Positive and Negative Mixtures in Relativistic Schrödinger Theory

S. Rupp^{1,2} and M. Sorg¹

The general formalism of relativistic Schrödinger theory (RST) is specialized to a scalar two-particle system with electromagnetic interactions (scalar helium atom). The set of dynamically allowed field configurations splits up into positive and negative mixtures and pure states. The static and spherically symmetric solutions are constructed by means of first-order perturbation theory for the case of an attractive Coulomb potential. The corresponding energy levels for the positive and negative mixtures resemble the emergence of ortho and para states in the conventional quantum theory. The associated energy eigenvalues predicted by the RST seem to undergo a certain kind of *mixture degeneracy* as the RST analog of the conventional *exchange degeneracy*. The charge densities of the positive mixtures assimilate, whereas the densities of the negative mixtures strongly resemble the bosonic (fermionic) matter of the conventional theory when the Pauli principle is applied.

1. INTRODUCTION AND SURVEY

Perhaps the most important and powerful notion in theoretical physics, being set up for the purposes of understanding the physical phenomena, is the "conservation law." This concept emerges in both classical and quantum physics with comparable significance, and therefore any conserved quantity surely represents some "element of reality" (in the sense of Einstein et al., 1935). But despite their profound meaning, the conservation laws are not understood completely because their true origin appears to be mysterious. At best, the conservation laws may be traced back to some physical "principle." Mostly such a principle is first grasped intuitively by its discoverer and is afterwards recast in mathematical terms in order to be verified (or falsified) by means of appropriate experiments and

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¹ Institut für Theoretische Physik der Universität Stuttgart, Stuttgart, Germany.

² To whom correspondence should be addressed at Institut für Theoretische Physik der Universität Stuttgart, Pfaffenwaldring 57, D 70550 Stuttgart, Germany.

observations. In the history of science, famous examples of this kind refer to the following:

- *Relativity Principle* (Einstein *et al.*, 1924), which inspired the development of special relativity (→ conservation of total four-momentum of closed systems),
- Equivalence Principle (Einstein et al., 1924; Stachel, 1987), underlying Einstein's gravitation (\sim local energy-momentum conservation $\nabla^{\mu}T_{\mu\nu} = 0$),
- Heisenberg's *Quantization Principles* (Heisenberg, 1930), where the conserved quantities are deduced from the Heisenberg equations of motion.

1.1. Pauli Principle

This paper deals with some questions centered around one of those fundamental principles, the "Pauli principle" (mostly, Pauli exclusion principle, e.g. Duck and Sudarshan, 1998). Originally the Pauli principle was set up in the form of an exclusion postulate so as to explain the spectral lines and the internal structure of atoms and molecules: any electronic quantum state defined in terms of single-particle quantum numbers can be occupied by only one electron so that no two electrons can have identical quantum numbers. More generally speaking, one might nowadays look upon the Pauli principle as the postulate of a fundamental dichotomy: elementary matter exists in two distinct forms, namely fermions (obeying the original exclusion principle) and bosons. The latter do not only disregard the exclusion postulate but, on the contrary, even tend (if not disturbed by thermal excitations) to crowd into one single-particle quantum state ($\sim Bose$ -*Einstein condensation*). The associated conservation law for this boson–fermion dichotomy of matter says that any particle must be either of the fermionic type or of the bosonic type, with exclusion of mixed types and of transitions between the two types. Recent experimental tests of this superselection rule yield the result that it is strictly obeyed: non-Pauli processes can only occur with a frequency less than 1 part in 10^{34} (Sudbery, 1990). Thus the boson–fermion conservation law stands on a comparably fundamental level as the energy-momentum conservation law (and its violation can therefore hardly be used to solve certain puzzles of contemporary physics, e.g. the solar-neutrino problem by means of non-Paulian burning of hydrogen (Plaga, 1989).

However from the purely theoretical point of view, a rigorous foundation of the Pauli principle presents some problems. It is possible to conceive a more general form of quantum theory ("*paraquantization*" (Ohnuki and Kamefuchi, 1982)), and within this general framework the original Pauli principle represents only a very special subcase. It seems not clear why para-bosons and para-fermions do not exist in nature. One merely may suppose that the validity of the ordinary Pauli principle might have to do something with the fact that our space–time has 1 + 3 dimensions, for in a 1 + 2 dimensional space–time a graded transition between the two types

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of matter is possible (see the theory of "anyons" in connection with the fractional quantum Hall effect (Wilczek, 1990)). Such an unclarified theoretical situation with the Pauli principle may facilitate to consider also alternative forms of the matter dichotomy, e.g. as it emerges in the relativistic Schrödinger theory (RST) (Sorg, 1992, 1997a,b). For a comparison of both alternative approaches to the matter dichotomy, it is instructive to consider some concrete physical situation where the predictions can be directly opposed to one another: the two-electron atoms.

1.2. Ortho and Para States

In principle, one tests the Pauli claim by confining some particles to a bounded region of three-space (e.g. two electrons around the nucleus of a helium atom) and looks at their energy distribution. The *exact* energy level scheme $\{E_n\}$ as solution of the Schrödinger eigenvalue problem

$$\hat{H}_{(1,2)}\Psi_{(1,2)} = E_n \Psi_{(1,2)} \tag{1.1}$$

is not obtainable in most cases, but in order to obtain the desired *qualitative* energy distribution one may be satisfied to know the levels approximately by means of perturbation theory. Furthermore, neglecting the spin interactions, the electronic wave functions factorize in a spatial part and a spin part so that the spatial part alone may be either symmetric or antisymmetric. Thus, for the spinless approximation one tries the following entangled single-particle states for the spatial part of the wave function (Blochincev, 1964):

$${}^{(S)}\psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_{\rm I}(\vec{r}_1)\cdot\psi_{\rm II}(\vec{r}_2) + \psi_{\rm I}(\vec{r}_2)\cdot\psi_{\rm II}(\vec{r}_1))$$
(1.2a)

$${}^{(A)}\psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_{\rm I}(\vec{r}_1)\cdot\psi_{\rm II}(\vec{r}_2)-\psi_{\rm I}(\vec{r}_2)\cdot\psi_{\rm II}(\vec{r}_1)), \qquad (1.2b)$$

which are exact solutions of the two-particle Schrödinger equation (1.1) when the electronic interactions \hat{H}_{int} ($\Rightarrow \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$) are switched-off (\rightsquigarrow exchange degeneracy). The standard procedure of first-order perturbation theory then yields for the

The standard procedure of first-order perturbation theory then yields for the energy corrections ${}^{(1)}E_{12}$ of the unperturbed two-particle states (1.2) as a consequence of the electronic interactions

$$^{(1)}E_{12} = U_{\rm C} \pm E_{\rm G}.\tag{1.3}$$

Here the positive (negative) sign corresponds to the symmetrized (antisymmetrized) trial functions (1.2). Consequently, the first-order energy levels (E_B) of the helium atom are found to be split up into the well-known parahelium (A) and orthohelium (S) states, thus eliminating the exchange degeneracy:

$$^{(1,2)}E_{\mathrm{B},\mathrm{S}} \cong -^{(0)}E_{\mathrm{B},1} - {}^{(0)}E_{\mathrm{B},2} + U_{\mathrm{C}} + E_{\mathrm{G}}$$
(1.4a)

$$^{(1,2)}E_{\rm B,A} \cong -^{(0)}E_{\rm B,1} - {}^{(0)}E_{\rm B,2} + U_{\rm C} - E_{\rm G}.$$
 (1.4b)

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Here the exact single-particle binding energies have been denoted by ${}^{(0)}E_{B,a}(a = 1, 2)$; they build up the zero-order approximation of the exact result. Moreover, the "*Coulomb integral*" $U_{\rm C}$ is due to the classical electrostatic interaction energy of the single-particle charge distributions $\rho_{\rm I} (\Rightarrow |\psi_{\rm I}|^2)$ and $\rho_{\rm II} (\Rightarrow |\psi_{\rm II}|^2)$, i.e.

$$U_{\rm C} = e^2 \int dV_1 \, dV_2 \, \frac{\rho_{\rm I}(\vec{r}_1) \cdot \rho_{\rm II}(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|},\tag{1.5}$$

and finally the "*exchange integral*" E_G (being responsible for the splitting into the para and ortho states) is given by

$$E_{\rm G} = e^2 \int dV_1 \, dV_2 \, \frac{\psi_{\rm I}^*(\vec{r}_1)\psi_{\rm II}(\vec{r}_1)\psi_{\rm II}^*(\vec{r}_2)\psi_{\rm I}(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|}.$$
 (1.6)

The numerical coincidence of the first-order approximations (1.4) with the experimental numbers is bad: for instance, for the energy difference of ortho and para states associated with the 1*s* and 2*s* single-particle states one finds in the conventional first-order approximation (Grau, 1993)

$$^{(1,2)}E_{\rm B,S} - {}^{1,2}E_{\rm B,A} = 2E_{\rm G} \cong 2.38 \,\,{\rm eV}$$
 (1.7)

whereas the experimental value is only 0.8 eV (see Martin, 1883, 1987). Nevertheless the predicted qualitative splitting of the helium levels into the ortho and para sublevels is found to be actually realized in nature and this (together with a lot of similar effects in atomic and molecular physics) is generally believed to be an experimental verification of the (ordinary) Pauli principle. Clearly, the numerical coincidences of the corresponding theoretical and experimental values may be further improved by applying more subtle approximation techniques (Drake, 1996), taking into account the screening of the nuclear charge. However, in the present paper we are satisfied with a comparison of the first-order approximations of the conventional theory and RST; see Fig. 1. (Contrary to the case of the conventional theory, the first-order approximation scheme of RST already implies the screening of the nuclear charge (Rupp *et al.*, 2000).

The conclusion, to be drawn from such a result, surely must be that the boson-fermion dichotomy of matter is adequately expressed by the Pauli principle. Furthermore, since this principle could be incorporated successfully into the conventional quantum theory, the latter framework thus appears to have received additional support of its "truth." However these conclusions cannot imply that the conventional quantum theory is the only theoretical framework capable of accounting for the matter dichotomy. Indeed we shall demonstrate subsequently that RST is also able to predict such a dichotomic phenomenon, albeit in a somewhat different manner; and the corresponding theoretical predictions are comparable to those of the conventional quantum theory, especially concerning the emergence



Fig. 1. Total energy ${}^{(1)}E_{12}$ in first-order approximation. The RST first-order approximation (solid lines) for the two-particle interaction energy ${}^{(1)}E_{12}$ (5.23) approaches the pure-state result for $C_* \rightarrow \infty$ (i.e. ${}^{(1)}E_{12}(\infty) = U_{\rm C}$). On the other hand the experimental values ${}^{(S)}E_{12}$, ${}^{(A)}E_{12}$) are adopted for C_* in the vicinity of the minimally possible values C_{\pm} . The numerical coincidence with the experimental values ${}^{(S)}E_{12} = 9.63$ eV and ${}^{(A)}E_{12} = 8.83$ eV occurs for $C_*^{(+)} = 0.62$ and $C_*^{(-)} = 1.13$. This supports the hypothesis that the electrons in a real atom may actually be in an RST mixture rather than in a pure state. In contrast to this, the first-order prediction (1.3) of conventional quantum theory yields the following results (Grau, 1993):

⁽¹⁾
$$E_{12}(S) = U_{\rm C} + E_{\rm G} \cong 11.422 \text{ eV} + 1.194 \text{ eV} = 12.616 \text{ eV}$$

⁽¹⁾ $E_{12}(A) = U_{\rm C} - E_{\rm G} \cong 11.422 \text{ eV} - 1.194 \text{ eV} = 10.228 \text{ eV}.$

of some kind of degeneracy phenomenon (see Fig. 1). More concretely, the exchange degeneracy of the symmetrized and antisymmetrized states (1.2) of the conventional theory finds its RST counterpart in form of the *mixture degeneracy* referring to the fact that positive and negative mixtures have the same binding energy, at least in the vicinity of the pure states. Whether the present mixture degeneracy is broken by the interelectronic interactions in the same way as the conventional exchange degeneracy (1.3) requires further clarification (in a separate paper).

1.3. Survey of RST Results

In RST, the matter dichotomy arises via the dynamical subdivision of the set of mixture configurations into two subsets: *positive and negative mixtures* (the



Fig. 2. Mixtures and pure states. The relativistic von Neumann equation (2.5) subdivides the density configuration space into three subsets: the pure states occupy the *Fierz cone* $\sigma_* = 0$, positive mixtures ($\sigma_* = 1$) are geometrically represented by the two-parted hyperboloid, and the negative mixtures ($\sigma_* = -1$) by the one-parted hyperboloid. The mixtures approach the pure states for $\zeta \to \infty$. The general RST dynamics forbids a change of the mixture type, cf. (3.60). The positive (negative) mixtures may be considered as the RST counterparts of the bosonic (fermionic) matter of the conventional quantum theory.

intermediate configurations are the pure states; see Fig. 2). Anyone of these two RST mixtures exhibits some striking features reminding one strongly of the corresponding properties of fermionic and bosonic matter in the conventional theory: the single-particle densities $\rho_a(x)$ of both particles (a = 1, 2) tend to assimilate $(\rho_1(x) \cong \rho_2(x) \rightsquigarrow charge \ fusion)$ in the positive mixture case (resembling the Bose–Einstein condensation of bosonic matter), whereas these densities recede from one another in the negative mixture case ($\sim charge \ separation$), resembling rather the Pauli exclusion mechanism for fermions. Thus the positive (negative) mixtures may be considered as RST analog of bosonic (fermionic) matter of the

conventional theory. As indicated by our preliminary perturbative results (Fig. 1), this behavior then may lead to a similar ortho-para splitting of the helium levels in RST similarly as it is encountered in the conventional theory. Just as in the latter case, the negative mixtures (\Leftrightarrow fermions) seem to have lower energy eigenvalue than the positive mixtures (\Leftrightarrow bosons), cf. the conventional splitting (1.4).

Our procedure of developing these results is the following:

In Section 2 we briefly sketch the general structure of RST insofar as it is relevant for the present question of matter dichotomy. Next, in Section 3, the general structure is specialized down to the \mathbb{C}^2 -realization of RST with an abelian gauge group (i.e. $U(1) \times U(1)$). At this stage, there arises the matter dichotomy in a most natural way, namely through the observation that the density configuration space is four-dimensional and is naturally equipped with a pseudo-Euclidean metric. It is well known that such a geometry is characterized by a cone structure, i.e. in the present case by a "*Fierz cone*" representing geometrically the pure states. The "positive mixtures" are then represented by those points of the configuration space which have positive squared distance from the origin (~ interior of the Fierz cone) and similarly the "negative mixtures" occupy the "exterior" cone regions with negative squared distance from the origin (see Fig. 2). Thus the Fierz cone plays here a similar part as does the light cone in special relativity. The analogous construction for the \mathbb{R}^2 -realization of RST has been discussed in a preceding paper (Mattes and Sorg, 1999a). The general RST dynamics forbids transitions from positive to negative mixtures (and vice versa), similarly as in special relativity a particle cannot be accelerated (decelerated) from subluminal (superluminal) velocity to superluminal (subluminal) velocity.

In Section 4, the interrelationships between mixtures and pure states are studied in detail. The important point here is that all the physical densities as well as the dynamical equations can be written in such a form that the transitions from mixtures to pure states (and vice versa) can be continuously performed. There exists a "*mixture variable*" (ζ) which measures the "purity" of a field configuration $(\zeta = \infty)$: pure state; $\zeta < \infty$: mixture). In order to restrict the discussion to these mixture effects exclusively, one neglects certain components of the Hamiltonian (the "exchange fields"). This simplification enables one to eliminate the mixture variables completely in favor of the pure-state variables so that we can describe the mixtures exclusively in terms of the pure-state variables and some integration constant C_* (i.e. the "mixture parameter"). However the corresponding dynamical equations for the pure-state variables now become highly nonlinear for the mixture case and acquire their usual linear form for the pure states only when the *mixture parameter* (C_*) adopts its pure-state value ($C_* \Rightarrow \infty$). Thus the latter parameter is a nice handle to change the purity of the field configuration continuously from one extremal case ($C_* \rightarrow \infty$: pure states) to a certain other extreme situation ($C_* \rightarrow C_+ = 0$: positive mixture limit; $C_* \rightarrow C_- = 1$: negative mixture limit).

In Section 5, the treatment of the static and spherically symmetric field configurations is presented in great detail in order to prepare the investigation of 2-electron atoms in the last section. Similarly as in conventional quantum theory, it is also very difficult in RST to find the exact solutions for such an intricate physical situation, and therefore one is forced to develop an adequate perturbation theory. In the corresponding first-order approximation, one then gets the energy eigenvalues and the charge distribution for the two-particle system. This then yields some amazing results concerning the matter dichotomy mentioned previously:

- For any value of the mixing parameter C_* , the first-order perturbation results say that the positive mixtures have greater energy eigenvalue than the negative mixtures just as is true for the symmetric case (1.4a) in comparison to the antisymmetric case (1.4b) of the conventional theory (see Fig. 1).
- The RST energy eigenvalues depend upon the mixing parameter C_{*} in such a way that in the pure-state limit (C_{*} → ∞) the results of the conventional theory with vanishing exchange energy E_G (1.6) are reproduced (i.e. neglection of the splitting into para and ortho states). This means that passing over from an RST pure state to an RST mixture implies the splitting into para and ortho states.
- In the conventional theory, the first-order exchange energy E_G (1.6) (producing the para–ortho splitting) is in bad agreement with the experimental data. It is true that the corresponding RST results depend upon the mixing parameter C_* whose value cannot be fixed within the present perturbation order, but there exist values for C_* such that the first-order RST results become arbitrarily close to the experimental data (see Fig. 1). It is true that the reliability of first-order perturbation theory for this range of the mixing parameter C_* remains to be clarified but the emergence of the mixture degeneracy for the pure-state limit $C_* \rightarrow \infty$ is safely established.
- The charge densities of the positive and negative mixtures exhibit a rather different pattern: while the densities ρ_a of positive mixtures assimilate $(\rho_1(x) \approx \rho_2(x))$ and thus demonstrate *charge fusion*, the densities of negative mixtures recede from one another and try to occupy different regions of space ((*charge separation*); see Fig. 3). Thus the positive mixtures strongly resemble the bosonic matter and the negative mixtures the fermionic matter of the conventional theory.

Clearly the conventional theory provides us with the possibility to produce more realistic predictions by taking account of the electron spins, but this possibility exists also for the RST. Indeed, there is no problem with the Dirac theory of the spinning electron, which may be considered as nothing else than a special \mathbb{C}^4 -realization of RST (see Mattes and Sorg, 1999b; Sigg and Sorg, 1997; Sorg, 1997b).



Fig. 3. Electrostatic charge distributions ${}^{(0)}\rho_a$. (a) For the pure states ($\sigma_* = 0$ or $C_* \Rightarrow \infty$), both charge distributions ${}^{(0)}\rho_a$ (4.7) coincide with the squares $({}^{(0)}L_a)^2$ of the amplitudes. (b) But for the negative mixtures ($\sigma_* = -1$) there occurs a complete *charge separation* in the limit case $C_* \Rightarrow C_-$ (=1). The first charge is confined to the *interior* region $y < y_*$ (=3.1633), ${}^{(0)}\rho_1 \neq 0$, ${}^{(0)}\rho_2 \equiv 0$, and from this region the second particle is kept off. Conversely, the first particle cannot invade in this limit the exterior region $y > y_*$ which is exclusively occupied by the second particle: ${}^{(0)}\rho_1 \equiv 0$, ${}^{(0)}\rho_2 \neq 0$. (c) For the positive mixtures ($\sigma_* = +1$), both charge distributions ${}^{(0)}\rho_a$ are *fused* into one another ${}^{(0)}\rho_1 \equiv {}^{(0)}\rho_2$ in the limit $C_* \Rightarrow 0$ and then together occupy all three-space ($0 \le y < \infty$).



Fig. 3. (Continued)

2. RELATIVISTIC SCHRÖDINGER THEORY

Let us first collect the relevant results of some preceding papers into the following sketch of the fundamental building blocks of RST in order to sufficiently elucidate the peculiarities of that theory.

2.1. Wave Function and Intensity Matrix

In RST, matter is described by an (Hermitian) *intensity operator* $\mathcal{I}(x)$ (i.e. a matrix-valued section of the corresponding fiber bundle over space–time). In general, the intensity matrix \mathcal{I} is due to a mixture but in special situations it may be sufficient to deal exclusively with a wave function $\Psi(x)$ (i.e. the section of a complex or real vector bundle). In this latter case the intensity matrix \mathcal{I} degenerates to the tensor product of the wave function Ψ :

$$\mathcal{I} \to \Psi \otimes \bar{\Psi}.$$
 (2.1)

The necessary and sufficient condition for such a degeneration of \mathcal{I} is the *Fierz identity* (Mattes and Sorg, 1999b)

$$\mathcal{I}^2 - \mathcal{I} \cdot \operatorname{tr} \mathcal{I} = 0. \tag{2.2}$$

Whenever this identity is obeyed by \mathcal{I} , it is said that matter is described by the *pure* state Ψ (2.1). In order to obtain some measure for the "purity" of \mathcal{I} one defines

the *Fierz deviator* $\mathcal{D}_{\rm F}$ through (Mattes and Sorg, 1999b)

$$\mathcal{D}_{\mathrm{F}} := \mathcal{I} \cdot \mathrm{tr} \, \mathcal{I} - \mathcal{I}^2 \tag{2.3}$$

and thus a necessary condition for purity is the vanishing of the Fierz deviation $\Delta_{\rm F}$

$$\Delta_{\mathrm{F}} := \mathrm{tr} \, \mathcal{D}_{\mathrm{F}}.\tag{2.4}$$

Concerning the relationship between mixtures and pure states, there does not exist such a rigorous distinction between both concepts in RST as in conventional quantum theory (in atomic physics) where one traditionally deals mainly with the pure states. It was not until recently that one considers the decay of pure states into mixtures as a most natural process (Giulini et al., 1996) and thus acknowledges the concept of mixture as being of equal (or even higher) relevance as the pure states. However in RST, the relationship between mixtures and pure states is more intimate in the sense that the matter configuration is a mixture in one region of space-time and is a pure state in an other region (determined by the zeros of the Fierz deviation Δ_F (2.4)). Subsequently we will present an example of this kind, namely the mass-eigenvalue problem of a scalar two-particle system being bound by the electrostatic Coulomb force (i.e. pointlike force center). With neglection of the exchange effects, such a system can be parametrized by two (scalar) amplitude fields $L_a(x)$ and a mixing parameter C_* , which is an integration constant and measures the purity of the matter configuration ($C_* \rightarrow \infty$: pure state, $C_* < \infty$: mixture). Thus, besides the globally pure states ($C_* = \infty$) there are the mixtures $(C_* < \infty)$ which may, however, degenerate *locally* to a pure state, namely at the zeros of the amplitude fields L_a . Since these amplitudes tend to zero (for localized configurations) at spatial infinity, one has a pure state outside $(r \rightarrow \infty)$ but a mixture inside $(r \rightarrow 0)$. Whether such mixtures are equipped with a greater or a smaller binding energy in comparison to the pure states is the main concern of the present investigation.

2.2. Hamiltonian Dynamics

The motion of matter is governed by the field equation for the intensity operator \mathcal{I} , i.e. the relativistic von Neumann equation (RNE)

$$\mathcal{D}_{\mu}\mathcal{I} = \frac{i}{\hbar c} [\mathcal{I} \cdot \bar{\mathcal{H}}_{\mu} - \mathcal{H}_{\mu} \cdot \mathcal{I}].$$
(2.5)

Here, the *Hamiltonian* \mathcal{H}_{μ} is a $\mathcal{GL}(N, \mathbb{C})$ -valued one-form which in general is neither Hermitian nor anti-Hermitian. It is to be determined from its field equations, namely the *integrability condition*

$$\mathcal{D}_{\mu}\mathcal{H}_{\nu} - \mathcal{D}_{\nu}\mathcal{H}_{\mu} + \frac{i}{\hbar c}[\mathcal{H}_{\mu}, \mathcal{H}_{\nu}] = i\hbar c\mathcal{F}_{\mu\nu}$$
(2.6)

and the conservation equation

$$\mathcal{D}^{\mu}\mathcal{H}_{\mu} - \frac{i}{\hbar c}\mathcal{H}^{\mu}\cdot\mathcal{H}_{\mu} = -i\hbar c \left[\left(\frac{\mathcal{M}c}{\hbar} \right)^2 + i\mathcal{G} \right].$$
(2.7)

The mass operator \mathcal{M} is assumed to be covariantly constant

$$\mathcal{D}_{\mu}\mathcal{M} = 0, \tag{2.8}$$

which can easily be achieved for identical particles by simply putting

$$\mathcal{M} = M \cdot \mathbf{1},\tag{2.9}$$

where *M* is the particle mass. But obviously the *Hamiltonian dynamics* [(2.6) and (2.7)] is based upon two new objects { $\mathcal{G}, \mathcal{F}_{\mu\nu}$ }, which must now be explained in some detail.

First consider the bundle curvature $\mathcal{F}_{\mu\nu}$ which is closely related to the principle of *minimal coupling* of matter and gauge fields. The gauge covariance of RST is namely ensured by consistent use of the gauge covariant derivative \mathcal{D} , e.g. for the Hamiltonian \mathcal{H}_{μ} :

$$\mathcal{D}_{\mu}\mathcal{H}_{\nu} := \nabla_{\mu}\mathcal{H}_{\nu} + [\mathcal{A}_{\mu}, \mathcal{H}_{\nu}]. \tag{2.10}$$

The coordinate-covariant derivative over pseudo-Riemannian space–time is denoted here by ∇ and \mathcal{A}_{μ} is the *bundle connection* one-form which takes its values in the Lie algebra of the gauge group. The corresponding *curvature* $\mathcal{F}_{\mu\nu}$ is defined as usual

$$\mathcal{F}_{\mu\nu} := \nabla_{\mu}\mathcal{A}_{\nu} - \nabla_{\nu}\mathcal{A}_{\mu} + [\mathcal{A}_{\mu}, \mathcal{A}_{\nu}]$$
(2.11)

and thus obeys the well-known Bianchi identity

$$\mathcal{D}_{\lambda}\mathcal{F}_{\mu\nu} + \mathcal{D}_{\mu}\mathcal{F}_{\nu\lambda} + \mathcal{D}_{\nu}\mathcal{F}_{\lambda\mu} \equiv 0.$$
(2.12)

Furthermore, the curvature $\mathcal{F}_{\mu\nu}$ enters the integrability condition (2.6) on the righthand side, and therefore it is just that condition which ensures the validity of the *bundle identity* for the intensity matrix \mathcal{I}

$$[\mathcal{D}_{\mu}\mathcal{D}_{\nu} - \mathcal{D}_{\nu}\mathcal{D}_{\mu}]\mathcal{I} = [\mathcal{F}_{\mu\nu}, \mathcal{I}].$$
(2.13)

For the special case (2.1), where the matter system is in a pure state Ψ , the RNE (2.5) is replaced by the relativistic Schrödinger equation (RSE)

$$i\hbar c\mathcal{D}_{\mu}\Psi = \mathcal{H}_{\mu}\cdot\Psi, \qquad (2.14)$$

where

$$\mathcal{D}_{\mu}\Psi \, \doteqdot \, \partial_{\mu}\Psi + \mathcal{A}_{\mu}\cdot\Psi,$$

and the integrability condition (2.6) then ensures the validity of the bundle identity for Ψ :

$$[\mathcal{D}_{\mu}\mathcal{D}_{\nu} - \mathcal{D}_{\nu}\mathcal{D}_{\mu}]\Psi \equiv \mathcal{F}_{\mu\nu} \cdot \Psi.$$
(2.15)

Thus, it should have become obvious that the meaning of the integrability condition (2.6) refers to the intrinsic consistency of the system of field equations for matter.

2.3. Gauge Field

The field equation for the gauge field itself is chosen as the (generalized) Maxwell equation

$$\mathcal{D}^{\mu}\mathcal{F}_{\mu\nu} = 4\pi\alpha\mathcal{J}_{\nu}.$$
(2.16)

Here the coupling operator α must be covariantly constant ($\mathcal{D}_{\mu}\alpha \equiv 0$) in order that the Maxwell equations (2.16) automatically imply the charge conservation law as usual

$$\mathcal{D}^{\mu}\mathcal{J}_{\mu} \equiv 0, \qquad (2.17)$$

namely via the bundle identity for the curvature $\mathcal{F}_{\mu\nu}$

$$\mathcal{D}^{\mu}\mathcal{D}^{\nu}\mathcal{F}_{\mu\nu} \equiv 0. \tag{2.18}$$

Sometimes it may also be convenient to recast the gauge field equations in component form. To this end, decompose the connection A_{μ} and its curvature $\mathcal{F}_{\mu\nu}$ with respect to the generators $\{\tau^a\}$ of the gauge group (more precisely, holonomy group) as follows:

$$\mathcal{A}_{\mu} = A_{a\mu}\tau^a \tag{2.19a}$$

$$\mathcal{F}_{\mu\nu} = F_{a\mu\nu}\tau^a. \tag{2.19b}$$

The field strengths $F_{a\mu\nu}$ read then in terms of the gauge potentials $A_{a\mu}$

$$F_{a\mu\nu} = \nabla_{\mu}A_{a\nu} - \nabla_{\nu}A_{a\mu} \tag{2.20}$$

where we have restricted ourselves to an abelian gauge group (i.e., $[\tau^a, \tau^b] = 0$), e.g. to the product group $U(1) \times U(1) \times U(1) \times \cdots \times U(1)$ for an electromagnetic *N*-particle system (Mattes *et al.*, 1999).

A similar decomposition for the current \mathcal{J}_{μ} reads

$$\mathcal{J}_{\mu} = j_{a\mu} \tau^a \tag{2.21}$$

so that the abstract conservation law (2.17) yields the N conservation laws

$$\nabla^{\mu} j_{a\mu} = 0 \tag{2.22}$$

where

$$a = 1, \dots, N \tag{2.23}$$

for the N charged particles; furthermore, the abstract Maxwell equations (2.16) become more concretely

$$\nabla^{\mu}F_{a\mu\nu} = 4\pi\alpha j_{a\nu}.$$
(2.24)

(For identical particles we can consider the coupling matrix α as an ordinary real number.)

2.4. Convertor and Currents

Next turn to the second new object in the Hamiltonian dynamics, namely the *convertor* \mathcal{G} in the conservation equation (2.7), and observe that this equation is responsible for the conservation laws (2.22). Remember here that our total field system consists of the RNE (2.5), the Hamiltonian dynamics [(2.6) and (2.7)], and the Maxwell equation (2.16). But this system can be closed only through specifying the current \mathcal{J}_{μ} in terms of the matter field, i.e. the intensity matrix \mathcal{I} (or the wave function Ψ , resp.). Clearly this specification of the currents $j_{a\mu}$ in terms of the matter field must be performed in such a way that the conservation laws (2.22) are *automatically* obeyed as a direct consequence of the operator equations for \mathcal{I} and \mathcal{H}_{μ} ! This requirement will then reveal the meaning of the convertor \mathcal{G} on the right-hand side of the conservation equation (2.7).

In order to get the desired link between the currents $j_{a\mu}$ and the intensity matrix \mathcal{I} we introduce the (Hermitian) velocity operators $v_{a\mu}$ ($=\bar{v}_{a\mu}$) and put

$$j_{a\mu} = \operatorname{tr}(\mathcal{I} \cdot v_{a\mu}). \tag{2.25}$$

This ansatz converts the conservation requirement for the currents $j_{a\mu}$ (2.22) to the following condition upon the velocity operators:

$$\nabla^{\mu} j_{a\mu} = \operatorname{tr} \left\{ \mathcal{I} \cdot \left(\mathcal{D}^{\mu} v_{a\mu} + \frac{i}{\hbar c} [\bar{\mathcal{H}}^{\mu} \cdot v_{a\mu} - v_{a\mu} \cdot \mathcal{H}^{\mu}] \right) \right\} \stackrel{!}{=} 0.$$
(2.26)

In order to meet now with this condition we subject the velocity operators to the following requirement:

$$\mathcal{D}^{\mu}v_{a\mu} + \frac{i}{\hbar c}(\bar{\mathcal{H}}^{\mu} \cdot v_{a\mu} - v_{a\mu} \cdot \mathcal{H}^{\mu}) = \frac{\hbar}{Mc}\mathcal{G}_a$$
(2.27)

where the newly introduced (Hermitian) convertors G_a are required to obey the following algebraic constraint:

$$\operatorname{tr}(\mathcal{G}_a \cdot \mathcal{I}) = 0. \tag{2.28}$$

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Now it is easy to see that a solution of the requirement (2.27) for $v_{a\mu}$ is given by

$$v_{a\mu} = \frac{i}{2Mc^2} (\bar{\mathcal{H}}_{\mu} \cdot \tau_a + \tau_a \cdot \mathcal{H}_{\mu})$$
(2.29)

because by means of the conservation equation (2.7) we then immediately find the Hermitian convertors \mathcal{G}_a in terms of the former \mathcal{G} (2.7) as

$$\mathcal{G}_a = \frac{i}{2} (\tau_a \cdot \mathcal{G} + \bar{\mathcal{G}} \cdot \tau_a) \equiv \bar{\mathcal{G}}_a. \tag{2.30}$$

Indeed this is a nice result because it enables us to satisfy the original conservation requirement for the currents $j_{a\mu}$ (2.22), as ultimately expressed by that constraint (2.28), by simply putting

$$\mathcal{G} \cdot \mathcal{I} = 0. \tag{2.31a}$$

Additionally this algebraic constraint (2.31a), if transcribed to the wave function Ψ :

$$\mathcal{G} \cdot \Psi = 0, \tag{2.31b}$$

ensures the validity of the Klein-Gordon equation (KGE)

$$\mathcal{D}^{\mu}\mathcal{D}_{\mu}\Psi + \left(\frac{\mathcal{M}c}{\hbar}\right)^{2}\Psi = 0.$$
(2.32)

This is easily verified by differentiating once more the RSE (2.14) and applying just the conservation equation (2.7).

2.5. Energy–Momentum Density

Thus we have obtained now a closed system of equations of motion for our electromagnetic N-particle system. In order to gain further confidence into its intrinsic consistency, consider the energy–momentum conservation law

$$\nabla^{\mu}T_{\mu\nu} = f_{\nu}. \tag{2.33}$$

Here, the force density f_{ν} exerted upon the matter distribution emerges as the source of the matter energy–momentum density $T_{\mu\nu}$ and, according to the original Lorentzian idea, it should be composed of the currents $j_{a\mu}$ and field strengths $F_{a\mu\nu}$, i.e. one expects the following form:

$$f_{\nu} = \hbar c F_{a\mu\nu} j^{a\mu}. \tag{2.34}$$

However this result is actually obtained within the framework of our RST, provided we construct the energy–momentum density $T_{\mu\nu}$ of matter in the following way:

$$T_{\mu\nu} = \operatorname{tr}(\mathcal{I} \cdot \mathcal{T}_{\mu\nu}) \tag{2.35}$$

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and build up the *energy-momentum operator* $\mathcal{T}_{\mu\nu}$ in terms of the Hamiltonian \mathcal{H}_{μ}

$$\mathcal{T}_{\mu\nu} = \frac{1}{2Mc^2} [\bar{\mathcal{H}}_{\mu} \cdot \mathcal{H}_{\nu} + \bar{\mathcal{H}}_{\nu} \cdot \mathcal{H}_{\mu} - g_{\mu\nu} (\bar{\mathcal{H}}^{\lambda} \cdot \mathcal{H}_{\lambda} - (\mathcal{M}c^2))^2].$$
(2.36)

2.6. Polarization

Finally, let us also mention the effect of *polarization* of matter which will subsequently help us to classify the totality of possible field configurations into certain simple subcases. Although the Hamiltonian \mathcal{H}_{μ} is in general non-Hermitian $(\mathcal{H}_{\mu} \neq \tilde{\mathcal{H}}_{\mu})$, it is convenient to deal with Hermitian objects through the splitting

$$\mathcal{H}_{\mu} = \hbar c (\mathcal{K}_{\mu} + i \mathcal{L}_{\mu}), \qquad (2.37)$$

where the *kinetic field* \mathcal{K}_{μ} ($=\bar{\mathcal{K}}_{\mu}$) is the Hermitian part of the Hamiltonian \mathcal{H}_{μ} and the *localization field* \mathcal{L}_{μ} ($=\bar{\mathcal{L}}_{\mu}$) constitutes its anti-Hermitian part. Introducing this splitting into the velocity operators $v_{a\mu}$ (2.29) yields a decomposition of these objects into their *convection* and *polarization* parts

$$v_{a\mu} = {}^{(C)}v_{a\mu} + {}^{(P)}v_{a\mu}.$$
(2.38)

Here, the convection part ${}^{(C)}v_{a\mu}$ is determined by the kinetic field \mathcal{K}_{μ}

$$^{(C)}v_{a\mu} = \frac{i\hbar}{2Mc} \{\mathcal{K}_{\mu}, \tau_a\}$$
(2.39)

whereas the polarization part is rather related to the localization field \mathcal{L}_{μ} through

$$^{(P)}v_{a\mu} = \frac{\hbar}{2Mc} [\mathcal{L}_{\mu}, \tau_a].$$
(2.40)

Clearly this then yields an analogous splitting of the currents themselves:

$$j_{a\mu} = {}^{(C)}j_{a\mu} + {}^{(P)}j_{a\mu}$$
(2.41a)

$$^{(C)}j_{a\mu} = \operatorname{tr}\left(\mathcal{I} \cdot {}^{(C)}v_{a\mu}\right) \tag{2.41b}$$

$${}^{(\mathrm{P})}j_{a\mu} = \mathrm{tr}\big(\mathcal{I}\cdot{}^{(\mathrm{P})}v_{a\mu}\big). \tag{2.41c}$$

After all the essential ingredients of RST have been collected, we can turn to the two-particle systems being characterized by two independent and nontrivial "charge numbers" z_a (a = 1, 2)

$$z_a = \int_{(S)} j_{a\mu} \, dS^{\mu}, \tag{2.42}$$

which appear as the integrals of the currents $j_{a\mu}$ over some three-dimensional (space-like) hypersurface (S) of space-time. We will consider only identical particles and will then interpret the charge numbers z_a as dimensionaless quantum

numbers ($z_1 = z_2 = 1$). Thus the integrals (2.42) acquire the status of normalization conditions.

3. \mathbb{C}^2 -REALIZATION OF RST

For a two-particle system it should be self-evident that the minimal fiber dimension N for the vector bundle of wave functions is N = 2. Thus the wave functions $\Psi(x)$ have two components

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} L_1 e^{-i\alpha_1} \\ L_2 e^{-i\alpha_2} \end{pmatrix}$$
(3.1)

and the corresponding operators over the two-dimensional complex space \mathbb{C}^2 are $\mathcal{GL}(2, \mathbb{C})$ -valued objects. A thorough study of these operator sections is indispensable for the subsequent deductions of the two-particle wave equations. Thus we have to first clarify the *kinematical* fundamentals of the two-particle theory and then we can discuss its *dynamical* aspects.

3.1. Operator Basis and Gauge Group

As usual, the kinematics is discussed by reference to a certain operator basis. A Hermitian basis for the operators acting over the vector fiber \mathbb{C}^2 is given by two projectors $\mathcal{P}_a = (\bar{\mathcal{P}}_a)$

$$\mathcal{P}_1 \cdot \mathcal{P}_2 = 0 \tag{3.2a}$$

$$\mathcal{P}_1 + \mathcal{P}_2 = \mathbf{1} \tag{3.2b}$$

$$\operatorname{tr} \mathcal{P}_1 = \operatorname{tr} \mathcal{P}_2 = 1, \tag{3.2c}$$

which may be complemented by two further *permutators* $\Pi_a = \overline{\Pi}_a (a = 1, 2)$ such that the following algebra holds:

$$\{\Pi_a, \mathcal{P}_b\} = \Pi_a \tag{3.3a}$$

$$[\mathcal{P}_1, \Pi^a] = -[\mathcal{P}_2, \Pi^a] = i\varepsilon^a{}_b\Pi^b \tag{3.3b}$$

$$\{\Pi_a, \Pi_b\} = 2\delta_{ab} \cdot \mathbf{1} \tag{3.3c}$$

$$[\Pi_a, \Pi_b] = 2i\varepsilon_{ab}(\mathcal{P}_1 - \mathcal{P}_2). \tag{3.3d}$$

A convenient representation of this algebra is given by the Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$, i.e.

$$\mathcal{P}_1 = \frac{1}{2}(\mathbf{1} + \sigma_z) \tag{3.4a}$$

$$\mathcal{P}_2 = \frac{1}{2}(\mathbf{1} - \sigma_z) \tag{3.4b}$$

$$\Pi_1 = \sigma_x \tag{3.4c}$$

$$\Pi_2 = \sigma_y. \tag{3.4d}$$

This operator basis { \mathcal{P}_a , Π_b } is called the *single-particle basis* (SPB) because the projectors \mathcal{P}_a can be thought to project onto the single-particle subspaces of the total vector fiber $\mathbb{C}^2 = \mathbb{C}^1 \oplus \mathbb{C}^1$, so that the corresponding vector bundle of two-particle wave functions appears as the Whitney sum of the two single-particle bundles.

Similarly as in classical physics, a system of two point particles can be considered as one particle with internal degress of freedom (thus introducing the center-of-mass frame). In this sense the *extended-particle basis* {1, Q, Π_a } (EPB) is obtained from the SPB through

$$\mathcal{P}_1 + \mathcal{P}_2 = \mathbf{1} \tag{3.5a}$$

$$\mathcal{P}_1 - \mathcal{P}_2 \doteqdot \mathcal{Q}. \tag{3.5b}$$

Correspondingly, any operator can be expanded with respect to both basis systems where its components are then subject to the corresponding transformation relations. For instance, the intensity operator \mathcal{I} reads in the SPB formalism

$$\mathcal{I} = \rho_a \mathcal{P}^a + \frac{1}{2} s_a \Pi^a \tag{3.6}$$

(summation over double indices in opposite positions, the fiber metric is $g_{ab} = -\text{tr}(\tau_a \cdot \tau_b) \equiv \delta_{ab}$), or it can be specified in the EPB formalism as

$$\mathcal{I} = \frac{1}{2} (\rho \cdot \mathbf{1} + q \cdot \mathcal{Q} + s_a \Pi^a).$$
(3.7)

Evidently the corresponding transformation formulae are then given by

$$\rho = \rho_1 + \rho_2 \tag{3.8a}$$

$$q = \rho_1 - \rho_2. \tag{3.8b}$$

Similar relations also apply to the kinetic field \mathcal{K}_{μ}

$$\mathcal{K}_{\mu} = \begin{cases} K_{a\mu} \mathcal{P}^a + Q_{a\mu} \Pi^a, \quad (SPB) \qquad (3.9a) \end{cases}$$

$$\int_{\mu} \frac{1}{2} K_{\mu} \cdot \mathbf{1} + \frac{1}{2} k_{\mu} \mathcal{Q} + Q_{a\mu} \Pi^{a}, \quad \text{(EPB)}$$
(3.9b)

and to the localization field \mathcal{L}_{μ}

$$\mathcal{L}_{\mu} = \begin{cases} L_{a\mu} \mathcal{P}^a + N_{a\mu} \Pi^a, \quad (SPB) \quad (3.10a) \end{cases}$$

$$\sum_{\mu} = \left\{ \frac{1}{2} L_{\mu} \cdot \mathbf{1} + \frac{1}{2} l_{\mu} \mathcal{Q} + N_{a\mu} \Pi^{a}, \quad \text{(EPB)}. \right.$$
(3.10b)

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Furthermore, the single-particle generators τ_a for the electromagnetic twoparticle gauge group $U(1) \times U(1)$ are chosen as (a = 1, 2)

$$\tau_a = -i\mathcal{P}_a \tag{3.11}$$

and thus are covariantly constant

$$\mathcal{D}_{\mu}\tau_{a}=0. \tag{3.12}$$

And again, instead of decomposing the connection A_{μ} and curvature $\mathcal{F}_{\mu\nu}$ with respect to SPB (3.11) as shown in (2.19a) and (2.19b), one can resort to the EPB decomposition

$$\mathcal{A}_{\mu} = -i\hat{A}_{\mu} \cdot \mathbf{1} - ia_{\mu} \cdot \mathcal{Q}$$
(3.13a)

$$\mathcal{F}_{\mu\nu} = -i\hat{F}_{\mu\nu} \cdot \mathbf{1} - if_{\mu\nu}\mathcal{Q}, \qquad (3.13b)$$

with the EPB components being related to their SPB counterparts through

$$\hat{A}_{\mu} = \frac{1}{2} (A_{1\mu\nu} + A_{2\mu\nu}) \tag{3.14a}$$

$$a_{\mu} = \frac{1}{2} (A_{1\mu\nu} - A_{2\mu\nu}), \qquad (3.14b)$$

and similarly for the field strengths

$$\hat{F}_{\mu\nu} = \frac{1}{2}(F_{1\mu\nu} + F_{2\mu\nu})$$
(3.14c)

$$f_{\mu\nu} = \frac{1}{2}(F_{1\mu\nu} - F_{2\mu\nu}). \tag{3.14d}$$

Clearly, the mean gauge potential \hat{A}_{μ} generates the mean field strength $\hat{F}_{\mu\nu}$:

$$\hat{F}_{\mu\nu} = \nabla_{\mu}\hat{A}_{\nu} - \nabla_{\nu}\hat{A}_{\mu}, \qquad (3.14e)$$

and the analogous relationship holds for the *internal gauge potential* a_{μ} and *internal field strength* $f_{\mu\nu}$:

$$f_{\mu\nu} = \nabla_{\mu}a_{\nu} - \nabla_{\nu}a_{\mu}. \tag{3.14f}$$

The EPB formulation seems to be advantageous because it directly leads to the emergence of an SO(2) subbundle. Indeed the typical gauge element $S \in U(1) \times U(1)$ is written in the EPB form as

$$S = \exp(-iA \cdot \mathbf{1} - ia \cdot Q)$$

= $\exp(-iA \cdot \mathbf{1}) \cdot \exp(-iaQ)$ (3.15)
:= $S_{\operatorname{tot}(A)} \cdot S_{\operatorname{rel}(a)}$

and then it is found that the permutators Π_a transform as an SO(2) gauge doublet under the action of the *relative group* { S_{rel} }, i.e.

$$\mathcal{S} \cdot \Pi_a \cdot \mathcal{S}^{-1} = \mathcal{S}_{\text{rel}} \cdot \Pi_a \cdot \mathcal{S}_{\text{rel}}^{-1} = \Pi_b \cdot \mathring{\mathcal{S}}_a^b.$$
(3.16)

Here $\mathbf{\ddot{S}}$ is an SO(2) element of the relative group

$$\mathring{S}^{a}_{b} = \cos 2a \cdot \delta^{a}_{b} - \sin 2a \cdot \varepsilon^{a}_{b}$$
(3.17)

and $\varepsilon_{ab} = -\varepsilon_{ba}$ is the SO(2) invariant permutation tensor in two dimensions. The corresponding SO(2) subconnection $\mathring{\omega}^a_{b\mu}$ is immediately deduced from the original $U(1) \times U(1)$ connection \mathcal{A}_{μ} by means of the covariant derivative of the permutator doublet

$$\mathcal{D}_{\mu}\Pi_{a} = \Pi_{b} \cdot \mathring{\omega}^{b}_{a\mu} \tag{3.18a}$$

with

$$\mathring{\omega}^{b}_{a\mu} = -2a_{\mu} \cdot \varepsilon^{b}_{a}. \tag{3.18b}$$

Thus we arrive at the plausible result that the *internal* degree of freedom of the extended particle is gauged by the relative subgroup $\{S_{rel}\}$ alone. This internal degree of freedom is not affected at all by the action of the total subgroup $\{S_{tot}\}$ which is expected to refer to the *external* (i.e. center-of-mass) motion of the two-particle system. As a simple example for this mechanism, consider a general $U(1) \times U(1)$ gauge transformation of the intensity matrix \mathcal{I} :

$$\mathcal{I} \to \mathcal{I}' = \mathcal{S} \cdot \mathcal{I} \cdot \mathcal{S}^{-1}$$
$$= \frac{1}{2} (\rho \cdot \mathbf{1} + q \cdot \mathcal{Q} + s'_a \Pi^a). \tag{3.19}$$

Obviously, the total and relative densities ρ and q remain invariant whereas the *overlap densities* {*s*_{*a*}} transform as the components of an SO(2) vector field

$$s'_a = s_b \cdot \mathring{S}^b_a. \tag{3.20}$$

As a consequence the derivative of this vector must also be constructed in a gauge covariant way:

$$D_{\mu}s_{a} = \partial_{\mu}s_{a} - s_{b}\mathring{\omega}^{b}_{a\mu}.$$
(3.21)

3.2. Rotating Basis and Polarization Currents

The existence of the overlap densities s_a gives rise to a rotating but gauge invariant permutator doublet $\widehat{\Pi}$, $\widetilde{\Pi}$:

$$\widehat{\Pi} = \widehat{s}_a \Pi^a \tag{3.22a}$$

$$\widetilde{\Pi} = \varepsilon^{ab} \hat{s}_a \Pi_b, \qquad (3.22b)$$

where

$$\hat{s}_a = \frac{s_a}{s}, \quad s^2 = s^a s_a.$$

With respect to this *rotating basis* (RTB) $\{1, Q, \widetilde{\Pi}, \widehat{\Pi}\}$ the intensity matrix reads

$$\mathcal{I} = \frac{1}{2}(\rho \cdot \mathbf{1} + q\mathcal{Q} + s\widehat{\Pi}). \tag{3.23}$$

Subsequently we shall frequently make use of this decomposition of \mathcal{I} , together with an analogous decomposition of the *exchange fields* $Q_{a\mu}$ and $N_{a\mu}$ occurring in the Hamiltonian [(3.9) and (3.10)]:

$$Q_{a\mu} = {}^{(\parallel)}Q_{\mu} \cdot \hat{s}_a + {}^{(\perp)}Q_{\mu} \cdot \varepsilon_a^b \hat{s}_b \tag{3.24a}$$

$$N_{a\mu} = {}^{(\parallel)}N_{\mu} \cdot \hat{s}_a + {}^{(\perp)}N_{\mu} \cdot \varepsilon_a^b \hat{s}_b.$$
(3.24b)

The obvious advantage of the RTB is the gauge invariance of the operator components. Therefore in place of dealing with the gauge objects s_a , $Q_{a\mu}$, and $N_{a\mu}$ one can now resort to their gauge invariant counterparts s, ${}^{(\parallel)}Q_{\mu}$, ${}^{(\perp)}Q_{\mu}$, ${}^{(\parallel)}N_{\mu}$, and ${}^{(\perp)}N_{\mu}$. This enables us to write down subsequently the field equations in a gauge *invariant* way. (The RTB formalism has always been used for the treatments of Dirac's spinor theory as a possible \mathbb{C}^4 -realization of RST; see, e.g., Mattes and Sorg, 1999b.)

Finally, let us also discuss the polarization currents with respect to the change of basis from SPB to RTB. Originally the currents had been defined in their single-particle form $j_{a\mu}$ (2.25). Observing here too that splitting (2.41a)–(2.41c) into the convection and polarization parts yields for the first current by means of the two-particle Hamiltonian [(3.9) and (3.10)]

$$j_{1\mu} = {}^{(C)}j_{1\mu} + {}^{(P)}j_{1\mu}$$
(3.25a)

$${}^{(C)}j_{1\mu} = \frac{\hbar}{Mc} \left(\rho_1 K_{1\mu} + \frac{1}{2} s \cdot {}^{(\parallel)}Q_{\mu} \right)$$
(3.25b)

$${}^{(\mathrm{P})}j_{1\mu} = \frac{\hbar}{2Mc} \cdot \varepsilon^{ab} s_a N_{b\mu} \equiv \frac{\hbar}{2Mc} s \cdot {}^{(\perp)}N_{\mu}$$
(3.25c)

and similarly for the second current

$$j_{2\mu} = {}^{(C)}j_{2\mu} + {}^{(P)}j_{2\mu}$$
(3.26a)

$${}^{(C)}j_{2\mu} = \frac{\hbar}{Mc} \left(\rho_2 K_{2\mu} + \frac{1}{2} s \cdot {}^{(\parallel)}Q_{\mu} \right)$$
(3.26b)

$${}^{(\mathrm{P})}j_{2\mu} = -\frac{\hbar}{2Mc}\varepsilon^{ab}s_a N_{b\mu} \equiv -\frac{\hbar}{2Mc}s \cdot {}^{(\perp)}N_{\mu}. \tag{3.26c}$$

From this result we learn that, for the special case of a pure state Ψ (3.1), the polarization parts $^{(P)}j_{a\mu}$ can be different from zero only when the two wave functions ψ_a are overlapping and thus the overlap density *s* becomes nonzero!

The single-particle densities of a pure 2-particle state assume their corresponding special forms

$$\rho_1 = \operatorname{tr}(\mathcal{I} \cdot \mathcal{P}_1) \to \overline{\Psi} \cdot \mathcal{P}_1 \cdot \Psi = L_1^2 \tag{3.27a}$$

$$\rho_2 = \operatorname{tr}(\mathcal{I} \cdot \mathcal{P}_2) \to \overline{\Psi} \cdot \mathcal{P}_2 \cdot \Psi = L_2^2 \tag{3.27b}$$

$$s_1 = \operatorname{tr}(\mathcal{I} \cdot \Pi_1) \to \overline{\Psi} \cdot \Pi_1 \cdot \Psi = 2L_1L_2 \cos(\alpha_1 - \alpha_2)$$
 (3.27c)

$$s_2 = \operatorname{tr}(\mathcal{I} \cdot \Pi_2) \to \overline{\Psi} \cdot \Pi_2 \cdot \Psi = 2L_1L_2 \, \sin\left(\alpha_1 - \alpha_2\right) \qquad (3.27d)$$

$$s = \operatorname{tr}(\mathcal{I} \cdot \Pi) \to \Psi \cdot \Pi \cdot \Psi = 2L_1L_2.$$
 (3.27e)

From the last equation one can now see explicitly that the overlap scalar *s* actually is nonzero only for overlapping wave packets ψ_a . (Hint: convince yourself for the present pure-state case [(3.27a)–(3.27e)] that the Fierz identity (2.2) is satisfied, e.g. in the EPB form

$$\rho^2 - (q^2 + s^2) = 0. \tag{3.28}$$

Of course, the general form [(3.25a)-(3.26c)] for the single-particle currents does hold for the mixtures and not just for the pure states.

But now transcribe the single-particle currents $j_{a\mu}$ to their EPB forms J_{μ} , j_{μ}

$$J_{\mu} \doteqdot j_{1\mu} + j_{2\mu} \tag{3.29a}$$

$$j_{\mu} \doteqdot j_{1\mu} - j_{2\mu} \tag{3.29b}$$

and then find

$$J_{\mu} = \frac{\hbar}{2Mc} \left(\rho \cdot K_{\mu} + q \cdot k_{\mu} + 2s \cdot {}^{(\parallel)}Q_{\mu} \right)$$
(3.30a)

$$j_{\mu} = \frac{\hbar}{2Mc} \left(\rho \cdot k_{\mu} + q \cdot K_{\mu} + 2s \cdot {}^{(\perp)}N_{\mu} \right).$$
(3.30b)

This is a very satisfying result because the *total current* J_{μ} (3.30a) does not contain the polarization parts $(\sim^{(\perp)}N_{\mu})$, cf. (3.25c) and (3.26c), and is therefore built up exclusively by the convection parts of the single-particle currents. Indeed the total current J_{μ} must be considered as an *external* object which survives the point-particle limit $(q, s \mid \rightarrow 0)$ and therefore mainly describes the point-particle properties of the extended particle with a weak coupling to its intrinsic degrees of freedom. Observe also that it is the total current J_{μ} which has to carry the total charge number (N = 2) of the two-particle system, cf. (2.42)

$$\int_{(S)} J_{\mu} \cdot dS^{\mu} = \int_{(S)} j_{1\mu} \cdot dS^{\mu} + \int_{(S)} j_{2\mu} \cdot dS^{\mu} = 2, \qquad (3.31)$$

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whereas the *relative current* j_{μ} appears as a "neutral" current and therefore carries a trivial charge number:

$$\int_{(S)} j_{\mu} \cdot dS^{\mu} = \int_{(S)} j_{1\mu} \cdot dS^{\mu} - \int_{(S)} j_{2\mu} \cdot dS^{\mu} = 0.$$
(3.32)

However the internal degrees of freedom of the extended particle are described by the relative current j_{μ} (3.30b) which contains twice the polarization parts ($\sim^{(\perp)}N_{\mu}$) of the single-particle currents. Concerning the polarization part ($^{(P)}j_{a\mu}$, observe that such a quantity does not exist in a truly (scalar) single-particle theory where only single particle is present. Such a single-particle situation is to be described by the \mathbb{C}^1 -realization of RST (Mattes and Sorg, 1999a), which is the adequate description of point particles and coincides with the conventional Klein–Gordon theory. Thus we have to conclude that the polarization properties of either (scalar) particle of a two-particle system do arise by virtue of the presence of the other particle! This appears plausible because *scalar* particles cannot carry *intrinsic* polarization.

3.3. Integrability Condition

Now that the kinematics of the two-particle systems has sufficiently been clarified through the preceding considerations, one can turn to the dynamical aspects of those systems. First let us study somewhat closer the Hamiltonian dynamics [(2.6) and (2.7)] and defer the density dynamics (2.5) to the next subsection (the dynamical equations for the gauge field (2.16) are not discussed in the present paper; for their treatment, see Mattes *et al.*, 1999). The two-particle dynamics has already been investigated in a preceding paper (Mattes and Sorg, 1999c), but this was done in the SPB formalism which however seems not so convenient as the RTB formalism for the present purposes. Therefore it may be sufficient here to take over those dynamical SPB relations which are of interest in the present context, and transcribe them to their RTB from which then facilitates the subsequent investigations.

In this sense, consider first the integrability condition (2.6) which in the first place yields for the EPB localization field L_{μ} (3.10b) the following relation:

$$\nabla_{\mu}L_{\nu} - \nabla_{\nu}L_{\mu} = 0. \tag{3.33}$$

Thus the vector L_{μ} turns out to be a gradient field and therefore enables us to introduce an *amplitude field* L(x) through

$$L_{\mu} = \frac{\partial_{\mu}L^2}{L^2} = 2\frac{\partial_{\mu}L}{L}.$$
(3.34)

But in contrast to this pleasant result, the other localization coefficient l_{μ} (3.10b) surely is not a gradient field in general, because the integrability condition implies

a nontrivial curl relation:

$$\nabla_{\mu}l_{\nu} - \nabla_{\nu}l_{\mu} = 4 \big({}^{(\parallel)}N_{\mu} \cdot {}^{(\perp)}Q_{\nu} - {}^{(\parallel)}N_{\nu} \cdot {}^{(\perp)}Q_{\mu} - {}^{(\perp)}N_{\mu} \cdot {}^{(\parallel)}Q_{\nu} + {}^{(\perp)}N_{\nu} \cdot {}^{(\parallel)}Q_{\mu} \big).$$
(3.35)

The next interesting point refers to the kinetic fields K_{μ} and k_{μ} , cf. (3.9b). By means of the integrability condition, their curl is found to be related to the field strengths but this occurs in a rather different way for the total and relative parts, namely

$$\nabla_{\mu}K_{\nu} - \nabla_{\nu}K_{\mu} = 2\hat{F}_{\mu\nu} \tag{3.36a}$$

and

$$\nabla_{\mu}k_{\nu} - \nabla_{\nu}k_{\mu} = 2f_{\mu\nu} + 2G_{\mu\nu}, \qquad (3.36b)$$

where the *exchange field strength* $G_{\mu\nu}$ is found as

$$G_{\mu\nu} = 2 \Big({}^{(\parallel)}Q_{\mu} \cdot {}^{(\perp)}Q_{\nu} - {}^{(\parallel)}Q_{\nu} \cdot {}^{(\perp)}Q_{\mu} - {}^{(\parallel)}N_{\mu} \cdot {}^{(\perp)}N_{\nu} + {}^{(\parallel)}N_{\nu} \cdot {}^{(\perp)}N_{\mu} \Big).$$
(3.36c)

Observe here that the total kinetic field K_{μ} "feels" twice the mean field strength $\hat{F}_{\mu\nu}$! The reason is that the mean field $\hat{F}_{\mu\nu}$ refers to only one charge unit by its very definition (3.14c) but on the other hand the total kinetic field K_{μ} is related to the total J_{μ} (3.30a) with its double charge number (3.31). This is seen more clearly by reconstructing these currents in terms of the corresponding velocity operators \mathcal{V}_{μ} and ν_{μ} which yields

$$J_{\mu} = \operatorname{tr}(\mathcal{I} \cdot \mathcal{V}_{\mu}) \tag{3.37a}$$

$$j_{\mu} = \operatorname{tr}(\mathcal{I} \cdot \nu_{\mu}), \qquad (3.37b)$$

with the *total velocity operator* V_{μ} being identical to the total kinetic field \mathcal{K}_{μ} (up to a constant factor)

$$\mathcal{V}_{\mu} := v_{1\mu} + v_{2\mu} = \frac{\hbar}{Mc} \mathcal{K}_{\mu}.$$
 (3.38)

Thus the total velocity V_{μ} is of purely convective nature (cf. the velocity splitting (2.38) and (2.39)), whereas the relative velocity v_{μ}

$$v_{\mu} := v_{1\mu} - v_{2\mu} = \frac{1}{2Mc^2} (\bar{\mathcal{H}}_{\mu} \cdot \mathcal{Q} + \mathcal{Q} \cdot \mathcal{H}_{\mu})$$
(3.39)

contains also a polarization part $^{(P)}v_{\mu}$

$$v_{\mu} = {}^{(C)}v_{\mu} + {}^{(P)}v_{\mu}, \qquad (3.40)$$

which together with its convective counterpart ${}^{(C)}v_{\mu}$ is found in the RTB form as

$${}^{(C)}v_{\mu} = \frac{\hbar}{2Mc} \{\mathcal{K}_{\mu}, \mathcal{Q}\} = \frac{\hbar}{2Mc} (K_{\mu} \cdot \mathcal{Q} + k_{\mu} \cdot \mathbf{1})$$
(3.41a)

$${}^{(\mathrm{P})}v_{\mu} = \frac{i\hbar}{2Mc}[\mathcal{Q}, \mathcal{L}_{\mu}] = \frac{\hbar}{Mc} \big({}^{(\perp)}N_{\mu} \cdot \widehat{\Pi} - {}^{(\parallel)}N_{\mu} \cdot \widetilde{\Pi}\big).$$
(3.41b)

In any case, the convective nature (3.38) of the total current J_{μ} (3.37a) together with its double charge number (3.31) makes it plausible that the curl of K_{μ} should be *twice* the mean field $\hat{F}_{\mu\nu}$ as it is expressed by Eq. (3.36a).

But the curl relation for the relative kinetic field k_{μ} (3.36b) has some striking features too. Evidently this field does not only "feel" the internal field strength $f_{\mu\nu}$, being defined through Eq. (3.14d), but also the *exchange field strength* $G_{\mu\nu}$ (3.36c). It is easy to see that this field obeys the following condition in a pseudo-Riemannian space–time:

$$\nabla_{\mu}G_{\nu\lambda} + \nabla_{\nu}G_{\lambda\mu} + \nabla_{\lambda}G_{\mu\nu} \equiv 0, \qquad (3.42)$$

which is necessary and sufficient in order that an *exchange potential* G_{μ} exists so that $G_{\mu\nu}$ is just its curl:

$$G_{\mu\nu} = \nabla_{\mu}G_{\nu} - \nabla_{\nu}G_{\mu}. \tag{3.43}$$

Consequently we can rewrite the curl relation for k_{μ} (3.36b) as

$$\nabla_{\mu}' k_{\nu} - \nabla_{\nu}' k_{\mu} = 2f_{\mu\nu} \tag{3.44}$$

so that now the modified field $'k_{\mu}$

$${}^{\prime}k_{\mu} := k_{\mu} - 2G_{\mu} \tag{3.45}$$

exclusively "feels" the internal field strength $f_{\mu\nu}$ and nothing else.

Subsequently we shall make use of the modified field k_{μ} in place of the original k_{μ} . For instance, the SO(2) covariant derivative of the unit vector \hat{s}_a defined in Eqs. (3.22a) and (3.22b) is found as (Mattes and Sorg, 1999c)

$$D_{\mu}\hat{s}_{a} = \varepsilon_{a}^{b}\hat{s}_{b} \cdot {}^{\prime}k_{\mu}. \tag{3.46a}$$

Or similarly, the derivatives of the RTB operators are computed as

$$\mathcal{D}_{\mu}\widehat{\Pi}_{a} = k_{\mu} \cdot \widetilde{\Pi} \tag{3.46b}$$

$$\mathcal{D}_{\mu}\widetilde{\Pi}_{a} = -k_{\mu}\cdot\widehat{\Pi}.$$
(3.46c)

Furthermore it should also be mentioned that the exchange potential G_{μ} enters not only the modified kinetic field k_{μ} (3.45) but also plays an important part for the remaining integrability conditions upon the Hamiltonian coefficients $Q_{a\mu}$ and $N_{a\mu}$ which read in the RTB version

$$\nabla_{\mu}^{(\parallel)}Q_{\nu} - \nabla_{\nu}^{(\parallel)}Q_{\mu} = l_{\mu} \cdot {}^{(\perp)}N_{\nu} - l_{\nu} \cdot {}^{(\perp)}N_{\mu} + 2({}^{(\perp)}Q_{\mu} \cdot G_{\nu} - {}^{(\perp)}Q_{\nu} \cdot G_{\mu})$$
(3.47a)

$$\nabla_{\mu}{}^{(\perp)}Q_{\nu} - \nabla_{\nu}{}^{(\perp)}Q_{\mu} = -l_{\mu} \cdot {}^{(\parallel)}N_{\nu} + l_{\nu} \cdot {}^{(\parallel)}N_{\mu} - 2({}^{(\parallel)}Q_{\mu} \cdot G_{\nu} - {}^{(\parallel)}Q_{\nu} \cdot G_{\mu})$$
(3.47b)

$$\nabla_{\mu}^{(\parallel)}N_{\nu} - \nabla_{\nu}^{(\parallel)}N_{\mu} = -l_{\mu} \cdot {}^{(\perp)}Q_{\nu} + l_{\nu} \cdot {}^{(\perp)}Q_{\mu} + 2\left({}^{(\perp)}N_{\mu} \cdot G_{\nu} - {}^{(\perp)}N_{\nu} \cdot G_{\mu}\right)$$
(3.47c)

$$\nabla_{\mu}{}^{(\perp)}N_{\nu} - \nabla_{\nu}{}^{(\perp)}N_{\mu} = l_{\mu} \cdot {}^{(\parallel)}Q_{\nu} - l_{\nu} \cdot {}^{(\parallel)}Q_{\mu} - 2({}^{(\parallel)}N_{\mu} \cdot G_{\nu} - {}^{(\parallel)}N_{\nu} \cdot G_{\mu}).$$
(3.47d)

This system may look somewhat complicated but it admits the pleasant possibility of putting three of the exchange fields to zero $({}^{(\parallel)}Q_{\mu} = {}^{(\perp)}N_{\mu} = G_{\mu} \equiv 0)$ and retaining the other two $({}^{(\parallel)}N_{\mu} \neq 0, {}^{(\perp)}Q_{\mu} \neq 0)$. We shall make use of this possibility in the next section.

3.4. Conservation Equation

Similar to the preceding discussion of the integrability condition (2.6), the closer inspection of the conservation equation (2.7) will also yield a deeper insight into the structure of RST. Here the first point arises with the convertor \mathcal{G} which enters the abstract conservation equation on its right-hand side (2.7). Clearly before we can exploit this equation in a similar way as was done with the integrability condition, one must first determine the convertor \mathcal{G} from its algebraic constraint (2.31a) where the intensity matrix \mathcal{I} is given in its RTB form by equation (3.23).

The solution for \mathcal{G} in terms of \mathcal{I} is most conveniently expressed by a certain reparametrization of the latter operator. For that purpose rewrite the densities ρ , q, and s of the intensity operator \mathcal{I} in terms of the amplitude field L (3.34) in the following way:

$$\rho = Z_{\rm T} \cdot L^2 \tag{3.48}$$

$$q = Z_{\rm R} \cdot L^2 \tag{3.49}$$

$$s = Z_0 \cdot L^2, \tag{3.50}$$

thus introducing the *renormalization factors* Z_T , Z_R , and Z_O . Consequently the intensity operator \mathcal{I} (3.23) can be written as

$$\mathcal{I} = \mathcal{Z} \cdot L^2, \tag{3.51}$$

with the *renormalization operator* Z being parametrized by the renormalization factors through

$$\mathcal{Z} = \frac{1}{2} (Z_{\mathrm{T}} \cdot \mathbf{1} + Z_{\mathrm{R}} \cdot \mathcal{Q} + Z_{\mathrm{O}} \cdot \widehat{\Pi}).$$
(3.52)

Thus the previous algebraic constraint upon the convertor \mathcal{G} (2.31a) is recast into the form

$$\mathcal{G} \cdot \mathcal{Z} = 0 \tag{3.53}$$

from which we have to determine \mathcal{G} in terms of the renormalization factors Z_T , Z_R , and Z_O . This is a simple algebraic problem with a four-parametric solution which can easily be found but will not be presented here because our main interest concerns the mixtures and for these the convertor \mathcal{G} must always vanish (consequently we will put $\mathcal{G} \equiv 0$ from now on).

With this presumption, consider first the localization coefficient L_{μ} (3.10b) for which the conservation equation says

$$\nabla^{\mu}L_{\mu} + \frac{1}{2}(L^{\mu}L_{\mu} + l^{\mu}l_{\mu} - K^{\mu}K_{\mu} - k^{\mu}k_{\mu}) + 2\left[\left(\frac{Mc}{\hbar}\right)^{2} + {}^{(\parallel)}N_{\mu} \cdot {}^{(\parallel)}N^{\mu} + {}^{(\perp)}N_{\mu} \cdot {}^{(\perp)}N^{\mu} - {}^{(\parallel)}Q_{\mu} \cdot {}^{(\perp)}Q_{\mu} \cdot {}^{(\perp)}Q_{\mu} \cdot {}^{(\perp)}Q^{\mu}\right] = 0.$$
(3.54)

Sometimes it may be more instructive to work with the amplitude field L(x) in place of the localization field L_{μ} (3.34); the present equation (3.54) then reads in terms of L

$$\Box L + \left[\left(\frac{Mc}{\hbar} \right)^2 + \frac{1}{4} (l^{\mu} l_{\mu} - K^{\mu} K_{\mu} - k^{\mu} k_{\mu}) + {}^{(\parallel)} N_{\mu} \cdot {}^{(\parallel)} N^{\mu} + {}^{(\perp)} N_{\mu} \cdot {}^{(\perp)} N^{\mu} - {}^{(\parallel)} Q_{\mu} \cdot {}^{(\parallel)} Q^{\mu} - {}^{(\perp)} Q_{\mu} \cdot {}^{(\perp)} Q^{\mu} \right] \cdot L = 0.$$
(3.55)

This *amplitude equation* plays an important part in RST because it essentially is the relativistic counterpart of Schrödinger's nonrelativistic equation from which the energy eigenvalues of the system are to be determined (in RST one should rather speak of a *mass-eigenvalue problem*; this can be solved exactly for the Coulomb force in the single-particle case (Mattes and Sorg, 1999c)). Observe also that the amplitude equation (3.55) contains the second localization coefficient which, however, is not a gradient field, cf. (3.35). Therefore the abstract integrability condition (2.6) does not admit, in general, a second amplitude field, obeying a second amplitude equation, but instead we have to keep the original equation for l_{μ} corresponding to Eq. (3.54) for L_{μ} :

$$\nabla^{\mu}l_{\mu} + L^{\mu}l_{\mu} - K^{\mu}k_{\mu} = 0.$$
(3.56)

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Finally, let us write down the source equations for both kinetic fields

$$\nabla^{\mu} K_{\mu} + L^{\mu} \cdot K_{\mu} + l^{\mu} \cdot k_{\mu} + 4 \left({}^{(\parallel)} Q_{\mu} \cdot {}^{(\parallel)} N^{\mu} + {}^{(\perp)} Q_{\mu} \cdot {}^{(\perp)} N^{\mu} \right) = 0 \quad (3.57a)$$
$$\nabla^{\mu} k_{\mu} + L^{\mu} \cdot k_{\mu} + l^{\mu} \cdot K_{\mu} = 0, \quad (3.57b)$$

and similarly for the remaining Hamiltonian coefficients

$$\nabla^{\mu(\|)}Q_{\mu} - {}^{(\perp)}Q_{\mu} \cdot {}^{\prime}k^{\mu} + L^{\mu} \cdot {}^{(\|)}Q_{\mu} + K^{\mu} \cdot {}^{(\|)}N_{\mu} = 0 \qquad (3.58a)$$

$$\nabla^{\mu(\perp)}Q_{\mu} + {}^{(\parallel)}Q_{\mu} \cdot {}^{\prime}k^{\mu} + L^{\mu} \cdot {}^{(\perp)}Q_{\mu} + K^{\mu} \cdot {}^{(\perp)}N_{\mu} = 0 \qquad (3.58b)$$

$$\nabla^{\mu(\|)} N_{\mu} - {}^{(\perp)} N_{\mu} \cdot {}^{\prime} k^{\mu} + L^{\mu} \cdot {}^{(\|)} N_{\mu} + K^{\mu} \cdot {}^{(\|)} Q_{\mu} = 0 \qquad (3.58c)$$

$$\nabla^{\mu(\perp)} N_{\mu} + {}^{(\parallel)} N_{\mu} \cdot {}^{\prime} k^{\mu} + L^{\mu} \cdot {}^{(\perp)} N_{\mu} + K^{\mu} \cdot {}^{(\perp)} Q_{\mu} = 0.$$
(3.58d)

3.5. Density Dynamics

The RNE (2.5) is the field equation for the intensity matrix \mathcal{I} whose RTB decomposition (3.23) led us to the total density ρ , relative density q, and overlap density s. Therefore one could now transcribe the RNE into the corresponding field equations for these individual densities. However, in the meantime we have already introduced the associated renormalization factors Z_T , Z_R , and Z_O [(3.48)–(3.50)] and therefore we can at once translate the density dynamics for ρ , q, and s into the corresponding *renormalization dynamics*

$$\partial_{\mu} Z_{\mathrm{T}} = Z_{\mathrm{R}} \cdot l_{\mu} + 2Z_{\mathrm{O}} \cdot {}^{(\parallel)} N_{\mu} \tag{3.59a}$$

$$\partial_{\mu} Z_{\rm R} = Z_{\rm T} \cdot l_{\mu} - 2 Z_{\rm O} \cdot {}^{(\perp)} Q_{\mu} \tag{3.59b}$$

$$\partial_{\mu} Z_{\mathrm{O}} = 2 \big(Z_{\mathrm{T}} \cdot {}^{(\parallel)} N_{\mu} + Z_{\mathrm{R}} \cdot {}^{(\perp)} Q_{\mu} \big). \tag{3.59c}$$

This system admits a first integral in the form

$$Z_{\rm T}^2 - \left(Z_{\rm R}^2 + Z_{\rm O}^2\right) = \sigma_*,\tag{3.60}$$

where the *mixture index* σ_* is a constant and can be chosen without loss of generality as $\sigma_* = 0, \pm 1$. By introducing the densities (3.48)–(3.50) into the component form (3.28) of the Fierz identity (2.2), we see that the value $\sigma_* = 0$ stands for the *pure states* which therefore may be parametrized by the *mixture variable* ζ and *overlap angle* ξ_0 as

$$Z_{\rm T} = \frac{1}{2} e^{\zeta} \tag{3.61a}$$

$$Z_{\rm R} = \frac{1}{2} e^{\zeta} \cdot \cos \xi_{\rm o} \tag{3.61b}$$

$$Z_{\rm O} = \frac{1}{2} e^{\zeta} \cdot \sin \xi_{\rm o}. \tag{3.61c}$$

For $\sigma_* = +1$ we have the *positive mixtures*

$$Z_{\rm T} = \cosh \zeta \tag{3.62a}$$

$$Z_{\rm R} = \sinh \zeta \cdot \cos \xi_0 \tag{3.62b}$$

$$Z_{\rm O} = \sinh \zeta \cdot \sin \xi_{\rm o}, \qquad (3.62c)$$

and for $\sigma_* = -1$ the *negative mixtures*

$$Z_{\rm T} = \sinh \zeta \tag{3.63a}$$

$$Z_{\rm R} = \cosh \zeta \cdot \cos \xi_0 \tag{3.63b}$$

$$Z_{\rm O} = \cosh \zeta \cdot \sin \xi_{\rm o}. \tag{3.63c}$$

For the subsequent computations it is convenient to collect all three cases into one formula by putting

$$Z_{\rm II} \doteqdot \sqrt{Z_{\rm R}^2 + Z_{\rm O}^2} \tag{3.64}$$

so that we have for all three cases

$$Z_{\rm R} = Z_{\rm II} \cdot \cos \xi_{\rm o} \tag{3.65a}$$

$$Z_{\rm O} = Z_{\rm II} \cdot \sin \xi_0 \tag{3.65b}$$

with

$$Z_{\rm T}^2 - Z_{\rm II}^2 = \sigma_*; ag{3.66}$$

see also Fig. 2.

The interesting point with this threefold subdivision of the density configuration space lies in the fact that the pure states, albeit separated kinematically from the mixtures, can be approximated by the latter with unlimited precision, namely through the limit process $\zeta \to \infty$. Whether this kinematically possible process is also admitted by the dynamics must be studied seperately. For such a purpose, it is convenient to consider directly the field equations for the internal variables ζ and ξ_0 . Here, one combines the two localization coefficients l_{μ} and ${}^{(\parallel)}N_{\mu}$ into two new vectors g_{μ} and h_{μ}

$$g_{\mu} = 2^{(\parallel)} N_{\mu} \cdot \cos \xi_{\rm o} - l_{\mu} \cdot \sin \xi_{\rm o}$$
(3.67a)

$$h_{\mu} = 2^{(\parallel)} N_{\mu} \cdot \sin \xi_{0} + l_{\mu} \cdot \cos \xi_{0},$$
 (3.67b)

and then the desired field equations for ζ and ξ_0 are deduced from the original renormalization dynamics (3.59) as

$$\partial_{\mu}\zeta = h_{\mu} \tag{3.68a}$$

$$\partial_{\mu}\xi_{\rm o} = 2\left({}^{(\perp)}Q_{\mu} + \frac{Z_{\rm T}}{2Z_{\rm II}} \cdot g_{\mu}\right). \tag{3.68b}$$

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But with the introduction of two new dynamical variables (g_{μ}, h_{μ}) one also wants to know their field equations which are easily deduced from the corresponding equations for the old pair $(l_{\mu}, {}^{(\parallel)}N_{\mu})$. Thus the curl relations for the new vectors read

$$\nabla_{\mu}g_{\nu} - \nabla_{\nu}g_{\mu} = \frac{Z_{\mathrm{T}}}{Z_{\mathrm{II}}}[h_{\mu} \cdot g_{\nu} - h_{\nu} \cdot g_{\mu}] + 4\left[{}^{(\perp)}N_{\mu}\left(\cos\xi_{\mathrm{o}} \cdot G_{\nu} + \sin\xi_{\mathrm{o}} \cdot {}^{(\parallel)}Q_{\nu}\right)\right]$$

$$- {}^{(\perp)}N_{\nu} \cdot \left(\cos\xi_{0} \cdot G_{\mu} + \sin\xi_{0} \cdot {}^{(\parallel)}Q_{\mu}\right) \right]$$
(3.69a)

$$\nabla_{\mu}h_{\nu} - \nabla_{\nu}h_{\mu} = 0. \tag{3.69b}$$

The last equation is of course trivial because h_{μ} has already been revealed to be a gradient field, cf. (3.68a). Analogously, the source equations for the new vectors are easily written down (Rupp *et al.*, 2000) but are supressed here because they can subsequently be reformulated as wave equations for two scalar fields ζ and χ . Here, the first scalar ζ has already been introduced through Eq. (3.68a) in connection with the new vector h_{μ} , and the second scalar χ generates the other new vector g_{μ} in a similar way

$$g_{\mu} = Z_{\rm II} \cdot \partial_{\mu} \chi, \qquad (3.70)$$

provided we resort to those simplified configurations which have vanishing exchange fields ${}^{(\parallel)}Q_{\mu}$, ${}^{(\perp)}N_{\mu}$, and G_{μ} :

$$G_{\mu} = {}^{(\perp)}N_{\mu} = {}^{(\parallel)}Q_{\mu} \equiv 0. \tag{3.71}$$

Subsequently we will mainly be occupied with this kind of field systems. The vanishing of the three exchange fields (3.71) leaves us with some constraints upon the remaining fields; for instance the source equation (3.58a) for the vanishing $(\mathbb{I})Q_{\mu}$ fixes the directional derivative of the overlap angle ξ_0 along the relative kinetic field k_{μ} as

$$k^{\mu} \cdot \partial_{\mu} \xi_{0} = (K^{\mu} g_{\mu}) \cos \xi_{0} + (k^{\mu} h_{\mu}) \sin \xi_{0} + \frac{Z_{T}}{Z_{II}} g^{\mu} k_{\mu}.$$
(3.72)

A similar constraint is implied by the source equation (3.58d) for the vanishing ${}^{(\perp)}N_{\mu}$:

$$K^{\mu} \cdot \partial_{\mu} \xi_{0} = (k^{\mu} g_{\mu}) \cos \xi_{0} + (k^{\mu} h_{\mu}) \sin \xi_{0} + \frac{Z_{T}}{Z_{II}} g^{\mu} K_{\mu}.$$
(3.73)

4. MIXTURES AND PURE STATES

The relationship between mixtures and pure states requires some clarification. The reason here is that the Fierz identity (2.2) establishes some algebraic constraint for the pure states which therefore must have a reduced number of degrees of freedom in comparison to the mixtures. On the other hand, the result of Fig. 3

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says that the pure states occupy the (two-dimensional) Fierz cone and the mixtures occupy the (two-dimensional) hyperboloids and thus both the mixtures and the pure states appear to possess the same number of degrees of freedom. But this cannot be true because the pure states can be considered as the limit configuration $\zeta \rightarrow \infty$, and therefore the internal variable ζ must drop out for the description of pure states. In what way can this cancellation of ζ be conceived? A first hint comes from combining both reparametrizations (3.27a)–(3.27e) and (3.48)–(3.50) of the physical densities (ρ , q, s) with (3.62) for the case of the pure states:

$$\rho \Rightarrow L_1^2 + L_2^2 = \frac{1}{2}e^{\zeta} \cdot L^2 \doteqdot 'L^2$$
(4.1a)

$$q \Rightarrow L_1^2 - L_2^2 = \frac{1}{2}e^{\zeta} \cdot L^2 \cos \xi_0 = L^2 \cos \xi_0$$
 (4.1b)

$$s \Rightarrow 2L_1L_2 = \frac{1}{2}e^{\zeta} \cdot L^2 \sin \xi_0 = L^2 \sin \xi_0.$$
 (4.1c)

Obviously the dropping of ζ can occur through absorption into the amplitude field L in order to generate a *modified amplitude field* $'L^2 (=\frac{1}{2}e^{\zeta} \cdot L^2)$ as the proper external variable for the localization properties of the 2-particle system. As a consequence it should be possible to recast all the 2-particle equations in a form which contains both the mixture index σ_* and the mixture variable ζ in addition to the modified amplitude field 'L so that the pure-state form of that equation is obtained by either putting σ_* to zero *or* by letting ζ tend to infinity. The remaining variables 'L and ξ_0 are then sufficient to describe the pure states.

4.1. Currents

As a first example for this procedure consider both currents J_{μ} (3.29a) and j_{μ} (3.29b). Observing here the reparametrizations of the physical densities ρ , q, and s in terms of the renormalization factors $Z_{\rm T}$, $Z_{\rm R}$, and $Z_{\rm O}$ (3.65) actually yields the desired form of the currents, namely for the total current

$$J_{\mu} = \frac{1}{2} \left(\frac{Z_{\rm T}}{Z_{\rm II}} - 1 \right) \cdot \frac{\hbar}{2Mc} K_{\mu} \cdot {}^{\prime}L^2 + \mathring{J}_{\mu}$$
(4.2a)

$$\mathring{J}_{\mu} = \frac{\hbar}{2Mc} \{ K_{\mu} + \cos \xi_{0} \cdot k_{\mu} + 2 \sin \xi_{0} \cdot {}^{(\parallel)}Q_{\mu} \} \cdot {}^{\prime}L^{2}, \qquad (4.2b)$$

and similarly for the relative current

$$j_{\mu} = \frac{1}{2} \left(\frac{Z_{\rm T}}{Z_{\rm II}} - 1 \right) \cdot \frac{\hbar}{2Mc} K_{\mu} \cdot {}^{\prime}L^2 + \mathring{j}_{\mu}$$
(4.3a)

$$\mathring{j}_{\mu} = \frac{\hbar}{2Mc} \{ k_{\mu} + \cos \xi_{o} \cdot K_{\mu} + 2 \,{}^{(\perp)}N_{\mu} \cdot \sin \xi_{o} \} \cdot {}^{\prime}L^{2}. \tag{4.3b}$$

Here we have made use of the modified amplitude field 'L(x) which has already been mentioned in connection with the pure states [(4.1a)–(4.1c)] and whose general definition reads

$$L \doteq \sqrt{Z_{\mathrm{II}}} \cdot L.$$
 (4.4)

Indeed this is just the desired result, for the pure-state forms \mathring{J}_{μ} (4.2b) and \mathring{j}_{μ} (4.3b) are recovered by *either* putting the mixture index σ_* to zero in the general form for J_{μ} (4.2a) or j_{μ} (4.3a) or by letting the mixture variable ζ tend to infinity, cf. the reparametrizations [(3.62)–(3.66)] for the renormalization factors.

Remarkably, for our special situation (3.71), the pure-state contributions J_{μ} (4.2b) and j_{μ} (4.3b) to the complete currents J_{μ} (4.2a) and j_{μ} (4.3a) are exclusively built up by the pure-state variables 'L and ξ_0 but not by the mixture variables ζ and χ , even if one has a true mixture:

$$\mathring{J}_{\mu} \Rightarrow \frac{\hbar}{2Mc} \{ K_{\mu} + \cos \xi_{0} \cdot k_{\mu} \} \cdot {}^{\prime}L^{2}$$
(4.5a)

$$\overset{\circ}{j}_{\mu} \Rightarrow \frac{\hbar}{2Mc} \{k_{\mu} + \cos\xi_{o} \cdot K_{\mu}\} \cdot {}^{\prime}L^{2}.$$
(4.5b)

This peculiarity is expressed even more clearly when we return again to the singleparticle currents $j_{a\mu}$ (3.25a)–(3.26c) which become by means of the present simplification requirement (3.71)

$$j_{1\mu} \Rightarrow \frac{\hbar}{Mc} \rho_1 K_{1\mu} \tag{4.6a}$$

$$j_{2\mu} \Rightarrow \frac{\hbar}{Mc} \rho_2 K_{2\mu}.$$
 (4.6b)

Obviously the mixture degree of freedom has been hidden here completely behind the scalar single-particle densities ρ_a . In the general mixture case these may be parametrized by the pure-state variables 'L, ξ_0 and by the mixture variable ζ in the following form:

$$\rho_1(x) = g_w(x) \cdot (L_1(x))^2 + g_s(x) \cdot (L_2(x))^2$$
(4.7a)

$$\rho_2(x) = g_w(x) \cdot (L_2(x))^2 + g_s(x) \cdot (L_1(x))^2.$$
(4.7b)

Here the space–time dependent *structure functions* g_w and g_s are defined in terms of the renormalization factors as

$$g_w = \frac{1}{2} \left(\frac{Z_{\rm T}}{Z_{\rm II}} + 1 \right) \tag{4.8a}$$

$$g_s = \frac{1}{2} \left(\frac{Z_{\rm T}}{Z_{\rm II}} - 1 \right) \tag{4.8b}$$

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and furthermore the single-particle amplitudes L_a through

$$L_1 = L \cdot \cos\frac{\xi_0}{2} \tag{4.9a}$$

$$L_2 = L \cdot \sin \frac{\xi_0}{2}. \tag{4.9b}$$

Thus for the limit case of the pure states ($\zeta \to \infty$) one has for the structure functions $g_w \Rightarrow 1$ and $g_s \Rightarrow 0$, and this then identifies the scalar densities ρ_a (4.7) with the square of the moduli of the single-particle wave functions ψ_a (3.1). However, for the more general case of a true mixture, such a 2-component wave function $\Psi = \{\psi_a\}, a = 1, 2$ as given in (3.1), is not sufficient to describe the mixture degree of freedom! (Similar arguments as those holding for the currents do apply to other physical densities also, e.g. the energy–momentum density $T_{\mu\nu}$ (Rupp *et al.*, 2000).)

4.2. Gauge Interactions

The mixture degree of freedom becomes physically active via the currents as the sources of the electromagnetic field which itself is responsible for the gauge interactions among the particles. Thus, a mixture configuration will generate certain changes of the pure-state interactions which, e.g., may become manifest as changes of the energy eigenvalues of bound systems (see as given later). More concretely, the electromagnetic interactions are constructed in the following way:

In the SPB formalism, Maxwell's equations read (a = 1, 2)

$$\nabla^{\mu}F_{a\mu\nu} = 4\pi\alpha_* \cdot j_{a\nu}, \qquad (4.10)$$

where the curvature components $F_{a\mu\nu}$ have already been defined by Eq. (2.19b), the single-particle currents $j_{a\mu}$ obey the cross-relation (4.13), and α_* is the electromagnetic coupling constant $(=\frac{e^2}{\hbar c})$. In order to exclude the *direct* particle selfinteractions, the curvature components $F_{a\mu\nu}$ also obey a cross-relation with respect to the electromagnetic fields $F_{a\mu\nu}$ generated by the single-particle currents $j_{a\mu}$:

$$F_{1\mu\nu} = {}^{(\text{ex})}F_{\mu\nu} + {}^{\prime}F_{2\mu\nu} \tag{4.11a}$$

$$F_{2\mu\nu} = {}^{(\text{ex})}F_{\mu\nu} + {}^{\prime}F_{1\mu\nu}.$$
(4.11b)

By virtue of this construction, any one of both particles feels the external field $^{(ex)}F_{\mu\nu}$ and the field $'F_{b\mu\nu}$ of the *other* particle but not its *own* field, i.e. the Maxwell equations are required to connect the currents and field strengths in the following way:

$$\nabla^{\mu} F_{a\mu\nu} = 4\pi \alpha_* \cdot j_{a\nu}, \qquad (4.12)$$

where

$$\nabla^{\mu \text{ (ex)}} F_{\mu\nu} \equiv 0.$$

As a consequence, the comparison of both Maxwell equations (4.10) and (4.12) yields the cross-relation for the currents

$$j_{1\mu} \equiv j_{2\mu} \tag{4.13a}$$

$$j_{2\mu} \equiv j_{1\mu}, \tag{4.13b}$$

where the proper currents $j_{a\mu}$ on the right are to be identified with the RST currents defined by Eq. (2.25).

For the present simplified situation (3.71), the source currents $j_{a\mu}$ are specified by Eqs. (4.6a) and (4.6b) and thus contain the mixture effect exclusively via the single-particle densities ρ_a (4.7). Since the first (second) density $\rho_1(\rho_2)$ also contains the second (first) amplitude field $L_2(L_1)$ with the structure function g_s as a kind of weight factor (relative to g_w), there arise *self-interactions* for the mixtures in an *indirect* way. In order to see this in some detail, recall that the Maxwell equations (4.10) for the curvature components $F_{a\mu\nu}$ imply the wave equations for the connection components $A_{a\mu}$ (2.20):

$$\Box A_{a\mu} = 4\pi \alpha_* \cdot j_{a\mu}. \tag{4.14}$$

Applying the Lorentz gauge $\nabla^{\mu} A_{a\mu} \equiv 0$, the formal solution is given here by

$$A_{a\mu}(x) = {}^{(\text{ex})}A_{\mu}(x) + \int d^{4}x' \,\tilde{D}(x-x')\,' j_{a\mu}(x') \tag{4.15}$$

with an appropriate Green's function $\tilde{D}(x, x')$:

$$\Box \tilde{D}(x, x') = \delta^4(x - x').$$
 (4.16)

(The specification of the Green's function $\tilde{D}(x, x')$ will require an extra argument.) Consequently the gauge potentials $A_{a\mu}(x)$ are also cross-related to the currents

$${}^{\prime}\!A_{2\mu} \equiv A_{1\mu}(x) = {}^{(\text{ex})}\!A_{\mu}(x) + \alpha_* \int d^4 x' \,\tilde{D}(x, x') \,j_{2\mu}(x) \qquad (4.17a)$$

$${}^{\prime}\!A_{1\mu} \equiv A_{2\mu}(x) = {}^{(\text{ex})}\!A_{\mu}(x) + \alpha_* \int d^4 x' \,\tilde{D}(x, x') \,j_{1\mu}(x). \tag{4.17b}$$

On the other hand the gauge potentials influence the single-particle wave functions ψ_a (3.1) via their covariant derivatives as usual

$$\mathcal{D}_{\mu}\Psi = \partial_{\mu}\Psi + \mathcal{A}_{\mu}\Psi, \qquad (4.18)$$

i.e. in components

$$D_{\mu}\psi_{1} = \div \partial_{\mu}\psi_{1} - i A_{1\mu}\psi_{1} \tag{4.19a}$$

$$D_{\mu}\psi_2 = \doteqdot \partial_{\mu}\psi_2 - i A_{2\mu}\psi_2. \tag{4.19b}$$

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Therefore the first (second) amplitude field $L_1(L_2)$ acts back to the first (second) wave function $\psi_1(\psi_2)$ by entering the second (first) current $j_{2\mu}(j_{1\mu})$ which itself generates the first (second) gauge potential $A_{1\mu}(A_{2\mu})$ acting on the first (second) wave function $\psi_1(\psi_2)$, i.e. in symbolical and self-evident notation

$$L_1(L_2) \stackrel{g_s}{\underset{(4.6-4.7)}{\Longrightarrow}} j_{2\mu}(j_{1\mu}) \stackrel{\tilde{D}}{\underset{(4.17)}{\Rightarrow}} A_{1\mu}(A_{2\mu}) \stackrel{D_{\mu}}{\underset{(4.19)}{\Rightarrow}} \psi_1(\psi_2).$$
(4.20)

Observe here that this kind of self-interaction is not identical to the usual mechanism in which the *mutual* gauge forces are active. As is well known, the latter forces are working in such a way that the first (second) amplitude field $L_1(L_2)$ enters the first (second) current $j_{1\mu}(j_{2\mu})$, which generates the second (first) connection component $A_{2\mu}(A_{1\mu})$ acting on the second (first) wave function $\psi_2(\psi_1)$; in symbolical notation

$$L_1(L_2) \stackrel{g_w}{\underset{(4.6-4.7)}{\longrightarrow}} j_{1\mu}(j_{2\mu}) \stackrel{\tilde{D}}{\underset{(4.17)}{\Rightarrow}} A_{2\mu}(A_{1\mu}) \stackrel{D_{\mu}}{\underset{(4.19)}{\Rightarrow}} \psi_2(\psi_1).$$
(4.21)

It is important here to remark that in the first step the mutual gauge interactions (4.21) rely upon the structure function $g_w(\zeta)$ (4.8a) whereas the former *self-interactions* (4.20) rely upon the structure function $g_s(\zeta)$ (4.8b). Thus the conventional gauge interactions survive the pure-state limit ($g_w(\zeta \to \infty) \Rightarrow 1$) whereas the self-interactions do not ($g_s(\zeta \to \infty) \Rightarrow 0$). Through this argument it becomes obvious that the self-interactions are essentially mediated by the mixture variable ζ and thus the peculiarities of this unconventional type of interaction will be elucidated by considering the wave equation for ζ (see as given later).

One must concede that the description of mixtures in terms of vector potentials $A_{a\mu}$ and single-particle wave functions ψ_a may appear somewhat artificial and uneffective. A formalism more manageable than this (ψ , A)-formalism is the (L, K)-formalism, which relies upon the use of the localization (amplitude) and kinetic fields in place of wave functions and vector potentials. The unconventional self-interaction chain (4.20) reads then in the (L, K)-formalism

$$L_1(L_2) \stackrel{g_s}{\underset{(4.6-4.7)}{\Rightarrow}} j_{2\mu}(j_{1\mu}) \stackrel{\alpha \tilde{D}}{\underset{(4.25)}{\Rightarrow}} K_{1\mu}(K_{2\mu}) \stackrel{\Box}{\underset{(4.31)}{\Rightarrow}} L_1(L_2).$$
(4.22)

whereas the conventional gauge interaction (4.21) is transcribed as

$$L_1(L_2) \stackrel{g_w}{\underset{(4.6-4.7)}{\Rightarrow}} j_{1\mu}(j_{2\mu}) \stackrel{\alpha\tilde{D}}{\underset{(4.25)}{\Rightarrow}} K_{2\mu}(K_{1\mu}) \stackrel{\Box}{\underset{(4.31)}{\Rightarrow}} L_2(L_1).$$
(4.23)

The first step, leading from the amplitudes L_a to the currents $j_{a\mu}$, is the same as in the (ψ, A) -formalism [(4.20) and (4.21)] and runs via Eqs. (4.6) and (4.7), but the second and third steps (symbolized by $\alpha \tilde{D}$ and the d'Alambertian \Box) require some explanation. Here, the third step (\Box) refers to the wave equations for the amplitude fields L_a , which contain the kinetic fields $K_{a\mu}$ and shall be presented at length subsequently; but the second step $(\alpha \tilde{D})$ is only a minor modification of the inversion process (4.17), namely by resorting to the kinetic fields $K_{a\mu}$ in place of the vector potentials $A_{a\mu}$, and it can be elucidated by the following argument:

Both the connection components $A_{a\mu}$ and the kinetic fields $K_{a\mu}$ have the curvature components $F_{a\mu\nu}$ as their curl, cf. (2.20), together with the SPB formulation of the integrability conditions (2.6) for the kinetic fields reading

$$\nabla_{\mu}K_{a\nu} - \nabla_{\nu}K_{a\mu} = F_{a\mu\nu}. \tag{4.24}$$

Therefore both vector fields $A_{a\mu}$ and $K_{a\mu}$ may differ at most by some gradient field $(\partial_{\mu}\alpha)$

$$K_{a\mu} = \partial_{\mu}\alpha_a + A_{a\mu}. \tag{4.25}$$

Thus the relationship (\tilde{D}) between the currents and the vector potentials (4.17) is also transferred to the kinetic fields, apart from the additional emergence of the scalar fields $\alpha_a(x)$. The latter are necessary in order to guarantee the homogeneous transformation behavior (here invariance) of the kinetic fields under a change of gauge (parametrized by the $U(1) \times U(1)$ group parameters $a_b(x)$, b = 1, 2)

$$K_{a\mu} \Rightarrow K'_{a\mu} \equiv K_{a\mu} \tag{4.26}$$

whereas the gauge potentials $A_{a\mu}$ and scalar fields α_a transform *inhomogeneously*

$$A_{b\mu} \Rightarrow 'A_{b\mu} - \partial_{\mu}a_b \tag{4.27a}$$

$$\alpha'_b(x) \Rightarrow \alpha_b(x) + a_b(x).$$
 (4.27b)

(see the reconstruction of the wave function ψ from the variables of the (L, K)-formalism in Mattes and Sorg (1999a). These new scalar fields $\alpha_a(x)$ stand in close relation to the mass eigenvalues (M_a) which will be further elucidated later.

The final step (\Box) of the interaction chains (4.22) and (4.23) now consists in specifying the wave equations for the amplitude fields L_a , which will then clearly display the coupling between the kinetic and amplitude fields.

4.3. Wave Equations

Up to now we have been mainly concerned with the kinematical setting whose internal consistency has been found to be guaranteed by the integrability condition (2.6). The dynamical equations, as the complementing building block of RST, must now be considered. The starting point here is the conservation equation (2.7) which can be transcribed to the corresponding wave equations for the scalar fields introduced earlier: amplitude field 'L(x) (4.4), overlap angle ξ_o (3.61)–(3.65), and the mixture variables ζ and χ (3.70). Remember here that in place of the pure-state variables 'L and ξ_o one could also resort to the single-particle amplitudes L_a (4.9).

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Transcribing the former amplitude equation for L(x) (3.55) to the new variable ${}^{\prime}L(x)$ (4.4) yields

$$\Box' L + L \cdot \left\{ \left(\frac{Mc}{\hbar} \right)^2 - \frac{1}{4} [K^{\mu} K_{\mu} + k^{\mu} k_{\mu} + \partial^{\mu} \xi_0 \cdot \partial_{\mu} \xi_0] - \frac{1}{2} \frac{Z_{\rm T}}{Z_{\rm II}} \cos \xi_0 (K^{\mu} k_{\mu}) \right\}$$
$$= \frac{\sigma_*}{4 Z_{\rm II}^2} (g^{\mu} g_{\mu} - h^{\mu} h_{\mu}). \tag{4.28}$$

Similarly the wave equation for the overlap angle ξ_o is deduced from the conservation equation for ${}^{(\perp)}Q_{\mu}$ (3.58b) via the first derivative of ξ_o (3.68b) as the following modified form of the well-known *Sine–Gordon equation* (Dodd *et al.*, 1982)

$$\Box \xi_{0} + {}^{\prime}L^{\mu} \cdot \partial_{\mu}\xi_{0} + \frac{Z_{\mathrm{T}}}{Z_{\mathrm{II}}} \sin \xi_{0}(K^{\mu}k_{\mu}) = -\frac{\sigma_{*}}{Z_{\mathrm{II}}^{2}}g^{\mu}h_{\mu}.$$
(4.29)

Here the use of a modified localization field L_{μ} is due to the transition from the amplitude L(x) to L(x) (4.4), i.e.

$${}^{\prime}L_{\mu} \doteq \frac{\partial_{\mu}{}^{\prime}L^{2}}{{}^{\prime}L^{2}} = L_{\mu} + \frac{Z_{\mathrm{T}}}{Z_{\mathrm{II}}}h_{\mu}.$$
 (4.30)

Observe again that the pure state forms of both wave equations (4.28) and (4.29) can be obtained in a twofold way, namely *either* by directly putting the mixture index σ_* to zero *or* by letting ζ tend to infinity for nonzero mixture index.

Alternatively, one might prefer to work with the single-particle amplitudes L_a (4.9) in place of the "external" amplitude field L(x) and overlap angle ξ_o . The corresponding amplitude equations for L_a are easily deduced from the present system [(4.28) and (4.29)] and read (a = 1, 2)

$$\Box L_a + L_a \cdot \left\{ \left(\frac{Mc}{\hbar} \right)^2 - K_{a\mu} K_a^{\mu} \right\} = -W_a^b L_b \tag{4.31}$$

(summation of indices in opposite positions). The coupling matrix elements $\{W_{ab}\}$ are found here to be of the following form:

$$W_{11} = -\sigma_* \frac{g^{\mu}g_{\mu} - h^{\mu}h_{\mu}}{(2Z_{\rm II})^2} - g_s \Big(K_{1\mu}K_1^{\mu} - K_{2\mu}K_2^{\mu}\Big)$$
(4.32a)

$$W_{22} = -\sigma_* \frac{g^{\mu}g_{\mu} - h^{\mu}h_{\mu}}{(2Z_{\rm II})^2} + g_s \left(K_{1\mu}K_1^{\mu} - K_{2\mu}K_2^{\mu}\right)$$
(4.32b)

$$W_{12} = -\sigma_* \frac{g^{\mu} h_{\mu}}{2Z_{\text{II}}^2} = -W_{21}.$$
(4.32c)

The present amplitude equations (4.31) have some interesting properties. First observe that they contain the kinetic fields $K_{a\mu}$ and thus the influence of the kinetic fields upon the amplitudes L_a is now clearly demonstrated (see the last step (\Box) for the gauge interaction schemes (4.22) and (4.23)). Second, the limit process

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 $\zeta \to \infty$ lets the coupling elements vanish ($W_{ab} \to 0$) and consequently we are left with two homogeneous amplitude equations

$$\Box L_a + L_a \cdot \left\{ \left(\frac{Mc}{\hbar} \right)^2 - K_{a\mu} K_a^{\mu} \right\} = 0, \qquad (4.33)$$

which describe a pure state ($\sigma_* = 0$). For this special case, the coupling between the two amplitude fields L_1 and L_2 occurs exclusively via the gauge interaction mechanism (4.23). Returning from the present (L, K)-formalism to the (ψ , A)formalism, one can reconstruct the components ψ_a of the two-particle wave function Ψ (3.1) and the single-particle wave functions ψ_a will then obey ordinary KGEs (see Mattes and Sorg, 1999a). However for true mixtures (i.e. $\sigma_* \neq 0$ and $0 < \zeta < \infty$) both matter degrees of freedom receive an additional *nongauge* coupling by virtue of the matrix elements W_{ab} which are governed, besides by the kinetic fields, essentially by the mixture variable ζ . Thus the dynamical features of this scalar field $\zeta(x)$ will determine the corresponding physical properties of the mixture interaction. Especially if one could find some wave equation for ζ one would assume that the mixture interactions also propagate with the (local) velocity of light just as is the case with the gauge interactions based upon the wave equations (4.14) for the vector potentials $A_{a\mu}$.

Indeed, such a wave equation for ζ can easily be deduced from the source equation for the vector field h_{μ} (3.67b). Remember here that this vector h_{μ} has already been revealed as the gradient field of the scalar ζ , cf. (3.68a), and thus the source equation for h_{μ} (to be deduced from the source equations for $(\parallel)N_{\mu}$ (3.58c) and for l_{μ} (3.56)) is nothing else than the desired wave equation for ζ :

$$\Box \zeta + L^{\mu} \cdot \partial_{\mu} \zeta - \frac{Z_{\mathrm{T}}}{Z_{\mathrm{II}}} \partial^{\mu} \zeta \cdot \partial_{\mu} \zeta = Z_{\mathrm{II}} \partial^{\mu} \chi \cdot \partial_{\mu} \xi_{\mathrm{o}} + \cos \xi_{\mathrm{o}} \cdot K^{\mu} k_{\mu}.$$
(4.34)

Obviously, the mixture variable ζ couples also to the other scalar variable χ so that we have to supply the wave equation for the latter variable χ in order to close the dynamical system. This wave equation is obtained in a similar way from the source equation for the other vector field g_{μ} which is related to the scalar χ by the former gradient condition (3.70). Thus one finds for χ the following wave equation:

$$\Box \chi + \left({}^{\prime}L^{\mu} + \frac{Z_{\mathrm{T}}}{Z_{\mathrm{II}}} \partial^{\mu} \zeta \right) \cdot \partial_{\mu} \chi = -\frac{1}{Z_{\mathrm{II}}} \sin \xi_{\mathrm{o}} \cdot (K^{\mu} k_{\mu}) - \frac{1}{Z_{\mathrm{II}}} h^{\mu} \cdot (\partial_{\mu} \xi_{\mathrm{o}} - Z_{T} \partial_{\mu} \chi). \quad (4.35)$$

The four wave equations (4.31), (4.34), and (4.35) are valid for that simplified situation defined by the requirement (3.71) for vanishing exchange fields G_{μ} , ${}^{(\perp)}N_{\mu}$, ${}^{(\parallel)}Q_{\mu}$ but nonzero exchange fields l_{μ} and ${}^{(\parallel)}N_{\mu}$. Obviously there can be no

hope to get an exact solution to such a highly non-linear and intricately coupled system. But fortunately the situation can be further simplified by neglection of the two remaining exchange fields ${}^{(\perp)}Q_{\mu}$ and ${}^{(\parallel)}N_{\mu}$. We shall readily see that, by this assumption, the mixture interaction becomes "local" (i.e. some kind of "overlap force" arises).

4.4. Vanishing Exchange Fields

It is not only for the sake of simplicity but it also provides us with a better understanding of the relationships between the exchange effects and mixture phenomena when we completely neglect the exchange fields (i.e. ${}^{(\perp)}Q_{\mu} = {}^{(\parallel)}N_{\mu} \equiv 0$) but retain the mixture character of the system (i.e. $\sigma_* = \pm 1$). In order to clearly see the specific kind of simplification which is produced by this neglection, write down both the exchange fields in terms of the mixture variables ζ and χ , cf. (3.68b), together with (3.70)

$${}^{(\perp)}Q_{\mu} \equiv \frac{1}{2}(\partial_{\mu}\xi - Z_{\mathrm{T}}\partial_{\mu}\chi) \stackrel{!}{=} 0$$

$$(4.36)$$

and

$${}^{(\parallel)}N_{\mu} \equiv \frac{1}{2}(\cos\xi_{0} \cdot Z_{\Pi} \cdot \partial_{\mu}\chi + \sin\xi_{0} \cdot \partial_{\mu}\zeta) \stackrel{!}{=} 0.$$

$$(4.37)$$

This system can be understood as a first integral of the wave equations for ζ (4.34) and χ (4.35) (Hint: check this by differentiating once more the system [(4.36) and (4.37)] and using the wave equations for ζ , χ , and ξ_0).

The point with the vanishing of all the exchange fields is now that the system [(4.36) and (4.37)] admits a formal solution, namely

$$\cos \xi_{0} = \begin{cases} \sqrt{1 + C_{*}^{2}} \cdot \cos \left(\chi - \chi_{*} \right), & \sigma_{*} = +1 \\ -\sqrt{C_{*}^{2} - 1} \cdot \sinh \left(\chi - \chi_{*} \right), & \sigma_{*} = -1 \end{cases}$$
(4.38a)

$$Z_{\rm II}(\zeta) = \frac{C_*}{\sin \xi_0}.$$
 (4.38b)

This solution establishes a rigid link between the mixture variables ζ , χ and the pure-state variable ξ_0 . Since the latter quantity is related to the single-particle amplitudes L_a via (cf. (4.9a) and (4.9b))

$$\sin \xi_{\rm o} = 2 \frac{L_1 L_2}{L_1^2 + L_2^2} \tag{4.39a}$$

$$\cos \xi_{\rm o} = \frac{L_1^2 - L_2^2}{L_1^2 + L_2^2},\tag{4.39b}$$

one can actually express the mixture variables ζ and χ through the single-particle amplitudes L_a . Thus what remains to be done is simply to eliminate the mixture variable ζ from the coupling matrix W_{ab} [(4.31) and (4.32)] by means of the relationships (4.38a) and (4.38b) via

$$\frac{g^{\mu}h_{\mu}}{2Z_{\mathrm{II}}^{2}} = -L_{1}L_{2}\frac{L_{1}^{2} - L_{2}^{2}}{\left(L_{1}^{2} + L_{2}^{2}\right)^{2}} \cdot \frac{(L_{1}\partial_{\mu}L_{2} - L_{2}\partial_{\mu}L_{1})(L_{1}\partial^{\mu}L_{2} - L_{2}\partial^{\mu}L_{1})}{\sigma_{*}L_{1}^{2}L_{2}^{2} + (C_{*}/2)^{2}\left(L_{1}^{2} + L_{2}^{2}\right)^{2}}$$
(4.40a)

$$\frac{g^{\mu}g_{\mu} - h^{\mu}h_{\mu}}{(2Z_{\Pi})^{2}} = \frac{4L_{1}^{2}L_{2}^{2} - (L_{1}^{2} - L_{2}^{2})^{2}}{(L_{1}^{2} + L_{2}^{2})^{2}} \cdot \frac{(L_{1}\partial_{\mu}L_{2} - L_{2}\partial_{\mu}L_{1})(L_{1}\partial^{\mu}L_{2} - L_{2}\partial^{\mu}L_{1})}{4\sigma_{*}L_{1}^{2}L_{2}^{2} + C_{*}^{2}(L_{1}^{2} + L_{2}^{2})^{2}}$$
(4.40b)

Observe also that the structure function g_s in front of the kinetic fields (4.32a) and (4.32b) within the coupling matrix W_{ab} can be expressed in terms of the amplitude fields as

$$\frac{Z_{\rm T}^2}{Z_{\rm II}^2} = 1 + \sigma_* \left(\frac{2}{C_*}\right)^2 \left(\frac{L_1 L_2}{L_1^2 + L_2^2}\right)^2 \equiv 1 + \sigma_* \frac{\sin^2 \xi_0}{C_*^2}.$$
 (4.41)

In this way, we actually see that the amplitude system (4.31) contains only pure-state variables where the nonlinearity induced by the coupling matrix W_{ab} is caused by the mixture effect. The latter may be parametrized by the *mixing parameter* C_* (4.38) so that for $C_* \to \infty$ the mixture system (4.31) tends again to the pure-state case (4.33). If the same elimination procedure of the mixture variable ζ in favor of the amplitude fields L_a is carried through for the singleparticle densities ρ_a (4.7), one gets these densities as exclusive functions of the amplitude fields. This result comes about via the structure functions g_w (4.8a) and g_s (4.8b) which both become functions of the amplitudes L_a by means of the link (4.41) between the renormalization factors and these amplitudes. The fact that any one of both densities ρ_a (a = 1, 2) is determined simultaneously by both amplitude fields may be considered as a kind of *fluid-dynamical entanglement* because a clear association of any one of the conserved currents $j_{a\mu}$ (a = 1, 2) to a definite amplitude field L_a is no longer possible for the mixtures.

Clearly the fortunate emergence of such a nice parameter C_* , admitting the continuous transition from mixtures to pure states, can be exploited in order to establish a perturbation expansion (in powers of C_*^{-n}) of the mixture results ($C_* < \infty$) around the pure-state results ($C_* = \infty$). However in order to get a qualitative picture of what happens for small enough values of C_* , far from the pure-state limit ($C_* \to \infty$), we cannot apply such an expansion but rather have to deal with the exact analytic expressions with respect to the mixing parameter.

5. PERTURBATIVE APPROACH

An approximative treatment of two-particle systems is possible in two ways: first, one can consider the electromagnetic interactions between the two particles (e.g. being trapped in an "external" force field) as a perturbation just as is done in conventional quantum mechanics. The unperturbed situation then refers to the presence of two noninteracting particles in the same external force field and thus would lead us to two bound single-particle states in the same external field as the point of departure for a perturbation expansion. Second, one may consider the mixture effects as a perturbation of the pure-state situation. Since the mixing parameter C_* , introduced through Eq. (4.38b) for the special case of vanishing exchange fields, admits to switch on and off the mixture effect continuously ($C_* \rightarrow \infty$: pure states) one may think here of a perturbation expansion in terms of powers of C_* . In contrast to this the perturbation expansion with respect to the interparticle interactions would be based upon the electromagnetic coupling constant $\alpha_* (= \frac{e^2}{\hbar c})$. Subsequently we shall treat both perturbative aspects on the same footing and will consider only the first-order approximation.

5.1. Single-Particle Concepts vs. Center-of-Mass Approach

The perturbative treatment of the electrostatic fields of the two particles will be considerably facilitated by our simplification assumptions (3.71). The reason is that the exchange field strength $G_{\mu\nu}$ (3.43) must necessarily vanish whenever the generating exchange potential G_{μ} is zero. Thus the general curl relation for the relative kinetic field k_{μ} (3.36b) reads simply

$$\nabla_{\mu}k_{\nu} - \nabla_{\nu}k_{\mu} = 2f_{\mu\nu} \tag{5.1}$$

and the modified field k_{μ} (3.45) can be identified with the original k_{μ} .

As a consequence, the SPB version of the EPB curl relation [(3.36a) and (3.36b)] could be simplified as shown in Eq. (4.24), where the properties of the SPB curvature components $F_{a\mu\nu}$ have already been described through Eqs. (4.11)–(4.13). According to that construction, any curvature component $F_{a\mu\nu}$ (a = 1, 2) is the sum of the external field $^{(ex)}F_{\mu\nu}$ and the single-particle field $'F_{b\mu\nu}$ being generated by the *other* particle. Thus the external field $^{(ex)}F_{\mu\nu}$, being felt by any one of both particles, appears to be "averted" by the field $'F_{b\mu\nu}$ of the other particle. Similarly the total kinetic field K_{μ} , feeling twice the mean field $\hat{F}_{\mu\nu}$ (3.36a), sees the double external field $^{(ex)}F_{\mu\nu}$ being averted through the sum of both single-particle fields

$$\nabla_{\mu}K_{\nu} - \nabla_{\nu}K_{\mu} = 2\hat{F}_{\mu\nu} = 2^{(\text{ex})}F_{\mu\nu} - (F_{1\mu\nu} + F_{2\mu\nu}).$$
(5.2)

More concretely, if the external field ${}^{(ex)}F_{\mu\nu}$ is due to a static point charge carrying z_{ex} charge units, then the total K_{μ} sees the double charge number $(2 \cdot z_{ex})$

being screened by two charge units $(2 = z_1 + z_2)$. This is very plausible because the total field K_{μ} describes the *external* (i.e. center-of-mass) motion of the twoparticle system, whereas the relative field k_{μ} rather refers to its *internal* degrees of freedom. The residual effect of the internal motion upon the external motion is then described by the sum of the single-particle fields on the right-hand side of Eq. (5.2). On the other hand, the external field ^(ex) $F_{\mu\nu}$ has no direct influence upon the internal motion as may be seen from the curl relation (5.1), with the internal field strength $f_{\mu\nu}$ (3.14d) being independent of the external ^(ex) $F_{\mu\nu}$:

$$f_{\mu\nu} \doteq \frac{1}{2}(F_{1\mu\nu} - F_{2\mu\nu}) = -\frac{1}{2}(F_{1\mu\nu} - F_{2\mu\nu}).$$
(5.3)

Thus there arise two possibilities for establishing a perturbation theory: (i) either one tries to solve the external problem alone (neglecting the internal degrees of freedom) and then one considers the internal motion as a perturbation or (ii) one tries to first solve both single-particle problems in the external field alone, cf. (4.33), and afterwards one considers the single-particle interactions W_{ab} (4.31) as a perturbation.

Subsequently we will carry through the second proposal based upon the single-particle concepts.

5.2. Perturbation Expansion

As usual in the conventional perturbation theory, one considers the field objects as a sum of individual terms whose magnitudes are decaying from order to order, i.e. we put for the amplitude fields

$$L_a(x) = {}^{(0)}L_a(x) + {}^{(1)}L_a(x) + {}^{(2)}L_a(x) + \cdots$$
(5.4)

and similarly for the kinetic fields

$$K_a(x) = {}^{(0)}K_a(x) + {}^{(1)}K_a(x) + {}^{(2)}K_a(x) + \cdots .$$
(5.5)

Substituting the amplitude exapansions (5.4) into the corresponding field equations (4.31), one just finds for the lowest-order approximation ${}^{(0)}L_a(x)$ the disentangled situation (4.33). i.e.

$$\Box^{(0)}L_a + {}^{(0)}L_a \left\{ \left(\frac{Mc}{\hbar}\right)^2 - {}^{(0)}K_{a\mu} \cdot {}^{(0)}K_a^{\mu} \right\} = 0.$$
 (5.6)

Furthermore it is assumed that the kinetic field does not feel the interparticle forces but only the external force, i.e. one puts in lowest order (cf. (4.25))

$${}^{(0)}K_{a\mu} = \partial_{\mu}{}^{(0)}\alpha_a + {}^{(\text{ex})}A_{\mu}.$$
(5.7)

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More concretely, for a static and spherically symmetric field configuration one puts (Rupp *et al.*, 2000)

$${}^{(\mathrm{ex})}A_{\mu} = A_{\mathrm{ex}}(r) \cdot \hat{t}_{\mu}, \qquad (5.8)$$

where *r* denotes the radial coordinate and $\hat{t}_{\mu} (= \partial_{\mu} x^0)$ is a unit vector pointing into the time direction ($\hat{t}^{\mu} \hat{t}_{\mu} = +1$). For instance, for the Coulomb potential with z_{ex} charge units placed in the origin (at r = 0) one has

$$A_{\rm ex}(r) = z_{\rm ex} \frac{\alpha_*}{r}.$$
(5.9)

Next, it should be evident that for such a symmetric situation the phase angles $\alpha_a(x)$ (4.27b) can only depend upon the time coordinate (x^0) in the following form:

$${}^{(0)}\alpha_a(x) = \frac{M_a c}{\hbar} \cdot x^0, \qquad (5.10)$$

where the integration constants M_a are the *mass eigenvalues* of the (bound) particles. As a consequence of these symmetry requirements, the zero-order kinetic fields ${}^{(0)}K_{a\mu} \doteq {}^{(0)}K_a(r) \cdot \hat{t}_{\mu}$ are found to be of the following form

$${}^{(0)}K_a(r) = \frac{{}^{(0)}M_a \cdot c}{\hbar} + z_{\rm ex}\frac{\alpha_*}{r},$$
(5.11)

where ${}^{(0)}M_a$ are the zero-order mass eigenvalues. For such a simple situation, the static form of the amplitude equations (5.6) reads

$$-\Delta^{(0)}L_a + {}^{(0)}L_a \left\{ \left(\frac{Mc}{\hbar}\right)^2 - \left({}^{(0)}K_a\right)^2 \right\} = 0$$
 (5.12)

and admits the well-known energy eigenfunctions ${}^{(0)}L_n(r)$ of the relativistic (scalar) hydrogen atom

$${}^{(0)}L_a(r) = \hat{L} \cdot \sqrt{\frac{z_{\text{ex}}^3}{\pi a_{\text{B}}^3}} \cdot L_a(y).$$
(5.13)

The eigenfunctions $L_n(y)$ are well known and may be looked up in any textbook about relativistic quantum mechanics (e.g., Messiah, 1965). Moreover, \hat{L} is some normalization constant which is unity for the pure states ($\sigma_* = 0$: $\hat{L} \Rightarrow 1$) but in general depends upon the mixing parameter C_* , and $a_B (= \frac{\hbar^2}{Me^2})$ is the Bohr radius.

Since our present endeavors aim at the mixture effects but not at the relativistic corrections, we can be satisfied with the nonrelativistic approximation to the eigenfunctions $L_n(y)$ which then become, e.g., for the single-particle ground state (1s)

$$L_1(y) = \exp(-y),$$
 (5.14)

or for the first excited state (2s)

$$L_2(y) = \frac{1}{\sqrt{8}} \cdot \left(1 - \frac{y}{2}\right) \exp\left(-\frac{y}{2}\right).$$
(5.15)

Correspondingly, the mass eigenvalues ${}^{(0)}M_a$ are also known exactly but for the present nonrelativistic limit we may be satisfied with working with the nonrelativistic binding energies ${}^{(0)}E_{\text{B},a}$ in lowest order

$${}^{(0)}E_{\mathrm{B},1} = \left(M - {}^{(0)}M_1\right) \cdot c^2 \cong \frac{1}{2} z_{\mathrm{ex}}^2 \frac{e^2}{a_{\mathrm{B}}}$$
(5.16a)

$${}^{(0)}E_{\mathrm{B},2} = \left(M - {}^{(0)}M_2\right) \cdot c^2 \cong \frac{1}{8} z_{\mathrm{ex}}^2 \frac{e^2}{a_{\mathrm{B}}}.$$
(5.16b)

5.3. Density Deformations

The present zero-order results are already sufficient in order to demonstrate certain RST peculiarities concerning the scalar densities ρ_a (4.7). The physical relevance of these densities originates from the fact that they essentially determine the interaction potentials $A_{a\mu}$ (4.17) via the currents $j_{a\mu}$ (4.6). Indeed one can easily show that in the first-order approximation these potentials $A_{a\mu}$ ($\Rightarrow A_a(r) \cdot \hat{t}_{\mu}$) can be written down in terms of the scalar densities as (Rupp *et al.*, 2000)

$${}^{\prime}A_{a}^{(1)}(r) = \alpha_{*} \int dV' \, \frac{{}^{(0)}\rho_{a}(\vec{r}')}{|\vec{r} - \vec{r}'|}.$$
(5.17)

Here the zero-order densities ${}^{(0)}\rho_a$ are obtained by introducing the zero-order amplitudes ${}^{(0)}L_a$ (5.13) into the defining equations (4.7). The resulting single-particle potentials ${}^{\prime}A_a^{(1)}$ (5.17) are then considered as first-order objects entering the first-order corrections ${}^{(1)}K_a$ of the kinetic fields (5.5) as follows:

$${}^{(1)}K_1(r) = \frac{{}^{(1)}M_1c}{\hbar} - {}^{\prime}A_2^{(1)}(r)$$
(5.18a)

$${}^{(1)}K_2(r) = \frac{{}^{(1)}M_2c}{\hbar} - {}^{\prime}A_1^{(1)}(r).$$
(5.18b)

Since the kinetic fields are acting back upon the amplitudes L_a according to the last step (\Box) of the interaction schemes (4.22) and (4.23), the influence of the densities ${}^{(0)}\rho_a$ upon the first-order mass corrections ${}^{(1)}M_a$ is evident. Observe

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here that these mass corrections themselves may be computed from the first-order amplitude equations

$$-\Delta^{(1)}L_a + {}^{(1)}L_a \left\{ \left(\frac{Mc}{\hbar}\right)^2 - \left({}^{(0)}K_a\right)^2 \right\} = 2{}^{(0)}L_a \left({}^{(0)}K_a \cdot {}^{(1)}K_a\right) - {}^{(1)}W_a^b \cdot {}^{(1)}L_b$$
(5.19)

which neccessarily must contain the first-order kinetic fields ⁽¹⁾ K_a (5.18). (The first-order mixture coupling elements ⁽¹⁾ W_{ab} are obtained by introducing the zero-order amplitudes ⁽⁰⁾ L_a into their defining equations (4.32) with observation of the scalar products (4.40).)

Now that the role of the densities ${}^{(0)}\rho_a$ has become clear, the interesting point with these densities refers to their deformation when the mixing parameter C_* varies from infinity (\rightarrow pure states) up to its minimal possible value which is $C_- = 1$ for the negative mixtures ($\sigma_* = -1$) and $C_+ = 0$ for the positive mixtures ($\sigma_* = +1$); see Fig. 3. For the pure states ($C_* = \infty$), the densities ${}^{(0)}\rho_a$ (4.7) coincide with the squares $({}^{(0)}L_a)^2$ of the amplitudes because here the structure function g_w (4.8a) is identical to unity and g_s (4.8b) vanishes. But with decreasing mixing parameter C_* the densities are deformed considerably away from their original amplitude shape and this deformation occurs for the two types of mixtures ($\sigma_* = \pm 1$) in a rather different way:

- (i) For the *positive* mixtures (σ_{*} = +1), both densities tend to become identical and arrive at the complete identity (⁽⁰⁾ρ₁ ≡ ⁽⁰⁾ρ₂) for the minimal possible value C₊ = 0 (→ *charge fusion*);
- (ii) However for the *negative* mixtures ($\sigma_* = -1$), both densities tend to recede from each other and thus try to occupy non-overlapping regions in three-space such that the complete *charge separation* is achieved for the minimal possible value $C_- = 1$ of the mixing parameter C_* .

Clearly, such a dichotomy of the behavior of the RST matter strongly reminds one of the corresponding boson–fermion dichotomy of matter in the conventional quantum theory. There the well-known Pauli exclusion principle says (among other things) that fermionic single-particle wave functions are reluctant to occupy the same region of three-space whereas the wave functions of bosonic particles even tend to fuse into a single one (as, e.g., during the process of Bose–Einstein condensation). Such a dichotomic behavior of matter must necessarily lead to experimental consequences, namely concerning the energy levels available for any type of matter bound by an attractive force. Here one would like to think that the fermionic matter occupies a lower energy level in comparison to the bosonic case because the charge separation (classically spoken) lowers the electrostatic interaction energy of the fermions whereas the charge fusion is expected to increase the interaction energy of the bosons. Indeed this expectation is realized in the conventional quantum theory (see Section 1) but it is also true in RST as can readily be demonstrated for the present two-particle situation described previously.

5.4. Two-Particle Interaction Energy

Suppose the present two-particle mass-eigenvalue problem (4.31) for the Coulomb potential $A_{ex}(r)$ (5.9) admits an exact solution. In this ideal situation, the perturbation expansion for the kinetic fields (5.5) would converge to the exact form

$$K_1(r) = \frac{M_1 c}{\hbar} + A_{\rm ex}(r) - A_2(r)$$
(5.20a)

$$K_2(r) = \frac{M_2 c}{\hbar} + A_{\rm ex}(r) - A_1(r)$$
(5.20b)

and thus both mass eigenvalues M_a would be known exactly. Also known exactly are the zero-order values ${}^{(0)}M_a$ which apply for the situation when the interparticle interactions (of both electromagnetic and mixture type) are switched-off, i.e. for $A_a \equiv 0$ and $C_* \rightarrow \infty$. The exact total mass M_{12} of the 2-particle system with switched-on interactions could then be defined as

$$M_{12} = \frac{1}{2} \{ {}^{(0)}M_1 + M_1 + {}^{(0)}M_2 + M_2 \}.$$
 (5.21)

This appears to be a plausible proposition because M_{12} reduces to the sum of the individual mass eigenvalues ${}^{(0)}M_a$ when the interactions are switched-off and thus $M_a \Rightarrow {}^{(0)}M_a$. Furthermore the interaction energy $(M_{12} - {}^{(0)}M_1 - {}^{(0)}M_2)$ is partitioned to both matter modes according to the scheme

$$M_{12} - \{{}^{(0)}M_1 + {}^{(0)}M_2\} = \frac{1}{2}(M_1 - {}^{(0)}M_1) + \frac{1}{2}(M_2 - {}^{(0)}M_2), \qquad (5.22)$$

i.e. both matter degrees of freedom contribute with the same weight $(\frac{1}{2})$.

In the first-order approximation one concludes from this for the total mass correction ${}^{(1)}M_{12}$ produced by the 2-particle interactions

$${}^{(1)}M_{12} = \frac{1}{2} \{ {}^{(1)}M_1 + {}^{(1)}M_2 \},$$
 (5.23)

where the individual mass corrections ${}^{(1)}M_a$ can be computed by means of the first-order amplitude equations (5.19) applying standard methods of perturbation theory (Rupp *et al.*, 2000). The result for the interaction energy ${}^{(1)}E_{12} = {}^{(1)}M_{12} \cdot c^2$ is plotted in Fig. 1 which demonstrates some interesting features (for the technical details, see Rupp *et al.*, 2000):

(i) For $C_* \to \infty$ (pure states) the mixture coupling vanishes (i.e. $W_{ab} \Rightarrow 0$) and we are left with two disentangled particles. These are described by the decoupled amplitude system (4.33) and are subject exclusively to the electrostatic gauge interactions, as it is symbolized by the interaction scheme (4.23) for the limit case $C_* \Rightarrow \infty$. Therefore one expects the interaction energy ${}^{(1)}E_{12}$ to be identical with the classical electrostatic interaction energy ($U_{\rm C}$) of the two charge clouds produced by the (normalized) single-particle amplitudes ${}^{(0)}L_a(\vec{r})$:

$$U_{\rm C} = e^2 \int dV \int dV' \, \frac{\left({}^{(0)}L_1(\vec{r})\right)^2 \cdot \left({}^{(0)}L_2(\vec{r}')\right)^2}{|\vec{r} - \vec{r}'|}.$$
 (5.24)

For the (1s, 2s)-configuration (5.13)–(5.16) one finds (either in the literature (Grau, 1993) or by explicit calculation)

$$U_{\rm C}(1s, 2s) = \frac{17}{81} z_{\rm ex} \frac{e^2}{a_{\rm B}} \approx 5.711 \cdot z_{\rm ex} \, [{\rm eV}]. \tag{5.25}$$

As shown by Fig. 1, this limit requirement is actually reproduced by our perturbative approach which therefore is reliable with respect to the gauge interactions.

- (ii) Now switching-on the mixture interactions means decreasing the value of the mixing parameter C_* from infinity to finite values ($C_* < \infty$). As the numerical results demonstrate (Fig. 1), the interaction energy ${}^{(1)}E_{12}$ decreases with decreasing C_* and thus tends toward the experimental values for the symmetric (S) and antisymmetric (A) 2-particle configurations. In this sense, the RST perturbation results come closer to the experimental values than the first-order predictions ($U_C \pm E_G$) of conventional quantum theory (cf. Section 1). Observe also that for identical values of the mixing parameter C_* , the interaction energy for the positive mixtures ($\sigma_* = +1$) is greater than for the negative mixtures ($\sigma_* = -1$). This supports the hypothesis of attributing the negative (positive) RST mixtures to fermionic (bosonic) matter.
- (iii) A certain problem arises for the present first-order perturbation result of RST when the mixing parameter C_* approaches its minimal value C_{\pm} (negative mixtures: $C_* \rightarrow C_- = 1$; positive mixtures: $C_* \rightarrow C_+ = 0$). In both cases, the interaction energy ${}^{(1)}E_{12}$ becomes infinite $({}^{(1)}E_{12} \rightarrow -\infty)$. Clearly, this signals a breakdown of the first-order approximation. Since the exact solution is not known, it is presently unclear what really happens when C_* approaches its minimally possible values C_{\pm} . Observe, however, that for the present first-order approximation one can fix the mixing parameter C_* in such a way ($C_* \Rightarrow C_*^{(\pm)}$) that the present first-order result exactly agrees with the experimental values (albeit the latter refer to *spinning* electrons whereas we are satisfied with the treatment of scalar charged particles).
- (iv) As is suggested by the numerical results of Fig. 3, there should exist a kind of *asymptotic mixture degeneracy* in the sense that not only for

the pure states themselves ($C_* = \infty$) but also in the vicinity of the pure states ($C_* \rightarrow \infty$) the energy eigenvalues ${}^{(1)}E_{12}$ of positive ($\sigma_* = +1$) and negative ($\sigma_* = -1$) mixtures become identical! This obvious suggestion will be clarified by an analytic computation for that asymptotic region (see a separate paper, by Rupp and Sorg, 2000). Such a mixture degeneracy represents the RST analog of the conventional exchange degeneracy, cf. the corresponding remarks in connection with Eqs. (1.2a) and (1.2b).

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