Relativistic wave equations for many-particle quantum systems

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In this paper, some concepts of nonrelativistic many-particle quantum mechanics (e.g., product states, density matrix) are generalized to the relativistic domain using a framework called relativistic Schrödinger theory (RST). By using a general ansatz, the RST framework is simplified considerably and some of its field equations are solved directly. The RST approach is then compared with nonrelativistic quantum mechanics (QM) for the case of a product state (conventional QM) and its RST analog. It is shown that relativistic wave equations can be derived from the RST formalism, so that they coincide in the nonrelativistic limit with the well-known Hartree equations.

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The dynamics of a state vector in nonrelativistic quantum mechanics is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle. \tag{1}$$

Likewise, the time development of a mixture configuration is given by the von Neumann equation

$$i\hbar \frac{d}{dt}\rho = [\hat{H},\rho]. \tag{2}$$

The quantities $|\Psi\rangle$ and ρ are elements of an infinite-dimensional *global* Hilbert space and must therefore be considered as nonlocal objects. For example, the state vector $|\Psi\rangle$ of an N-particle system depends on the time coordinate t and the three-coordinates $\vec{x}_i$ $(i=1,\ldots,N)$ at *different* points of three-space. Both Eqs. (1) and (2) are not Lorentz covariant, yet one may assume that they constitute the nonrelativistic limiting case of some relativistic framework. This is clearly true for the one-particle case: The Schrödinger equation (1) may be considered as the nonrelativistic limit of the Klein-Gordon equation

$$\mathcal{D}_\mu \mathcal{D}^\mu \psi + \left(\frac{Mc}{\hbar}\right)^2 \psi = 0, \tag{3}$$

(see Ref. [1]). The generalization of this result to a system of N particles is, however, difficult as the N space coordinates $\vec{x}_i$ of $|\Psi\rangle$ have to be replaced by N space-time coordinates $x_{i\mu}$, such that the vector $|\Psi\rangle$ depends on N individual particle times t_i. This makes the interpretation of the state vector difficult and necessitates the construction of one global time out of the N individual particle times, a difficult if not impossible task [2]. For the two-particle case, this has been done (cf. Bethe-Salpeter equation [3]), yet there still remain some unsolved problems [4]. In summary, there do not exist generally accepted relativistic wave equations for the N-particle case.

If one was able to find a relativistic generalization of Eqs. (1) and (2), it should be possible to derive such relativistic wave equations for the many-particle case. Some years ago, a framework named relativistic Schrödinger theory (RST) has been proposed [5,6] as a possible step in that direction. However, the RST field equations constitute a system of nonlinear partial differential equations, which up to now has been difficult to solve. In this paper, we solve most of the RST field equations using a general ansatz and show how RST deals with relativistic many-particle systems.

The essential difference between the RST approach and conventional quantum theory is the way in which many-particle states are constructed from one-particle states; whereas conventional QM constructs many-particle states as product states from one-particle states, e.g., for two particles (in coordinate space):

$$\Psi = \psi_1(\vec{x}_1,t)\cdot\psi_2(\vec{x}_2,t), \tag{4}$$

such that the total wave function depends on different points of space, the RST approach is considering the wave function of a many-particle system as being constructed as the direct sum of one-particle states at the *same* point of space-time:

$$\Psi(x_\mu) = \psi_1(x_\mu)\oplus\psi_2(x_\mu) = \begin{pmatrix}\psi_1(x_\mu)\\ \psi_2(x_\mu)\end{pmatrix}. \tag{5}$$

One of the results of this paper is to show that using the ansatz (4) in conventional QM and (5) in RST leads to the same wave equations in the nonrelativistic case, namely, the Hartree equations [7], which constitute a set of wave equations for the one-particle wave functions ψ_1 and ψ_2. The advantage of the RST approach over conventional QM lies in the fact that it produces a set of relativistic wave equations which reduce to the Hartree equations only in the nonrelativistic limit.

Of course, the wave vector (5) must obey some dynamical equation, which has been postulated in RST in close analogy to the nonrelativistic equation (1):

$$i\hbar c\mathcal{D}_\mu\Psi = \mathcal{H}_\mu\Psi, \tag{6}$$

$$(\mathcal{D}_\mu\Psi \equiv \partial_\mu\Psi + \mathcal{A}_\mu\Psi),$$

and is referred to in the following as relativistic Schrödinger equation (RSE). The state vector Ψ is a local sum (Whitney sum [8]) of N one-particle wave functions [constructed as in Eq. (5)]. The RSE is Lorentz and gauge covariant [5], and introduces as a new object the Hamiltonian field operator $\mathcal{H}_\mu$, which is not a fixed quantity as in conventional QM,

but obeys its own set of field equations. Furthermore, the Hamiltonian is non-Hermitian ($\mathcal{H}_\mu \neq \overline{\mathcal{H}}_\mu$), which does not reflect the fact that dissipation is present in the system, but merely that the local modulus ($\overline{\Psi}\Psi$) of the wave function Ψ is variable. For concrete applications, the Hamiltonian $\mathcal{H}_\mu$ may be considered as an $N\times N$ complex matrix of one-forms taking its values in the Lie algebra gl$(N,\mathbb{C})$.

As the relativistic analog of the von Neumann equation (2), the relativistic von Neumann equation (RNE) was proposed:

$$\mathcal{D}_\mu \mathcal{I} = \frac{i}{\hbar c}(\mathcal{I}\cdot\overline{\mathcal{H}}_\mu - \mathcal{H}_\mu\cdot\mathcal{I}) \tag{7}$$

$$\mathcal{D}_\mu \mathcal{I} \equiv \partial_\mu \mathcal{I} + [\mathcal{A}_\mu, \mathcal{I}].$$

The Hermitian intensity matrix $\mathcal{I}=\overline{\mathcal{I}}$ may be formally considered as the relativistic analog of the density matrix.

The essential new feature of the RST is clearly the usage of a Hamiltonian one-form $\mathcal{H}_\mu$ as a dynamical object. The field equations for $\mathcal{H}_\mu$ must be postulated in such a way that solutions to Eqs. (6) and (7) exist, which leads to the following curl equation:

$$\mathcal{D}_\mu \mathcal{H}_\nu - \mathcal{D}_\nu \mathcal{H}_\mu + \frac{i}{\hbar c}[\mathcal{H}_\mu, \mathcal{H}_\nu] = i\hbar c \mathcal{F}_{\mu\nu}, \tag{8}$$

referred to as the integrability condition. $\mathcal{F}_{\mu\nu}$ is the field strength operator of the gauge field $\mathcal{A}_\mu$ which carries the interaction and is defined as usual in Yang-Mills theory:

$$\mathcal{F}_{\mu\nu} = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu + [\mathcal{A}_\mu, \mathcal{A}_\nu]. \tag{9}$$

It obeys the Yang-Mills equations

$$\mathcal{D}^\mu \mathcal{F}_{\mu\nu} = 4\pi\alpha_* \mathcal{J}_\nu, \tag{10}$$

(α_* is the coupling constant) which reduce to the usual Maxwell equations in the Abelian case ($\alpha_* = e^2/\hbar c$).

The source equation for $\mathcal{H}_\mu$ guarantees the conservation of certain quantitites (such as charges, etc.) and differs for matter with and without spin. For spinless particles, we have

$$\mathcal{D}^\mu \mathcal{H}_\mu - \frac{i}{\hbar c}\mathcal{H}^\mu \mathcal{H}_\mu = -i\hbar c\left(\frac{\mathcal{M}c}{\hbar}\right)^2 \tag{11}$$

and for spin-1/2 particles,

$$\mathcal{D}^\mu \mathcal{H}_\mu - \frac{i}{\hbar c}\mathcal{H}^\mu \mathcal{H}_\mu = -i\hbar c\left(\frac{\mathcal{M}c}{\hbar}\right)^2 - i\hbar c \Sigma^{\mu\nu}\mathcal{F}_{\mu\nu}, \tag{12}$$

which is equivalent to [5]

$$\gamma_\mu \mathcal{H}^\mu = Mc^2 \mathbf{1} \tag{13}$$

[note that contracting Eq. (13) with $\gamma_\nu \mathcal{D}^\nu$ from the left yields Eq. (12)].

Until now, it was very difficult to obtain solutions to this coupled system of field equations. It was necessary to first solve the Hamiltonian dynamics (11)–(13) which subsequently admits to solve the RSE (6) for Ψ and the RNE (7) for $\mathcal{I}$. However, the link between the matter fields $\mathcal{I}$ and Ψ and $\mathcal{H}_\mu$ could have been obtained in a more direct way. We will show that both, the matter fields and the Hamiltonian may be constructed from the same object, a group element $g \in \mathrm{GL}(N,\mathbb{C})$.

The key point to obtain this result is the fact that the integrability condition (8) can be solved by the following ansatz for $\mathcal{H}_\mu$:

$$\mathcal{H}_\mu = i\hbar c(\mathcal{D}_\mu g)g^{-1} = i\hbar c[(\partial_\mu g)\, g^{-1} + \mathcal{A}_\mu], \tag{14}$$

$$(\mathcal{D}_\mu g \equiv \partial_\mu g + \mathcal{A}_\mu g)$$

with $g \in \mathrm{GL}(N,\mathbb{C})$. Note that Eq. (14) constitutes locally the general solution of Eq. (8) (see Ref. [9]). The Hamiltonian $\mathcal{H}_\mu$ is therefore identified as being the sum of the Maurer-Cartan form $(\partial_\mu g)g^{-1}$ of a group element $g \in \mathrm{GL}(N,\mathbb{C})$ and the gauge field $\mathcal{A}_\mu$, which take their values in the Lie algebra gl$(N,\mathbb{C})$ and in the gauge algebra, respectively, which is fixed by the type of interaction. The knowledge of the general form of $\mathcal{H}_\mu$ (14) makes it possible to solve the RSE (6) and the RNE (7) directly, which yields for the RSE

$$\Psi = g\Psi_* \tag{15}$$

(Ψ_* being a constant complex N vector) and

$$\mathcal{I} = g g_* \overline{g} \tag{16}$$

for the RNE (g_* being a constant Hermitian $N\times N$ matrix). The adjoint operator $\overline{g}$ is the Hermitian conjugate $g^\dagger$ multiplied by a constant unitary matrix (in the case of Klein-Gordon (KG) particles, this unitary matrix is **1**, and for Dirac particles, it is γ_0). By use of the ansatz (14), one finds that the conservation equation (11) is satisfied by putting

$$\mathcal{D}_\mu \mathcal{D}^\mu g - \left(\frac{Mc}{\hbar}\right)^2 g = 0, \tag{17}$$

where the mass operator $\mathcal{M}$ has been set proportional to unity ($\mathcal{M}\sim\mathbf{1}$ for indistinguishable particles), and for satisfying Eq. (13), one can put

$$i\hbar\gamma^\mu \mathcal{D}_\mu g = Mcg, \tag{18}$$

which are nothing else than the Klein-Gordon and Dirac equations for a group element g instead of a complex scalar ψ or a Dirac spinor Ψ. To recover the usual KG and Dirac equations, it is sufficient to let the operator equations (17) and (18) act upon the constant element Ψ_* and exploit the definiton of the wave function Ψ (15).

Although the main concern of our paper are the RST states (5), which constitute a subset of the pure states, it should be noticed that it is posssible to distinguish (as in conventional quantum mechanics) between pure states and mixtures in RST by using the following criterion [10]:

$$\det \mathcal{I} \begin{cases} >0 & : \text{ positive mixtures} \\ =0 & : \text{ pure states} \\ <0 & : \text{ negative mixtures} \end{cases} \tag{19}$$

(in conventional QM, one considers only the positive mixtures). Although the intensity matrix is a local quantity, varying from one space-time point to another space-time point, the sign of $\det \mathcal{I}$ is always fixed, as can be seen immediately from Eq. (16):

$$\det \mathcal{I} = \det(g\, g_* \overline{g}) = |\det(g)|^2 \det(g_*), \tag{20}$$

such that $\det \mathcal{I}$ depends only on the sign of the constant $\det(g_*)$. A pure state ($\det \mathcal{I}=0$) can therefore only be approached by a mixture if $\det(g) \Rightarrow 0$ in a region of space-time.

Most of the recent papers on RST have been considering mixture configurations [10,11]. Clearly, the relationship between mixtures and pure states is very important and interesting, however, if one wants to link RST and conventional QM, it is more instructive to consider a very simple case first, namely, that of two particles with electromagnetic interactions approximated by a pure state of the form (5) [being the equivalent of the product state (4) of conventional QM].

In conventional QM, the problem of two bound particles in the field of a nucleus (with charge Z) is given by the Schrödinger equation (1) and the following Hamiltonian $\hat{H}$:

$$\hat{H} = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - \frac{Ze^2}{|\vec{x}_1|} - \frac{Ze^2}{|\vec{x}_2|} + \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}. \tag{21}$$

To get a lowest-order approximative solution to Eq. (1), let us assume that this solution may be written as a product state of the form (4). The optimal single-particle wave functions ψ_1 and ψ_2 are then determined by minimizing the energy functional $E = \langle \Psi | \hat{H} | \Psi \rangle$ constructed from the static Schrödinger equation

$$E|\Psi\rangle = \hat{H}|\Psi\rangle \tag{22}$$

using the ansatz (4) for $|\Psi\rangle$ in time-independent form (see, e.g., Ref. [12]). The constraint that the one-particle wave functions have to be normalized to unity [$\int |\psi_i(x)|^2 dV = 1$] is taken into account by adding Lagrangian multipliers ϵ_i, such that the functional $\mathcal{F}$ to be minimized is of the following form:

$$\mathcal{F} = \langle \Psi | \hat{H} | \Psi \rangle - \sum_i \epsilon_i \left(\int |\psi_i(x)|^2 dV - 1 \right). \tag{23}$$

The result of this variation process are the Hartree equations

$$\left(-\frac{\hbar^2}{2M}\Delta_i - \frac{Ze^2}{\vec{x}_i} + V_i(\vec{x}_i) \right) \psi_i(\vec{x}_i) = \epsilon_i \psi_i(\vec{x}_i), \tag{24}$$

with the potentials V_i being defined as

$$V_i(\vec{x}_i) = \sum_{j \neq i} \int \frac{e^2}{|\vec{x}_i - \vec{x}_j|} |\psi_j(\vec{x}_j)|^2 d^3 x_j. \tag{25}$$

For our special problem of two particles, we put ($i,j = 1,2$).

The Lagrangian parameters ϵ_i are interpreted as the ionization energy of the ith particle under the assumption that all the other one-particle states remain unchanged (Koopmans' theorem [13]). The Hartree equations (24) are local equations for the ψ_i, i.e., involve only quantities at the same space point $\vec{x} = \vec{x}_i (i = 1, \ldots, N)$. However, they involve potentials which depend on an integration of the other wave functions $\psi_j (j \neq i)$ over the whole three-space. This is why the potentials (25) are considered as nonlocal quantities by some authors. These integrals may however be considered as being derived from a certain form of *local* Maxwell equations (see below).

How is the same problem treated in RST? Again, we restrict ourselves to the case of two particles. We then specialize the group element g to a 2×2 matrix, put one column to zero and retain only the other one. Equation (17) is then reduced to the following vector equation:

$$(\partial^\mu + \mathcal{A}^\mu)(\partial_\mu + \mathcal{A}_\mu) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} + \left(\frac{Mc}{\hbar} \right)^2 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0. \tag{26}$$

We now specialize the gauge field to the case of the electromagnetic interactions. We put [14]

$$\mathcal{A}_\mu = \frac{ie}{\hbar c} \begin{pmatrix} A_{2\mu} & 0 \\ 0 & A_{1\mu} \end{pmatrix} = \frac{ie}{\hbar c}(A_{2\mu}\mathcal{P}_1 + A_{1\mu}\mathcal{P}_2) \tag{27}$$

and using the Yang-Mills equations (10) in component form, we find

$$\partial^\mu F_{i\mu\nu} = 4\pi\alpha_* (j_{i\nu} + j_\nu^{(\mathrm{ex})}), \tag{28}$$

($i = 1,2$). The conserved currents $j_{i\nu}$ can be derived from the field equations (26) and are given by

$$j_{i\nu} = \frac{i\hbar}{2Mc} \left(\psi_i^* \partial_\nu \psi_i - \psi_i \partial_\nu \psi_i^* + 2\frac{ie}{\hbar c} A_{j\nu} \psi_i \psi_i^* \right), \tag{29}$$

($i,j = 1,2; i \neq j$). The external current $j_\nu^{(\mathrm{ex})} = (j_0^{(\mathrm{ex})}, \vec{j}^{(\mathrm{ex})})$ is generated by the static point charge of the nucleus [$j^{(\mathrm{ex})} \equiv j_0^{(\mathrm{ex})} = -Z\delta(\vec{x}), \vec{j}^{(\mathrm{ex})} = \vec{0}$]. By using the ansatz (27) for $\mathcal{A}_\mu$, the self-energy problem is avoided (for more details on this point, see Ref. [14]). Using the Lorentz gauge condition ($\partial^\nu A_{i\nu} = 0$), we get two wave equations from Eq. (28)

$$\Box A_{i\nu} = 4\pi e (j_{i\nu} + j_\nu^{(\mathrm{ex})}). \tag{30}$$

The equations for the matter fields (26) and the gauge fields (30) constitute the set of relativistic wave equations which have to be solved in the RST approach. Note that both magnetic as well as retardation effects are included into these equations, whereas the exchange interactions are neglected by the simplified ansatz (5).

We now consider a static solution to Eqs. (26) and (30) by making the following ansatz for the wave functions ψ_i:

$$\psi_i(x_\mu)=\psi_i(\vec{x})\exp\left[-\frac{i\epsilon_i}{\hbar}t\right]. \tag{31}$$

Note that both wave functions are taken at the *same* point of space-time, so that there is no distinction between different space positions $\vec{x}_1$, $\vec{x}_2$ for the two wave functions (i.e., $\vec{x}=\vec{x}_1=\vec{x}_2$). The four-potential $A_{i\nu}=(A_{i0},\vec{A}_i)$ is reduced to its static form by the ansatz $A_{i\nu}=(V_i(\vec{x}),0)$, such that only the zeroth component of the currents $j_{i\nu}$ is different from zero:

$$j_i(\vec{x})\equiv j_{i0}(\vec{x})=\frac{1}{Mc^2}(\epsilon_i-eV_j)\psi_i(\vec{x})\psi_i^*(\vec{x}). \tag{32}$$

Inserting the static form of the currents into Eq. (30) allows one to integrate this equation formally to yield

$$V_i(\vec{x})=e\int\frac{j_i(\vec{x}')+j^{(\mathrm{ex})}(\vec{x}')}{|\vec{x}-\vec{x}'|}d^3x'. \tag{33}$$

Equation (25) is simplified by this ansatz to

$$[\hbar^2c^2\Delta+(\epsilon_i-eV_j+Mc^2)(\epsilon_i-eV_j-Mc^2)]\psi_i(\vec{x})=0. \tag{34}$$

In order to compare with conventional QM, we now consider the nonrelativistic limit by first noting that the energy, ϵ_i is given by the rest mass plus the additional binding energy, $\epsilon_i=Mc^2+\epsilon_i'$. We now suppose that $\epsilon_i'-eV_j\ll Mc^2$ and obtain the following wave eqution:

$$\left(-\frac{\hbar^2}{2M}\Delta+e\,V_j\right)\psi_i(\vec{x})=\epsilon_i'\psi_i(\vec{x}). \tag{35}$$

One is easily convinced that Eq. (35) coincides with the Hartree equations (24) by noting that the currents j_i reduce in the nonrelativistic limit to

$$j_i(\vec{x})=\psi_i(\vec{x})\psi_i^*(\vec{x})=|\psi_i(\vec{x})|^2 \tag{36}$$

and therefore the potentials $V_i(\vec{x})$ are given by

$$V_i(\vec{x})=-\frac{Ze}{|\vec{x}|}+\int\frac{e\,|\psi_i(\vec{x}')|^2}{|\vec{x}-\vec{x}'|}d^3x'. \tag{37}$$

For the sake of simplicity, we have limited our discussion to the two-particle case, the generalization to the N-particle case is however obvious, as one just has to replace the two-particle ansatz (27) for the gauge potential $\mathcal{A}_\mu$ by

$$\mathcal{A}_\mu=\frac{1}{N-1}\frac{ie}{\hbar c}\sum_{i,j\neq i}A_{j\mu}\mathcal{P}_i. \tag{38}$$

The normalization factor $1/(N-1)$ is necessary so that the ith particle feels the *average* potential of the $(N-1)$ other particles, and the projectors $\mathcal{P}_i$ have been defined in Eq. (27) in an obvious way.

In summary, the RST formalism has been simplified considerably by making use of the ansatz (14) and the relationship between the matter fields $\mathcal{I}$ and Ψ and the Hamiltonian, one-form $\mathcal{H}_\mu$, has been clarified. Moreover, it has been shown using the special ansatz (5) that the RST formalism can be used to obtain relativistic many-particle wave equations (26) which take into account both magnetic as well as retardation effects and coincide with the Hartree equations in the nonrelativistic static limit. This has been made possible by a suitable choice of the gauge field operator $\mathcal{A}_\mu$ (27) and (38) in such a way that the self-energy problem is avoided. By making use of a nondiagonal operator $\mathcal{A}_\mu$, it should be possible to also derive a relativistic analog of the Hartree-Fock equations (in preparation). The RST formalism seems to allow the generalization of the nonrelativistic mixture concept to the relativistic domain; further investigations into this field are necessary. As a final point, it remains to be seen if the creation-annihilation processes of quantum field theory may also be included into the RST appproach.

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