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Variational two-particle wave equation in scalar quantum field theory

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We study two-particle systems in a model quantum field theory, in which scalar particles of different mass interact via a mediating scalar field. The Lagrangian of the model is reformulated using covariant Green's functions to solve for the mediating field in terms of the particle fields. This results in a Hamiltonian in which the mediating-field propagator appears directly in the interaction term. The variational method, with a simple Fock-state trial state, is used to derive a relativistic momentum-space two-particle wave equation. Non-relativistic and one-particle limits of the equation are determined and discussed briefly

Key words: *quantum field theory, two-particle wave equation*

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This paper is dedicated to Prof. Ihor Yukhnovsky on the occasion of his 75th birthday.

1. Introduction

In earlier papers [1, 2], a relativistic wave equation for a scalar particle-antiparticle system, interacting via a mediating scalar field, was derived variationally for the scalar Yukawa model (which is also called the Wick-Cutkosky model [3-6]). We consider the complementary problem of two scalar particles with different masses in the present paper. The model quantum field theory being studied is defined by the Lagrangian density ($\hbar = c = 1$)

$$\begin{aligned}\mathcal{L} \;=\; \sum_{k=1}^{2} \Big[&\partial^\nu \phi_k^\dagger(x)\, \partial_\nu \phi_k(x) - m_k^2 \phi_k^\dagger(x) \phi_k(x) - g_k \phi_k^\dagger(x) \phi_k(x)\, \chi(x) \\ &- \lambda_k (\phi_k^\dagger(x) \phi_k(x))^2 \Big] + \frac{1}{2} \partial^\nu \chi(x)\, \partial_\nu \chi(x) - \frac{1}{2} \mu^2 \chi^2(x), \qquad (1)\end{aligned}$$

where $\phi_1(x)$ and $\phi_2(x)$ are the scalar fields corresponding to the particles of masses m_1 and m_2 respectively, while $g_1, g_2, \lambda_1, \lambda_2$ are positive coupling constants. The mediating "chion" field can be massive ($\mu \neq 0$) or massless ($\mu = 0$).

The fields ϕ_k and χ satisfy the Euler-Lagrange equations

$$\partial^\nu \partial_\nu \chi(x) + \mu^2 \chi(x) = \rho(x), \tag{2}$$

where $\rho(x) = -g_1 \phi_1^\dagger(x)\phi_1(x) - g_2 \phi_2^\dagger(x)\phi_2(x)$,

$$\partial^\nu \partial_\nu \phi_k(x) + m_k^2 \phi_k(x) + 2\lambda_k(\phi_k^\dagger(x)\phi_k(x))\phi_k(x) = -g_k \phi_k(x)\chi(x), \tag{3}$$

and the conjugates of (3). Equation (2) has the formal solution

$$\chi(x) = \chi_0(x) + \int \mathrm{d}x'\, D(x-x')\, \rho(x'), \tag{4}$$

where $\mathrm{d}x = \mathrm{d}^N x\, \mathrm{d}t$ in $N+1$ dimensions, and $\chi_0(x)$ satisfies the homogeneous (or free field) equation (equation (2) with $\rho = 0$), while $D(x-x')$ is a covariant Green function (or chion propagator, in the terminology of QFT), such that

$$\left(\partial^\nu \partial_\nu + \mu^2\right) D(x-x') = \delta^{N+1}(x-x'). \tag{5}$$

Substitution of the formal solution (4) into equation (3) yields the equations

$$\begin{aligned} &\partial^\nu \partial_\nu \phi_k(x) + m_k^2 \phi_k(x) + 2\lambda_k(\phi_k^\dagger(x)\phi_k(x))\phi_k(x) = \\ &\quad = -g_k \phi_k(x)\chi_0(x) - g_k \phi_k(x) \int \mathrm{d}x' D(x-x')\rho(x'). \end{aligned} \tag{6}$$

Equations (6) are derivable from the action principle $\delta \int \mathrm{d}x\, \mathcal{L} = 0$, corresponding to the modified Lagrangian density

$$\begin{aligned} \mathcal{L} \;=\; & \sum_{k=1}^{2} \Big[\partial^\nu \phi_k^\dagger(x)\, \partial_\nu \phi_k(x) - m_k^2 \phi_k^\dagger(x)\phi_k(x) - g_k \phi_k^\dagger(x)\phi_k(x)\, \chi_0(x) \\ & \qquad - \lambda_k(\phi_k^\dagger(x)\phi_k(x))^2\Big] + \frac{1}{2}\int \mathrm{d}x' \rho(x) D(x-x')\rho(x'), \end{aligned} \tag{7}$$

provided that $D(x-x') = D(x'-x)$. (We suppress the Lagrangian density of the free chion field.)

The QFTs based on (1) and (7) are equivalent in the sense that they lead to the same invariant matrix elements in various order of covariant perturbation theory. The difference is that, in the formulation based on (7), the interaction term, which contains the propagator leads to Feynman diagrams involving virtual chions, while the term that contains χ_0 corresponds to diagrams that cannot be generated using the term with $D(x-x')$, such as those with external (physical) chion lines.

The Hamiltonian density corresponding to the Lagrangian (7) is given by

$$\mathcal{H}(x) = \mathcal{H}_{\phi_1}(x) + \mathcal{H}_{\phi_2}(x) + \mathcal{H}_\chi(x) + \mathcal{H}_I(x) + \mathcal{H}_{II}(x), \tag{8}$$

where

$$\mathcal{H}_{\phi_k}(x) = \dot{\phi}_k^\dagger(x)\dot{\phi}_k(x) + \nabla\phi_k^\dagger(x)\cdot\nabla\phi_k(x) + m_k^2\,\phi_k^\dagger(x)\phi_k(x), \tag{9}$$

$$\mathcal{H}_\chi(x) = \frac{1}{2}\dot{\chi}_0^2 + \frac{1}{2}(\nabla\chi_0)^2 + \frac{1}{2}\mu^2\chi_0^2, \tag{10}$$

$$\mathcal{H}_I(x) = \sum_{k=1}^{2} g_k\,\phi_k^\dagger(x)\phi_k(x)\chi_0(x), \tag{11}$$

$$\mathcal{H}_{II}(x) = -\frac{1}{2}\int \mathrm{d}x'\,\rho(x)D(x-x')\rho(x') + \sum_{k=1}^{2}\lambda_k(\phi_k^\dagger(x)\phi_k(x))^2, \tag{12}$$

and

$$D(x-x') = \int \frac{\mathrm{d}k}{(2\pi)^{N+1}}\mathrm{e}^{-\mathrm{i}k\cdot(x-x')}\frac{1}{\mu^2 - k\cdot k}, \tag{13}$$

where $\mathrm{d}k = d^{N+1}k$ and $k\cdot k = k^2 = k^\nu k_\nu$.

To specify our notation, we quote the Fourier decomposition of the fields in $N+1$ dimension:

$$\phi_k(x) = \int \mathrm{d}^N q\,[(2\pi)^N 2\omega(\mathbf{q}, m_k)]^{-\frac{1}{2}}[A_k(\mathbf{q})\mathrm{e}^{-\mathrm{i}q\cdot x} + B_k^\dagger(\mathbf{q})\mathrm{e}^{\mathrm{i}q\cdot x}], \tag{14}$$

where $\omega(\mathbf{p}, m) = \sqrt{\mathbf{p}^2 + m^2}$, $q\cdot x = q^\nu x_\nu$ and $q^\nu = (q^0 = \omega(\mathbf{q}, m_k), \mathbf{q})$, that is $q^2 = m_k^2$,

$$\chi_0(x) = \int \mathrm{d}^N k\,[(2\pi)^N 2\omega(\mathbf{k}, \mu)]^{-\frac{1}{2}}[d(\mathbf{k})\mathrm{e}^{-\mathrm{i}k\cdot x} + d^\dagger(\mathbf{k})\mathrm{e}^{\mathrm{i}k\cdot x}] \tag{15}$$

with $k^2 = \mu^2$. The momentum-space operators obey the usual commutation relations. The nonvanishing operators are

$$[A_i(\mathbf{p}), A_j^\dagger(\mathbf{q})] = [B_i(\mathbf{p}), B_j^\dagger(\mathbf{q})] = \delta_{ij}\,\delta^N(\mathbf{p}-\mathbf{q}), \tag{16}$$

$$[d(\mathbf{p}), d^\dagger(\mathbf{q})] = \delta^N(\mathbf{p}-\mathbf{q}). \tag{17}$$

These operators have the usual interpretation, namely that $A_k^\dagger$ are creation operators of the (free) scalar particles of mass m_k ($k = 1, 2$), $B_k^\dagger$ are the corresponding antiparticle creation operators, while $d^\dagger$ is the creation operator of the mediating-field quantum (which may be massive, $\mu > 0$, or massless, $\mu = 0$).

The Hamiltonian operator, $\hat{H} = \int \mathrm{d}^N x\,\hat{\mathcal{H}}(x)$, of the QFTheory is expressed in terms of the creation and the annihilation operators $A_k^\dagger$, A_k, $B_k^\dagger$, B_k, $d^\dagger$, d in the usual way. Since we are not interested in vacuum-energy questions in this work, we commute these operators so that they stand in normal order in the Hamiltonian.

2. Two-particle trial state and variational equations

We seek approximate two-particle states variationally by evaluating the expectation value of the Hamiltonian operator of the QFT given in equation (8). The simplest possible two-particle trial state is

$$|\,\psi_2\rangle = \int \mathrm{d}^N p_1\,\mathrm{d}^N p_2\,F(\mathbf{p}_1, \mathbf{p}_2)A_1^\dagger(\mathbf{p}_1)A_2^\dagger(\mathbf{p}_2)\,|\,0\rangle, \tag{18}$$

where $|0\rangle$ is the vacuum state annihilated by all the annihilation operators, A_k, B_k, d, of the theory, and $F(\mathbf{p}_1, \mathbf{p}_2)$ is an adjustable function to be determined variationally. Note that the commutation properties of the operators, together with the definition of $|\psi_2\rangle$, imply that $F(\mathbf{p}_1, \mathbf{p}_2) = F(\mathbf{p}_2, \mathbf{p}_1)$

We shall consider the simplified case with $\lambda_k = 0$ in this paper. The relevant matrix elements needed to implement the variational principle are

$$\begin{aligned}
&\langle\psi_2 |: \hat{H}_{\phi_1} + \hat{H}_{\phi_2} + \hat{H}_\chi :| \psi_2\rangle = \\
&\qquad = \int \mathrm{d}^N p_1 \, \mathrm{d}^N p_2 \, F^*(\mathbf{p}_1, \mathbf{p}_2) F(\mathbf{p}_1, \mathbf{p}_2) \Big[\omega(\mathbf{p}_1, m_1) + \omega(\mathbf{p}_2, m_2)\Big], \qquad (19) \\
&\langle\psi_2 |: \hat{H}_I :| \psi_2\rangle = 0, \qquad (20)
\end{aligned}$$

and

$$\begin{aligned}
&\langle\psi_2 |: \hat{H}_{II} :| \psi_2\rangle = \\
&= -\frac{g_1 g_2}{8(2\pi)^N} \int \mathrm{d}^N p \, \mathrm{d}^N q \, \mathrm{d}^N p' \, \mathrm{d}^N q' \, F^*(\mathbf{p}', \mathbf{q}') F(\mathbf{p}, \mathbf{q}) \, \delta^N(\mathbf{p} + \mathbf{q} - \mathbf{p}' - \mathbf{q}') \\
&\quad \times \mathrm{e}^{-\mathrm{i}(\omega(\mathbf{p}', m_1) - \omega(\mathbf{p}, m_1) + \omega(\mathbf{q}', m_2) - \omega(\mathbf{q}, m_2))t} \frac{1}{\sqrt{\omega(\mathbf{p}', m_1)\, \omega(\mathbf{p}, m_1)\, \omega(\mathbf{q}', m_2)\, \omega(\mathbf{q}, m_2)}} \\
&\quad \times \left[\frac{1}{\mu^2 - (p'_{(1)} - p_{(1)})^2} + \frac{1}{\mu^2 - (q'_{(2)} - q_{(2)})^2}\right], \qquad (21)
\end{aligned}$$

where $p_{(k)} = (\omega(\mathbf{p}, m_k), \mathbf{p})$.

We have normal-ordered the entire Hamiltonian, since this circumvents the need for mass renormalization which would otherwise arise. Not that there is a difficulty with handling mass renormalization in the present formalism (as shown in various earlier papers; see, for example, [6] and citations therein). It is simply that mass renormalization has no effect on the two-body states that we obtain in this paper. Furthermore, the approximate trial state (18), which we use in this work, is incapable of sampling loop effects.

We now specialize to the rest frame of the two-particle system. The momentum operator of this quantum field theory is given by

$$: \hat{\mathbf{P}} : = \int \mathrm{d}^N q \, \mathbf{q} \left[d^\dagger(\mathbf{q}) d(\mathbf{q}) + \sum_{k=1}^{2} \Big(A_k^\dagger(\mathbf{q}) A_k(\mathbf{q}) + B_k^\dagger(\mathbf{q}) B_k(\mathbf{q})\Big)\right]. \qquad (22)$$

The requirement that $: \hat{\mathbf{P}} : |\psi_2\rangle = 0$ implies that

$$F(\mathbf{p}_1, \mathbf{p}_2) = f(\mathbf{p}_1) \delta^N(\mathbf{p}_1 + \mathbf{p}_2) \qquad (23)$$

in the rest-frame of the two-particle system. Then, the matrix elements (19) and (21) reduce to

$$\langle\psi_2 |: \hat{H}_{\phi_1} + \hat{H}_{\phi_2} + \hat{H}_\chi :| \psi_2\rangle = \delta^N(0) \int \mathrm{d}^N p f^*(\mathbf{p}) f(\mathbf{p}) \Big[\omega(\mathbf{p}, m_1) + \omega(\mathbf{p}, m_2)\Big], \quad (24)$$

and

$$
\begin{aligned}
&\langle\psi_2 \,|\!: \hat{H}_{II} :\!|\, \psi_2\rangle = \\
&= -\frac{g_1 g_2}{8(2\pi)^N}\delta^N(0)\int \mathrm{d}^N p\,\mathrm{d}^N p'\, f^*(\mathbf{p}')f(\mathbf{p}) \\
&\quad\times \mathrm{e}^{-\mathrm{i}(\omega(\mathbf{p}',m_1)-\omega(\mathbf{p},m_1)+\omega(\mathbf{p}',m_2)-\omega(\mathbf{p},m_2))t}\frac{1}{\sqrt{\omega(\mathbf{p}',m_1)\,\omega(\mathbf{p},m_1)\,\omega(\mathbf{p}',m_2)\,\omega(\mathbf{p},m_2)}} \\
&\quad\times\left[\frac{1}{\mu^2-(p'_{(1)}-p_{(1)})^2}+\frac{1}{\mu^2-(p'_{(2)}-p_{(2)})^2}\right],
\end{aligned}
\tag{25}
$$

where $p_{(k)}^2 = m_k^2$.

We evaluate the matrix elements at $t = 0$, and choose $f(\mathbf{p})$ in accordance with the variational principle

$$
\delta\,\frac{\langle\psi_2|:\hat{H}:|\psi_2\rangle}{\langle\psi_2|\psi_2\rangle} = 0,
\tag{26}
$$

whereupon we find that $f(\mathbf{p})$ must be a solution of the momentum-space wave equation

$$
\begin{aligned}
&\Big[\omega(\mathbf{p},m_1)+\omega(\mathbf{p},m_2)-E\Big]f(\mathbf{p}) = \\
&= \frac{g_1 g_2}{8(2\pi)^N}\int \mathrm{d}^N p'\frac{f(\mathbf{p}')}{\sqrt{\omega(\mathbf{p},m_1)\omega(\mathbf{p}',m_1)\omega(\mathbf{p},m_2)\omega(\mathbf{p}',m_2)}} \\
&\quad\times\Bigg[\frac{1}{\mu^2+(\mathbf{p}'-\mathbf{p})^2-(\omega(\mathbf{p},m_1)-\omega(\mathbf{p}',m_1))^2} \\
&\qquad+\frac{1}{\mu^2+(\mathbf{p}'-\mathbf{p})^2-(\omega(\mathbf{p},m_2)-\omega(\mathbf{p}',m_2))^2}\Bigg],
\end{aligned}
\tag{27}
$$

where the Lagrange multiplier E represents the total rest-frame energy of the two-particle system, that is the total mass of a bound two-particle system. Note that the kernel (momentum-space potential) in this equation contains terms corresponding to one-chion exchange (this is perhaps more obvious from the manifestly covariant terms in equation (25)).

3. Nonrelativistic and one particle limit

In the nonrelativistic limit, $\mathbf{p}^2/m^2 \ll 1$, equation (27) reduces to

$$
\left[\frac{\mathbf{p}^2}{2m_r}-\epsilon\right]f(\mathbf{p}) = \frac{g_1 g_2}{4(2\pi)^N m_1 m_2}\int \mathrm{d}^N p'\, f(\mathbf{p}')\frac{1}{\mu^2+(\mathbf{p}'-\mathbf{p})^2},
\tag{28}
$$

where $m_r = m_1 m_2/(m_1+m_2)$ and $\epsilon = E - 2m$. In coordinate space, equation (28) is the usual time-independent Schrödinger equation for the relative motion of the two-particle system:

$$
-\frac{1}{2m_r}\nabla^2\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r}).
\tag{29}
$$

The potential $V(r)$ is an attractive Yukawa potential (due to one-chion exchange). In 3+1 dimensions it is, explicitly,

$$V(r) = -\alpha \frac{\mathrm{e}^{-\mu r}}{r}, \tag{30}$$

where $\alpha = \dfrac{g_1 g_2}{16\pi m_1 m_2}$ is the effective dimensionless coupling constant.

In the limit when one of the particles becomes very heavy, say $m_1 \to \infty$, equation (27) becomes, in $3+1$ dimensions,

$$\Big[\omega(\mathbf{p}, m_2) - \varepsilon\Big] f(\mathbf{p}) = \frac{\alpha}{2\pi^2} \int \mathrm{d}^3 p' f(\mathbf{p}') \sqrt{\frac{m_2}{\omega(\mathbf{p}, m_2)} \frac{m_2}{\omega(\mathbf{p}', m_2)}} \Bigg[\frac{1}{\mu^2 + (\mathbf{p}' - \mathbf{p})^2} - \frac{1}{2} \frac{(\omega(\mathbf{p}, m_2) - \omega(\mathbf{p}', m_2))^2}{[\mu^2 + (\mathbf{p}' - \mathbf{p})^2]\,[\mu^2 + (\mathbf{p}' - \mathbf{p})^2 - (\omega(\mathbf{p}, m_2) - \omega(\mathbf{p}', m_2))^2]} \Bigg], \tag{31}$$

where $\varepsilon = E - m_1$. This is a Salpeter-like equation, with a Yukawa-like potential and retardation terms in the kernel. In the non-relativistic limit, this equation reduces to the usual one-particle momentum-space Schrödinger equation with a Yukawa ($\mu > 0$) or Coulombic ($\mu = 0$) potential.

4. Concluding remarks

We have used the variational method to derive a relativistic two-particle wave equation (27) from the underlying scalar quantum field theory (the scalar Yukawa, or Wick-Cutkosky, model). The momentum-space potential describing the interaction between the two scalar particles corresponds to one-chion exchange (the mediating, or "chion", field is also a scalar field). The equation has only positive-energy solutions, that is, it is free of any negative-energy pathologies. It has the Schrödinger equation for the relative motion of the two particles (with a Yukawa interparticle potential) as its non-relativistic limit. It has a Salpeter-like equation, rather than a Klein-Gordon equation, as its one-body limit. That is not surprising, since the Klein-Gordon equation has negative-energy solutions, which do not (and should not) arise in the present formalism, since we use the standard Dirac ("filled-negative-energy-sea") vacuum.

The two-particle equation (27) cannot be solved analytically, even for a massless mediating field ($\mu = 0$), for either bound or scattering states. Nevertheless, approximate numerical or variational solutions can be readily obtained, as was done in the case of particle-antiparticle equations [1,2]. However, approximate solutions of equation (27) will be presented in a separate work.

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Варіяційне двочастинкове хвильове рівняння у скалярній квантовій теорії поля

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Ми вивчаємо двочастинкові системи в модельній квантовій теорії поля, в якій скалярні частинки різної маси взаємодіють через посередкове скалярне поле. Використовуючи коваріантні функції Ґріна для розв'язку посередкового поля в термінах частинкових полів, переформульовано ляґранжіян моделі. В результаті в гамільтоніяні виникає пропагатор посередкового поля прямо в члені, який описує взаємодію. Варіяційна метода з простим пробним фоковим станом використовується для того, щоб вивести релятивістичне двочастинкове хвильове рівняння в імпульс-просторі. Одержуються і обговорюються нерелятивістичні і одночастинкові границі цього рівняння.

Ключові слова: *квантова теорія поля, двочастинкове хвильове рівняння*

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