3\vec{r}\,'\,\frac{k_1(\vec{r})\cdot k_2(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\ . \qquad (3.60)$$

This energy functional refers again to the solutions of the RST system (3.37a)-(3.37b), but when one is satisfied with the Hartree-Fock equations (3.41a)-(3.41b), one can resort again to the non-relativistic limit (3.20a)-(3.20b) of the charge densities $k_a(\vec{r})$ and then one writes down the corresponding non-relativistic form of the energy functional $E_{\rm R}$ (3.60) as

$$E_{\rm R} \Rightarrow e^2 \iint {\rm d}^3\vec{r}\,{\rm d}^3\vec{r}\,'\,\frac{|\psi_1(\vec{r})|^2\cdot|\psi_2(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\ . \qquad (3.61)$$

Evidently, this is just the classical electrostatic interaction energy of the charge clouds generated by the two wave functions $\psi_1(\vec{r})$ and $\psi_2(\vec{r})$ and thus meets with our intuitive non-relativistic expectations.

Finally, consider the energy content $E_{\rm C}$ (2.71c) of the complex field modes and observe that this kind of energy owns the status of an *exchange energy* and thus is a truly non-classical phenomenon. Restricting ourselves again to the electrostatic approximation, the corresponding energy density ${}^{(\rm C)}T_{00}(\vec{r})$ is deduced from the general tensor ${}^{(\rm C)}T_{\mu\nu}$ (2.68) as

$${}^{(\rm C)}T_{00}(\vec{r}) = \frac{\hbar c}{4\pi\alpha_s}\sum_{j=1}^{3}\overset{*}{G}_{0j}G_{0j}\ . \qquad (3.62)$$

Here, the exchange field strengths G_{0j} can be expressed in terms of the exchange potential $B(\vec{r})$ via the general definition (3.24c) as

$$G_{0j} = -\exp\left(-i\frac{M_1 - M_2}{\hbar}c^2 t\right)\cdot\partial_j B(\vec{r})\,, \tag{3.63}$$

which simplifies again the energy density ${}^{(\mathrm{C})}T_{00}$ (3.62) into

$${}^{(\mathrm{C})}T_{00}(\vec{r}) = \frac{\hbar c}{4\pi\alpha_{\mathrm{s}}}\vec{\nabla}\overset{*}{B}(\vec{r})\cdot\vec{\nabla}B(\vec{r})\,. \tag{3.64}$$

Thus, the desired exchange energy E_{C} (2.71c) becomes, by means of partial integration and use of the Poisson equation (3.34b),

$$E_{\mathrm{C}} = \hbar c\int \mathrm{d}^3\vec{r}\,\overset{*}{B}(\vec{r})h^*(\vec{r}) = e^2\iint \mathrm{d}^3\vec{r}\,d^3\vec{r}\,'\frac{h^*(\vec{r})h(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,. \tag{3.65}$$

Observing here the non-relativistic limit (3.20c) of the exchange density $h(\vec{r})$ lets us arrive at the Hartree-Fock approximation of the exchange energy E_{C}:

$$E_{\mathrm{C}} \Rightarrow e^2\iint \mathrm{d}^3\vec{r}\,\mathrm{d}^3\vec{r}\,'\frac{\overset{*}{\psi}_2(\vec{r})\psi_1(\vec{r})\overset{*}{\psi}_1(\vec{r}\,')\psi_2(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,. \tag{3.66}$$

Since this exchange energy enters the internal gauge field energy E_{G} (3.55) with a minus sign, we ultimately arrive at its non-relativistic limit:

$$E_{\mathrm{G}} \Rightarrow e^2\iint \mathrm{d}^3\vec{r}\mathrm{d}^3\vec{r}\,' \times\frac{\overset{*}{\psi}_1(\vec{r})\psi_1(\vec{r})\overset{*}{\psi}_2(\vec{r}\,')\psi_2(\vec{r}\,') - \psi_1(\vec{r})\overset{*}{\psi}_1(\vec{r}\,')\psi_2(\vec{r}\,')\overset{*}{\psi}_2(\vec{r})}{|\vec{r}-\vec{r}\,'|}, \tag{3.67}$$

which is a well-known result of first-order perturbation theory for the interelectronic interactions in a helium atom.

Collecting the results, one finds the RST energy functional E_{T} to be of the following form:

$$\begin{aligned}E_{\mathrm{T}} = E_{\mathrm{M}} + E_{\mathrm{R}} - E_{\mathrm{C}} + E_{\mathrm{es}} = \\ Mc^2\sum_{a=1}^{2}Z_a^2 + 2\frac{\hbar^2}{2M}\sum_{a=1}^{2}\int \mathrm{d}^3\vec{r}\,\vec{\nabla}\overset{*}{\psi}_a(\vec{r})\cdot\vec{\nabla}\psi_a(\vec{r}) \\ +e^2\iint \mathrm{d}^3\vec{r}\mathrm{d}^3\vec{r}\,'\,\frac{k_1(\vec{r})\cdot k_2(\vec{r}\,') - \overset{*}{h}(\vec{r})\cdot h(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} \\ -\hbar c\int \mathrm{d}^3\vec{r}\,A_{\mathrm{ex}}(\vec{r})\big(k_1(\vec{r})+k_2(\vec{r})\big)\,.\end{aligned} \tag{3.68}$$

This energy functional is due to the RST eigenvalue system (3.37a)-(3.37b); however, when one is satisfied with the (non-relativistic) Hartree-Fock equations (3.41a)-(3.41b) one must resort to the corresponding Hartree-Fock functional E_{HF} as the non-relativistic limit of the RST functional E_{T} (3.68):

$$\begin{aligned}E_{\mathrm{T}} \Rightarrow E_{\mathrm{HF}} = 2Mc^2 + \frac{\hbar^2}{2M}\sum_{a=1}^{2}\int \mathrm{d}^3\vec{r}\,\vec{\nabla}\overset{*}{\psi}_a(\vec{r})\cdot\psi_a(\vec{r}) \\ +e^2\iint \mathrm{d}^3\vec{r}\,\mathrm{d}^3\vec{r}\,' \\ \times\frac{|\psi_1(\vec{r})|^2\cdot|\psi_2(\vec{r}\,')|^2 - \overset{*}{\psi}_2(\vec{r})\psi_1(\vec{r})\overset{*}{\psi}_1(\vec{r}\,')\psi_2(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} \\ -\hbar c\int \mathrm{d}^3\vec{r}\,A_{\mathrm{ex}}\left(|\psi_1(\vec{r})|^2 + |\psi_2(\vec{r})|^2\right).\end{aligned} \tag{3.69}$$

3.7 One-particle systems

Although the construction of the energy functional E_{T} has been performed along the generally accepted elements of relativistic field theory, one nevertheless wishes to have some kind of test of its physical truth. For such a purpose, the one-particle systems are well suited because here the two-particle eigenvalue system (3.37a)-(3.37b) degenerates to the ordinary (stationary) Klein-Gordon equation, whose solutions are known in analytic form. Consequently, one can compute the value of the proposed energy functional E_{T} upon those exact solutions of the one-particle theory and can then check whether the field energy E_{T} actually coincides with the mass eigenvalue (M_*c^2, say).

More concretely, extract the one-particle situation of the present two-particle case by putting

$$\psi_2(\vec{r}) = A_1(\vec{r}) = A_2(\vec{r}) = B(\vec{r}) \equiv 0\,, \tag{3.70a}$$

$$\psi_1(\vec{r}) \doteq \psi(\vec{r}) \tag{3.70b}$$

and find the corresponding one-particle KGE from the RST system (3.37a)-(3.37b) as

$$\frac{-\hbar^2}{2M}\,\Delta\psi(\vec{r}) + V_{11}(\vec{r})\cdot\psi(\vec{r}) = \frac{M_*^2 - M^2}{2M}c^2\cdot\psi(\vec{r}) \tag{3.71}$$

with the remaining potential $V_{11}(\vec{r})$ being cut down to

$$V_{11}(\vec{r}) \Rightarrow -\frac{\hbar^2}{2m}\left[\left(\frac{M_*c}{\hbar} + A_{\mathrm{ex}}(\vec{r})\right)^2 - \left(\frac{M_*c}{\hbar}\right)^2\right]. \tag{3.72}$$

For the Coulomb potential (3.53), the exact solutions of the one-particle eq. (3.71) are well known and presented in any textbook (*e.g.*, ref. [2]). The relativistic normalization condition for the one-particle solutions $\psi(\vec{r})$ is to be deduced from (3.22a) as

$$\int \mathrm{d}^3\vec{r}\,k(\vec{r}) = 1\,. \tag{3.73}$$

Here the charge density $k(\vec{r})$ is obtained from (3.18a) by applying the cutting prescription (3.70a)-(3.70b):

$$k(\vec{r}) = \frac{\hbar}{Mc}\left(\frac{M_*c}{\hbar} + A_{\mathrm{ex}}(\vec{r})\right)\overset{*}{\psi}(\vec{r})\psi(\vec{r})\,. \tag{3.74}$$

A similar simplification occurs also for the RST energy functional $E_{\rm T}$ (3.68) which reduces to the sum of matter energy ($E_{\rm M}$) and external interaction energy ($E_{\rm es}$):

$$\begin{aligned} E_{\rm T}[\psi] &\Rightarrow E_{\rm M}[\psi] + E_{\rm es}[\psi] \\ &= Mc^2 Z_*^2 + 2\,\frac{\hbar^2}{2M}\int {\rm d}^3\vec{r}\,\vec{\nabla}\overset{*}{\psi}(\vec{r})\cdot\vec{\nabla}\psi(\vec{r}) \\ &\quad -\hbar c\int {\rm d}^3\vec{r}\,A_{\rm ex}(\vec{r})\cdot k(\vec{r})\ . \end{aligned} \tag{3.75}$$

A very pleasant feature of this energy functional is now that its value upon the eigensolutions $\psi_{M_*}(\vec{r})$ of the eigenvalue problem (3.71) exactly yields the corresponding mass eigenvalue M_*:

$$E_{\rm T}[\psi_{M_*}] = M_* c^2\ . \tag{3.76}$$

This result holds for any member of the mass spectrum $\{M_*\}$, due to an *arbitrary* binding potential $A_{\rm ex}(\vec{r})$ [25], and thus supports the confidence into the RST energy functional $E_{\rm T}$ (3.68).

Observe, however, that the numerical identity (3.76) of field energy $E_{\rm T}$ and mass eigenvalue M_* can hold only for the one-particle systems; or, more concretely, the *many-particle* energy $E_{\rm T}$ cannot agree with the sum of mass eigenvalues! In order to see this more clearly for the present two-particle systems, one may reformulate the energy $E_{\rm T}$ (3.68) in terms of the mass eigenvalues M_a ($a = 1, 2$) so that the difference becomes obvious. To this end, one returns for a moment to the matter energy density ${}^{(\rm M)}T_{00}$ (3.42) and uses the relations (3.43) and (3.44) in order to eliminate from the corresponding matter functional $E_{\rm M}$ (2.71a) the spatial derivatives of the wave function Ψ, so that one finally ends up with the following form:

$$E_{\rm M} = \frac{\hbar}{M}\int {\rm d}^3\vec{r}\ \left(\mathcal{D}_0\bar{\Psi}\right)\left(\mathcal{D}_0\Psi\right)\ . \tag{3.77}$$

Next, one resorts here to the component form (3.11a)-(3.11b) of the covariant derivatives and thus finds for the stationary-field configuration (3.16a)-(3.17b)

$$\begin{aligned} \frac{\hbar^2}{M}\left(\mathcal{D}_0\bar{\Psi}\right)\cdot\left(\mathcal{D}_0\Psi\right) &= \left[\frac{M_1 c}{\hbar} + A_{\rm ex}(\vec{r}) + A_2(\vec{r})\right]\cdot k_1(\vec{r}) \\ &\quad + \left[\frac{M_2 c}{\hbar} + A_{\rm ex}(\vec{r}) + A_1(\vec{r})\right]\cdot k_2(\vec{r}) \\ &\quad + \hbar c\Big(B(\vec{r})h(\vec{r}) + \overset{*}{B}(\vec{r})\overset{*}{h}(\vec{r})\Big)\ . \end{aligned} \tag{3.78}$$

This result helps now putting the matter integral (3.77) into a very concise form, namely by inserting the static potentials $A_a(\vec{r}), B(\vec{r})$ (3.34a)-(3.34b) and afterwards observing the energy functionals $E_{\rm es}$ (3.51), $E_{\rm R}$ (3.59) and $E_{\rm C}$ (3.65) together with the normalization conditions (3.22a) for the charge densities $k_a(\vec{r})$. This procedure ultimately leads us to the following form of the matter energy $E_{\rm M}$ (3.77):

$$E_{\rm M} = M_1 c^2 + M_2 c^2 - E_{\rm es} - 2E_{\rm G}\ . \tag{3.79}$$

If this is substituted now into the total functional $E_{\rm T}$ (2.70), we arrive at the desired result

$$E_{\rm T} = M_1 c^2 + M_2 c^2 - E_{\rm G}\ . \tag{3.80}$$

Obviously, the total energy $E_{\rm T}$ is not simply the sum of mass eigenvalues $M_a c^2$, but the gauge field energy $E_{\rm G}$ ($= E_{\rm R} - E_{\rm C}$) must be subtracted. Indeed, this is a very plausible result because either of the two RST eigenvalue equations (3.37a)-(3.37b) takes account of the interelectronic interactions whose energy content enters therefore *both* mass eigenvalues M_1 and M_2. In order to annihilate this double counting of the interaction energy $E_{\rm G}$, one has to subtract it from the sum of eigenvalues as shown in eq. (3.80).

4 Numerical results

In order to evaluate the significance of RST for the relativistic effects, it is instructive to apply the preceding two-particle results to the helium atom. Here, one can compare the RST predictions for the energy levels $E_{\rm T}$ (3.68) with the corresponding predictions $E_{\rm HF}$ (3.69) of the Hartree-Fock approach in order to relate both to the observational data. However, such a comparison presents a certain problem because the two electrons of a real helium atom are spin-$\frac{1}{2}$ particles, obeying the Pauli exclusion principle, whereas the preceding RST and HF results refer to scalar particles. This circumstance requires some explanation.

First observe here that, in terms of the conventional theory, our scalar RST particles have to be described by *anti-symmetric* states corresponding to the Hartree-Fock ansatz

$$\Psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_{\rm I}(\vec{r}_1)\psi_{\rm II}(\vec{r}_2) - \psi_{\rm II}(\vec{r}_1)\psi_{\rm I}(\vec{r}_2)\right) \tag{4.1}$$

with orthonormal wave functions (3.21a)-(3.21b),

$$\int {\rm d}^3\vec{r}\,|\psi_{\rm I}(\vec{r})|^2 = \int {\rm d}^3\vec{r}\,|\psi_{\rm II}(\vec{r})|^2 = 1\,, \tag{4.2a}$$

$$\int {\rm d}^3\vec{r}\,\overset{*}{\psi}_{\rm I}(\vec{r})\psi_{\rm II}(\vec{r}) = 0\ . \tag{4.2b}$$

Such a procedure is justified when one is willing to neglect the spin interactions, because in this case the total anti-symmetric wave function factorizes into the space and spin parts, and when the spin part is symmetric the spatial part must be anti-symmetric (ortho-level system) in agreement with the spin-statistics theorem. Thus, when scalar RST is considered as the relativistic generalization of the scalar HF approach, the preceding RST results provide us with the possibility to study the relativistic effects in the ortho-level system of helium, albeit under neglection of the spin effects (*i.e.* fine structure). The para-level system may be treated within the framework of RST by simply omitting all the exchange terms occurring for the ortho-level system; *i.e.* the Hartree-Fock approach is substituted by the simpler Hartree approximation albeit in relativistic form.

4.1 One-particle spectrum

But even under neglection of the fine structure of the spectral lines, one cannot expect coincidence of the RST predictions with the experimental data. The reason is that a considerable part of the two-particle energy $E_{\rm T}$ consists in the sum of the one-particle energy eigenvalues $M_a c^2$ $(a = 1, 2)$, and the relativistic corrections of these single-particle mass eigenvalues are considerably different for spin-0 and spin-$\frac{1}{2}$ particles. For instance, for the Coulomb potential (3.53) one finds the single-particle ground-state energy $E_{\rm T} = M_* c^2$ as [26]

$$M_* = \begin{cases} M\sqrt{\frac{1}{2} + \sqrt{(\frac{1}{2})^2 - (z_{\rm ex}\alpha_{\rm s})^2}} = \\ \quad M\left(1 - \frac{1}{2} z_{\rm ex}^2 \alpha_{\rm s}^2 - \frac{1}{4} z_{\rm ex}^4 \alpha_{\rm s}^4 \dots\right), \text{ spin-0}, \\ M\sqrt{1 - (z_{\rm ex}\alpha_{\rm s})^2} = \\ \quad M\left(1 - \frac{1}{2} z_{\rm ex}^2 \alpha_{\rm s}^2 - \frac{1}{8} z_{\rm ex}^4 \alpha_{\rm s}^4\right), \text{ spin-}\frac{1}{2} \quad . \end{cases} \tag{4.3}$$

Here the upper case (spin-0) is the ground-state mass eigenvalue due to the stationary Klein-Gordon equation (3.71) for scalar particles; and, similarly, the lower case refers to the corresponding Dirac equation for spin-$\frac{1}{2}$ particles.

Observe now that the Schrödinger energy eigenvalue $E_{\rm S}$, as the non-relativistic limit of the mass defect, is actually the same for the bosonic and fermionic result (4.3):

$$E_{\rm S} = (M_* - M)\, c^2 \approx -\frac{1}{2} z_{\rm ex}^2 \alpha_{\rm s}^2 M c^2 = -\frac{z_{\rm ex}^2 e^4 M}{2\hbar^2} \tag{4.4}$$

but already the next higher relativistic correction ($\backsim z_{\rm ex}^4 \alpha_{\rm s}^4$) differs by a factor of two for both cases! Furthermore, the one-particle theories break down for different nuclear-charge numbers $z_{\rm ex}$, namely the bosonic case for $z_{\rm ex} = (2\alpha_{\rm s})^{-1} \approx 68$ and the fermionic case for $z_{\rm ex} \approx 137$ (see fig. 1). Therefore, it must appear as rather amazing that the present *scalar* RST predicts the two-particle spectrum in relatively good agreement with the experimental data for *fermions* for a restricted range of charge numbers $z_{\rm ex}$ (see fig. 4 above).

4.2 Two-particle spectrum

The existence of a singular endpoint (with vertical tangent in fig. 1) of the one-particle spectrum gives a hint on the qualitative features of the RST two-particle spectrum $\{E_{\rm T}\}$ (3.68). The numerical solutions of the RST system (3.37a)-(3.37b) demonstrate that the mutual interaction energy $E_{\rm G}$ (3.55) of the two electrons becomes dominated more and more by the sum of matter energy $E_{\rm M}$ (3.46a)-(3.46b) and external interaction energy $E_{\rm es}$ (3.51), when the charge number $z_{\rm ex}$ is increased. On the other hand, either of these two types of energy contributions is the sum of the corresponding one-particle energies $E_{\rm M}(a)$ and $E_{\rm es}(a)$ and therefore the characteristics of the one-particle spectrum must dominantly enter also the two-particle spectrum. This especially means that we have to expect the emergence of a singular endpoint for the two-particle spectrum, similarly to the one-particle situation of fig. 1.

Unfortunately, our numerical integrations of the relativistic two-particle equations (3.37a)-(3.37b) become spoiled by computational problems when the charge number $z_{\rm ex}$ tends to the critical one-particle value (*i.e.* $z_{\rm ex} \approx 68$); but the tendency of the two-particle spectrum to develop singular endpoints becomes evident already from our numerical results reaching up to $z_{\rm ex} \approx 60$ (see fig. 2). Observe here that the development of such singular endpoints is a truly relativistic effect which does not occur for the non-relativistic HF approach (curve (b) of fig. 2). On the other hand, the RST and HF predictions become identical for sufficiently weak external fields ($z_{\rm ex} \lesssim 20$, say). Evidently, this limit behavior for $z_{\rm ex} \lesssim 20$ and $z_{\rm ex} \gtrsim 60$ is sufficient to conclude that the relativistic two-particle energy $E_{\rm T}$ (3.68) is always smaller than its HF counterpart $E_{\rm F}$ (3.69): $E_{\rm T} < E_{\rm HF}$ (*i.e.* the relativistic binding energy $|E_{\rm T} - 2Mc^2|$ is always greater than its non-relativistic counterpart $|E_{\rm HF}|$ (3.69)). Since this relativistic effect is overestimated by the scalar theory (Klein-Gordon) in comparison to the spinor theory (Dirac), see fig. 1, the spinor predictions for the helium spectrum will be found to be closer to the experimental data, of course under neglection of the fine structure (see fig. 5).

4.3 Scalar wave functions and densities

Looking for an explanation for the relativistic enhancement of the two-particle binding energies (fig. 2) one will have to study the relativistic deformation of the wave functions. Here it is important to observe that both the RST and HF spectrum can be classified by pairs of one-particle states because when one switches off continuously the interelectronic interactions (*i.e.* putting in (3.38a)-(3.38d): $A_1(\vec{r}) \Rightarrow 0, A_2(\vec{r}) \Rightarrow 0, B(\vec{r}) \Rightarrow 0$), then one ends up with a pair of ordinary KGEs as displayed by eq. (3.71). Of course, the non-relativistic limit thereof is the ordinary Schrödinger equation

$$-\frac{\hbar^2}{2M} \Delta\psi(\vec{r}) - \hbar c A_{\rm ex}(\vec{r}) \cdot \psi(\vec{r}) = E\psi(\vec{r}) \ . \tag{4.5}$$

Using this "pair classification", the results of fig. 2 refer to the $(1s, 2s)$ pair of KGE states (3.71) for RST and to the corresponding Schrödinger states (4.5) for HF. When the interparticle interactions are neglected, both kinds of solutions are known in analytic form [2] and can therefore be used as the starting points for the iteration process in order to solve our RST system (3.37a)-(3.37b) or its non-relativistic version (3.41a)-(3.41b), respectively. Thus, the selected relativistic wave functions $\tilde{\psi}_a$ of lowest order are

$$1s: \qquad \tilde{\psi}_1 = \tilde{N}_1\, y^\nu \exp\left(-\frac{y}{\eta_1}\right), \tag{4.6a}$$

$$2s: \qquad \tilde{\psi}_2 = \tilde{N}_2\, y^\nu (y_* - y) \exp\left(-\frac{y}{\eta_2}\right) . \tag{4.6b}$$

Here we have rescaled the radial variable r to the dimensionless y through

$$y = \frac{z_{\rm ex} r}{a_{\rm B}}\,, \tag{4.7}$$

where $a_{\rm B}$ is the Bohr radius

$$a_{\rm B} = \frac{\hbar^2}{M e^2}\ . \tag{4.8}$$

The exponential parameter ν is found to be negative,

$$\nu = -\frac{1}{2}\left(1 - \sqrt{1-(2z_{\rm ex}\alpha_{\rm s})^2}\right)\,, \tag{4.9}$$

but it generates merely a weak singularity for the wave functions at the origin ($r = 0$) so that the energy functionals remain well defined. The widths η_a of the wave functions are given by ($a = 1, 2$)

$$\eta_a = \frac{M}{\tilde{M}_a}(\nu + a) \tag{4.10}$$

and the zeroth-order mass eigenvalues $\tilde{M}_a$ by

$$\tilde{M}_a = \frac{M}{\sqrt{1 + \dfrac{z_{\rm ex}^2\alpha_{\rm s}^2}{\left(a - \dfrac{1}{2} + \sqrt{\left(\dfrac{1}{2}\right)^2 - z_{\rm ex}^2\alpha_{\rm s}^2}\right)^2}}}\ . \tag{4.11}$$

Finally, the zero y_* of the first-excited state $\tilde{\psi}_2$ (4.6b) is

$$y_* = \eta_2(1+\nu) \tag{4.12}$$

and the normalization constants $\tilde{N}_a$ can be determined from (3.22a), *e.g.* for the ground state:

$$\tilde{N}_1^2 = \frac{2^{2+2\nu}}{4\pi\eta_1^{2+2\nu}\Gamma(2+2\nu)\left[(1+\nu)^2 + z_{\rm ex}^2\alpha_{\rm s}^2\right]}\ . \tag{4.13}$$

The pair of relativistic wave functions $\tilde{\psi}_a(\vec{r})$ (4.6a)-(4.6b) may be used as the point of departure for iteratively solving the RST system (3.37a)-(3.37b), but when one is satisfied with the non-relativistic HF equations (3.41a)-(3.41b), it is more adequate to resort to the non-relativistic counterpart ($\overset{\circ}{\psi}$, say) of those relativistic functions $\tilde{\psi}_a$:

$$\tilde{\psi}_1(\vec{r}) \Rightarrow \overset{\circ}{\psi}_1(\vec{r}) = \sqrt{\frac{z_{\rm ex}}{\pi a_{\rm B}^3}}\exp(-y)\,, \tag{4.14a}$$

$$\tilde{\psi}_2(\vec{r}) \Rightarrow \overset{\circ}{\psi}_2(\vec{r}) = \sqrt{\frac{z_{\rm ex}}{8\pi a_{\rm B}^3}}\left(1-\frac{y}{2}\right)\exp\left(-\frac{y}{2}\right)\ . \tag{4.14b}$$

Clearly, these are solutions of the ordinary Schrödinger equation (4.5), but their deviation from the relativistic solutions $\tilde{\psi}_a(\vec{r})$ (4.6a)-(4.6b) is very small and is hardly enhanced by the numerical iteration procedure so that the RST solutions of the relativistic system (3.37a)-(3.37b) remain very close to the corresponding solutions of the non-relativistic HF system (3.41a)-(3.41b).

However, the charge densities $k_a(\vec{r})$ (3.18a)-(3.18b) and the exchange density $h(\vec{r})$ (3.19) are more sensible with respect to the relativistic effect. Since these densities directly enter the relativistic energy functional $E_{\rm T}$ (3.68), the enhancement of the binding energy must be due to their relativistic deformation. Indeed fig. 3 shows a plot of the second charge density $k_2(\vec{r})$ for the $(1s, 2s)$ state from which it is clearly seen that the RST density (curve (a)) is shifted towards the origin ($r = 0$) in comparison to its HF counterpart (curve (b)). The same effect occurs also for the other densities $k_1(\vec{r})$ and $h(\vec{r})$. As a consequence of this relativistic shrinking of the extension of the charge distributions, the negative electrostatic interaction energy $E_{\rm es}$ (3.51) becomes dominantly smaller and therefore responsible for the observed enhancement of the $(1s, 2s)$ binding energy, fig. 2.

4.4 Spectral lines

The most immediate test of the theoretical predictions naturally must refer to the frequencies of the photons which are emitted during the transitions between the stationary states. For the present test of scalar RST, we restrict ourselves to the transition from the $(1s, 2s)$ state of the ortho-helium to the $(1s, 1s)$ state of the para-system. Observe that the present scalar RST can refer to both the para- and ortho-system where, under neglect of the magnetic (*i.e.* spin) interactions, the space parts of the conventional quantum states are anti-symmetric so that the exchange terms enter the HF equations with a minus sign, cf. (3.41a)-(3.41b). However, the ground state $(1s, 1s)$ belongs to the para-system with symmetric spatial wave functions and must therefore, in the conventional HF approach, be described by the Hartree approximation being based upon a simple product ansatz. But this situation can be treated also by our present scalar form of RST, namely by simply omitting the exchange terms for both the relativistic system (3.37a)-(3.37b) and for its non-relativistic limit (3.41a)-(3.41b).

Thus, the frequency ω of the emitted photons for the transition $(1s, 2s) \rightarrow (1s, 1s)$ is determined by

$$\hbar\omega = E_{\rm T}(1s, 2s) - E_{\rm T}(1s, 1s)\,, \tag{4.15}$$

whose non-relativistic approximation is given by substituting here the HF functional $E_{\rm HF}$ (3.69) in place of $E_{\rm T}$ (3.68). Figure 4 shows a plot of the relative deviations Θ,

$$\Theta = \frac{\omega - \omega_{\rm exp}}{\omega_{\rm exp}}\,, \tag{4.16}$$

of the RST and HF predictions from the experimental values which are taken from ref. [29]. Here, a pleasant effect occurs in favor of the present scalar RST which consists in the result that for small nuclear charge (*i.e.* $z_{\rm ex} \lesssim 10$) the scalar RST predictions come closer to the experimental values than the corresponding HF predictions by some 50% or more, see fig. 4. However, for stronger external fields ($z_{\rm ex} \gtrsim 15$, say) the exaggeration of that relativistic effect of fig. 1 by the scalar fields becomes dominant and

the scalar RST predictions become even worse than the corresponding HF results.

4.5 RST for fermions

Surely, the deviations of the scalar RST predictions from the experimental data for strong external fields $z_{\rm ex} \gtrsim 20$ (fig. 4) may appear somewhat disappointing. However, the origin of this deficiency has nothing to do with RST itself but simply points at the fact that the real electrons are fermions, not bosons. Thus, one will expect that the RST predictions will meet better with the observations in strong external fields when RST is adapted to fermion systems. Remember here that a single Dirac particle has considerably smaller binding energy (in strong external fields) in comparison to a Klein-Gordon particle (see fig. 1), and it is just this effect of exaggeration of the scalar Klein-Gordon theory which is the origin of failure of the corresponding *scalar* RST predictions for $z_{\rm ex} \gtrsim 20$ (fig. 4).

In order to verify this claim, one elaborates RST for fermion systems [26] and carries through the same numerical studies as for the preceding case of bosons. In short, one may mention that the gauge field system has the same structure for fermions as for bosons, and it is only the matter subsystem which undergoes certain modifications: the Klein-Gordon eq. (2.6) for spin-0 particles is replaced by the two-particle Dirac equation,

$$i\hbar c \Gamma^\mu (\mathcal{D}_\mu \Psi) = \mathcal{M} c^2 \Psi \,, \tag{4.17}$$

which may be deduced from the corresponding RSE (2.1) by means of the spinor analogue of the conservation equation (2.5) for bosons [27]:

$$\Gamma^\mu \cdot \mathcal{H}_\mu = \mathcal{M} c^2 \ . \tag{4.18}$$

Here the (8×8)-matrices Γ_μ are the generators of an eight-dimensional representation of the Clifford algebra $C(1,3)$:

$$\Gamma_\mu \Gamma_\nu + \Gamma_\nu \Gamma_\mu = 2 g_{\mu\nu} \cdot \mathbf{1} \ , \tag{4.19}$$

and simultaneously the object Γ_μ plays the part of the total velocity operator v_μ (2.9) of the scalar case, *i.e.* the total fermionic current j_μ is given by

$$j_\mu = {\rm tr}(\mathcal{I} \cdot \Gamma_\mu) \,. \tag{4.20}$$

Carrying now through all the computations necessary to solve the fermionic analogue of the bosonic mass eigenvalue problem (3.37a)-(3.37b) lets us arrive at the frequency ω of the photons emitted during the transition $(1s_{1/2}, 2s_{1/2}\ {}^3S_1) \to (1s_{1/2}, 1s_{1/2}\ {}^1S_0)$:

$$\hbar\omega = E_{\rm T}(1s_{1/2}, 2s_{1/2}\ {}^3S_1) - E_{\rm T}(1s_{1/2}, 1s_{1/2}\ {}^1S_0) \ . \tag{4.21}$$

Clearly, this is the fermion analogue of the bosonic situation (4.15), where we have again restricted ourselves to work in the electrostatic approximation. Nevertheless, in view of its approximative character, this fermionic result (4.21) is very encouraging (fig. 5): namely, on the one hand it preserves the improvement of the bosonic RST result over the non-relativistic HF situation (fig. 4) for moderate external-field strengths ($z_{\rm ex} \lesssim 10$), and on the other hand the fermionic result (4.21) avoids the bosonic overestimation of the binding energy in the strong-field regime $z_{\rm ex} \gtrsim 20$ (fig. 4). Quite on the contrary, it is just for the strong external fields ($z_{\rm ex} \gtrsim 30$) that the fermionic RST predictions come closer and closer to the experimental values.

The origin of this pleasant result for the strong fields is closely related to the circumstance that the photon frequency ω (4.21) deviates from the experimental value up to some 3-4% in the weak-field regime $z_{\rm ex} \lesssim 4$. The common reason for both effects is namely that the interelectronic interaction energy $E_{\rm G}$ constitutes a relatively large fraction of the total energy $E_{\rm T}$ for *weak* fields but is *negligible for strong fields* ($|E_{\rm G}| \ll |E_{\rm T}|$), so that in the strong-field limit the total energy $E_{\rm T}$ is practically identical to the sum of single-particle mass eigenvalues (*i.e.* $E_{\rm T} \sim M_1 c^2 + M_2 c^2$). However, the single-particle eigenvalues M_a for non-interacting particles are correctly described by the single-particle Dirac equation, which is part of RST, and therefore the fermionic RST predictions are relatively precise in the strong-field regime (fig. 5). On the other hand, in the weak-field regime, the neglection of the magnetic interactions among the electrons must necessarily spoil the precision of the present scalar RST predictions because the neglected magnetostatic energy presents here a considerable part of the total energy $E_{\rm T}$.

4.6 Ground-state interaction energy

It may appear now that these relatively precise RST predictions for strong external fields ($z_{\rm ex} \gtrsim 30$ in fig. 5) are exclusively due to the increasing dominance of the single-particle eigenvalues $M_a c^2$ over the interelectronic interactions $E_{\rm G}$ for building up the total energy $E_{\rm T}$ (3.80). However, this is not the whole truth because we are able to demonstrate that the *electrostatic* interactions are still taken into account to an amazingly correct extent by our electrostatic approximation, even for very strong external fields! In order to give a brief demonstration of this effect, we consider the ground-state interaction energy between the two electrons in the highly ionized helium-like ions (*i.e.* with large nuclear charge $z_{\rm ex} \gtrsim 30$). Fortunately, this interaction energy ($\Delta E_{\rm exp}$, say) is accessible to direct measurement [19]; and, on the other hand, this quantity appears theoretically as the difference of the two-particle ground-state energy $E_{\rm T}(2)$ and the double one-particle ground-state energy $E_{\rm T}(1)$:

$$\Delta E_{\rm RST} = E_{\rm T}(2) - 2E_{\rm T}(1) \ . \tag{4.22}$$

In principle, this difference can be computed with high precision within the framework of RST but, in agreement with the foregoing neglection of the magnetic interactions, we are satisfied to work here again in the electrostatic approximation. Denoting the corresponding result

by $\Delta E^{(\mathrm{e})}_{\mathrm{RST}}$, one defines

$$\Delta E^{(\mathrm{e})}_{\mathrm{RST}} \doteq E^{(\mathrm{e})}_{\mathrm{T}}(2) - 2E_{\mathrm{T}}(1)\,, \tag{4.23}$$

where $E^{(\mathrm{e})}_{\mathrm{T}}(2)$ is the two-particle ground-state energy E_{T} (3.80) to be computed by means of the spin version [26] of the RST system (3.37a)-(3.37b), however under neglection of the magnetic contributions. Concerning the one-particle energy $E_{\mathrm{T}}(1)$, one can refer to the mass energy relation (3.76) with the mass eigenvalue M_* being given by eq. (4.3) which may then further be improved by the Lamb-shift contribution [19].

The comparison of our calculations for the energy difference $\Delta E^{(\mathrm{e})}_{\mathrm{RST}}$ (4.23) with the corresponding experimental values ΔE_{exp} (see table 1) demonstrates now that the interelectronic interaction for the helium-like ground state is met by RST roughly up to 1–11% (fourth column). Thus, the electrostatic approximation turns out to be not too bad and simultaneously hints at the order of magnitude of the (neglected) magnetic interactions. Clearly for increasing nuclear charge, ranging from germanium ($z_{\mathrm{ex}} = 32$) up to bismuth ($z_{\mathrm{ex}} = 83$), the electrons become more and more relativistic, which enhances the magnetic contributions to the energy difference and thus the electrostatic approximation must necessarily become worse.

However, this failure of the electrostatic approximation just meets with the estimate of the magnetic interaction energy $\Delta E^{(\mathrm{m})}_{\mathrm{RST}}$ presented in sect. 1. The last column of the table displays the values for the prefactor f_* (1.10) which measures the relative fraction of the magnetic contribution to the ground-state interaction energy ΔE. Recall here that, according to those arguments leading to the estimate (1.10), the quantity f_* should be (nearly) independent of the nuclear charge z_{ex}, which is actually the case up to $z_{\mathrm{ex}} \approx 66$ (dysprosium). This result supports the RST picture of the cooperation of electric and magnetic interactions in order to build up the relativistic energy E_{T} of the stationary bound many-particle systems, as proposed by eq. (3.80). Clearly, this qualitative picture must now be converted to a quantitative approach by solving the original RST eigenvalue problem due to the two-particle eq. (4.17) with high precision and comparing the results to the corresponding observational data.

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