Kramers equations for atoms

H. Pilkuhn
Institut für Theoretische Kernphysik, Universität Karlsruhe, Kaiserstrasse 12, Postfach 6980, D-7500 Karlsruhe 1, Federal Republic of Germany

Received 4 February 1988; final version 23 March 1988

Starting from the Dirac-Breit equation in the Weyl representation, eliminating all components with at least one dotted index and omitting the resulting higher powers of the Breit operator, one obtains a new, four-component “Kramers-type” equation for two charged spinor particles in external fields. Alternatively, the equation is derived from the QED $S$-matrix including external potentials, using a two time formalism and eliminating the relative time. It has the usual factorizing orbital solutions in the limit of very large external fields, and reduces to the modern “effective onebody” equations with relativistic two-body kinematics for binary atoms in the limit of vanishing external fields. The application to helium-like Rydberg states is mentioned.

PACS: 11.10.Q; 31.30.J

1. Introduction

The relativistic wave equations of Schrödinger and Dirac were intended by their inventors for a single particle in a given four-potential $A^a(r,t)$. However, it was soon realized that they apply primarily to field operators which create particles and remove antiparticles, and that $A^a$ contains an operator piece $A^a_{op}$ in addition to the external potential $A^a_{ext}$. In particular, the relativistic Schrödinger equation, now known as Klein-Gordon equation, was shown to be correct for a scalar field operator [1]. With the notation

$$\pi^0 = i \partial_t + eA^0, \quad \pi = -iV + eA \quad \text{(units} \ h = c = 1\text{)},$$

it reads

$$(\pi^0 - K) \psi = 0, \quad K = K_0 + e(\mathbf{B} - i\mathbf{E}).$$

(1.1)

From the field equations, one can derive the original single-particle equations as approximations, the corrections (selfenergy shift, vacuum polarization, anomalous magnetic moment, etc.) being small in practically all cases. This development has shown that Dirac’s original reservation against equations with second-time derivatives was unjustified.

After the resurrection of the spinless equation [1], Kramers [2] published his version of the Dirac equation: if one uses two-component Weyl spinors ($\psi_R, \psi_L$) in the Dirac equation ($\psi_R = \text{righthand = undotted spinor}, \psi_L = \text{lefthand = dotted spinor}$) and eliminates one Weyl spinor, say $\psi_L$, one obtains a second-order equation for the other one:

$$(\pi^0 - K) \psi_R = 0, \quad K = K_0 + e\sigma(\mathbf{B} - i\mathbf{E})$$

(1.2)

with $\mathbf{B} = \text{rot} \mathbf{A}, \mathbf{E} = -\partial_t \mathbf{A} - \nabla A^0$, and $\sigma$ = Pauli matrices (see Sect. 2 for details). The equation has twice as many solutions as the Dirac equation (which depends also on the sign of $m$), but provides nevertheless a convenient basis for QED [3] as well as an approximate (in the above sense) one-electron equation [4]. In fact, in several one-electron cases the Kramers equation is more convenient than the original Dirac equation [5, 6].

Systems with two relativistic spin-$\frac{1}{2}$ particles occur in very different cases. When Breit derived his 16-component Dirac-Breit equation [7] he envisaged the helium atom, but the equation gives also all relativistic $x^2$-recoil corrections for free “binary atoms” such as hydrogen and positronium (in the latter case, one must add an “annihilation potential” in the triplet $S$-state, which we shall ignore). Apart from the regrettable fact that the Breit operator $B_D$ [(1.8) below] makes sense only in lowest-order perturbation theory [8], the equation is thus quite powerful. (In binary atoms with a heavy partner, $m_2^2 \gg m_1^2$, one can treat particle 2 nonrelativistically and then transform the Dirac-Breit equation into an “effective Dirac equa-
tion" with reduced mass \( \mu = m_1 m_2 / (m_1 + m_2) \), which again has exact solutions [9].

In contrast with this early and far-reaching development for two spin-\( \frac{1}{2} \) particles, systems with two spinless particles were first treated in 1971 by Todorov [10, 11], but only for free binary atoms. This late start is understandable in view of the lack of precision experiments on such systems, but logically the spinless case should have come first. This is so because in the basic field equations, the Kramers equation is obtained from the Klein-Gordon equation by adding the term \( e_\alpha (\mathbf{B} - iE) \) of (1.2).

The Todorov equation is time-independent and applies in the \( cm \) system, \( p_1 + p_2 = 0, \ P_1^0 + P_2^0 = E = \text{total cm energy} \). Defining \( \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \) and \( V(r) = V_{12}(r) = e_1 e_2 / r, \) the equation has for \( r \to \infty \) solutions \( \sim e^{ikr} \), where \( k \) is the \( cm \) momentum of two free particles of masses \( m_1 \) and \( m_2 \):

\[
k^2 = \lambda / 4 E^2, \quad \lambda = E^4 - 2E^2(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2.
\]

(1.3)

Bound states have positive-imaginary \( k \), as usual. Apart from a \( \delta(r) \) operator, the Todorov equation reads

\[
[(e - V_{12})^2 - \mu_b^2 + V^2] \psi = 0,
\]

\[
e^2 = - \frac{E^2 - m_1^2 - m_2^2}{2E}, \quad \mu_b = \frac{m_1 m_2}{E}.
\]

(1.4)

The relation \( e^2 - \mu_b^2 = k^2 \) justifies the name "relativistic reduced mass" for \( \mu_b \). Bound states have \( E \) near \( m_1 + m_2 \) for \( e_1 e_2 < 0 \) (and near \( -m_1 - m_2 \) for \( e_1 e_2 > 0 \)), but the equation remains valid also for \( E \to \pm \infty \), contrary to the Breit equation in the corresponding spinor case.

The heuristic arguments leading to the relativistic two-body kinematics were immediately transferred to the spinor case [11, 12]. As it seemed unlikely that such a complicated energy dependence could arise from a hamiltonian equation \( i \partial_t \psi = H \psi \) with a single time \( t \) for two particles, the interest moved to the Bethe-Salpeter equation [13, 14] with its two times, which has the additional advantage of admitting external potentials [15]. However, as the two-time problem remained difficult, the present state of the art for binary atoms is largely heuristic [16].

The first differential equation for two relativistic spinless particles including external potentials was published only last year [17]. It shows that the energy dependence (1.3) does follow from the usual single-time formalism. As the hamiltonian version of the basic Klein-Gordon field equation contains two components, the corresponding two-particle equation contains four components. Elimination of the three auxiliary components leads to the final equation for two spinless particles in a static potential \( V(r) \),

\[
K_{00} \psi = 0
\]

\[
K_{00} = \pi^0 - \{ \pi^0, K_{10} + K_{20} \} + \Delta K_0 \frac{1}{\pi^0} \Delta K_0 + K_{bo}
\]

\[
\pi_0 = \pi_e - V_{12}, \quad \pi_e = E - V(r_1) - V(r_2)
\]

(1.5)

where \( \{ \pi^0, K \} \) denotes the anticommutator \( \pi^0 K + K \pi^0 \)

\[
\Delta K_0 = K_{10} - K_{20} = m_1^2 + p_1^2 - m_2^2 - p_2^2
\]

(1.6)

and \( K_{bo} \) is the Breit operator for spinless particles

\[
K_{bo} = 4 V_{12} [p_1 p_2 + r^{-2} \mathbf{r} \cdot (p_1 p_2)] \]

(1.7)

For \( V(r_2) = V(r_1) = 0, -p_2 = p_1 = p \), (1.5) comes close to Todorov’s equation (1.4), because the fourth order derivatives disappear from the operator \( \Delta K_0 (\pi^0)^{-1} \Delta K_0 \), which reduces to \( (m_1^2 - m_2^2)^2 / (E - V_{12}) \). In fact, after a transformation of a part of \( K_{bo} \), which is consistent with the precision of the equation (the necessary steps are given in Sect. 5, including spin), the Todorov equation is a special case of (1.5). The fact that it contains four different powers of \( E \) derives from the four coupled equations of the type \( H \psi = E \psi \).

In the present paper, this success of the single-time formalism is repeated for two spinor particles, and the connection with the two-time formalism is demonstrated. We start with the 16-component Dirac-Breit equation in the Weyl representation, eliminate the 12 components with one or two dotted indices and obtain again (1.5) for the spin-independent terms. Only the Breit interaction (i.e. the exchange of transverse photons) is treated differently. In principle, it is added after the reduction to four components. This method is explained in the second half of Sect. 4. In Sect. 3, however, we start with the original Breit operator,

\[
B_D = - V_{12}(\alpha_1 \alpha_2 + \alpha_1, \alpha_2)/2
\]

(1.8)

\( \alpha_i \) being the \( 4 \times 4 \) Dirac "velocity" matrix of particle \( i \), and \( \alpha_{i\mathbf{r}} = \alpha_i \mathbf{r} / r = \alpha_i \mathbf{r} \) the component of \( \alpha_i \) along \( \mathbf{r} \).

In this way one first obtains the Kramers version of the Dirac-Breit equation, (2.13) below. It has the same defect as the original Dirac-Breit equation, of course: all operators derived from higher powers of \( B_D \) are too large. This is so because the operator \( \alpha \) has the meaning of velocity only between positive energy states, where the "small components" of the Dirac spinor are indeed small. The relations \( \alpha_0^2 = \alpha_{\mathbf{r}}^2 = \alpha_0 \mathbf{r}^2 = 1 \) show that \( \alpha^2 \) is not the square of the velocity. One way of avoiding this is by means of projection operators on positive energy states [13], but this makes the equation mathematically unpleasant; la-