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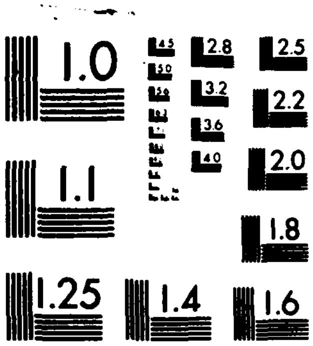

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Fock-Tani Representation for Electron-Hydrogen Scattering

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Abstract

A canonical transformation method previously applied to positron-hydrogen scattering has been used to derive the Fock-Tani Hamiltonian for electron-hydrogen scattering. The transformed Hamiltonian exhibits the H^- bound and resonance channels as explicit terms in the second-quantized interaction. This representation is expected to be useful for inclusion of these channels as intermediate states in the many-body Green's function approach to evaluation of S-matrix elements.

Quantum field theoretic Green's functions are a useful tool for calculation of elastic and inelastic electron-atom, atom-atom, and atom-molecule scattering cross sections[1-5]. The S-matrices for such processes are expressible in terms of single-particle Green's functions[2]. The extension to reactive scattering cross sections normally requires more complicated Bethe-Salpeter transition amplitudes[6], which are harder to determine accurately. This difficulty can be circumvented in some cases by an appropriate change of representation, such that the new field operators for the appropriate composite states satisfy elementary particle commutation relations. The contributions of these composite states to reactive scattering cross sections are then already manifested in certain new single-particle Green's functions in the new representation. The application of such a representation, the Fock-Tani representation[7,8] to positron-hydrogen scattering has recently been described[9-11]. The same approach can be applied to electron-hydrogen scattering, for the purpose of incorporating the contributions of the bound H^- channel and the H^- resonance channels into the field-theoretic calculation of cross sections. In this note we shall exhibit and discuss the Fock-Tani representation Hamiltonian for this problem. The derivation is almost the same as that given previously for positron-hydrogen scattering and will not be included here. The application to calculation of H^- bound and resonance channel contributions to electron-hydrogen scattering cross sections is in progress.

The previously-used canonical transformation method[9] yields the following expression for the Hamiltonian:

$$H = H_0 + V$$

$$H_0 = \sum_\alpha \epsilon_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha + \int dx\ \hat{e}^\dagger(x) H(x) \hat{e}(x)$$

$$V = \sum_{\alpha\beta}' \hat{a}^\dagger_\alpha (\alpha|H|\beta) \hat{a}_\beta$$

$$+ 2^{-1/2} \sum_\alpha \int dx_1 dx_2 \left[\hat{e}^\dagger(x_1) \hat{e}^\dagger(x_2) (x_1 x_2|H|\alpha) \hat{a}_\alpha + \text{h.c.} \right]$$

$$+ \frac{1}{2} \int dx_1 dx_2 dx_1' dx_2'\ \hat{e}^\dagger(x_1) \hat{e}^\dagger(x_2) (x_1 x_2|H|x_1' x_2') \hat{e}(x_2') \hat{e}(x_1') \ . \tag{1}$$

Here $\hat{e}(x)$ and $\hat{e}^\dagger(x)$ are Fock annihilation and creation operators for electrons, satisfying Fermi anticommutation relations. The argument x stands for ($\vec{r}$, σ) with $\vec{r}$ the electron position, σ (= ↑ or ↓) its spin z-component variable, and $\int dx = \sum_\sigma \int d^3\vec{r}$. The $\hat{a}$ and $\hat{a}^\dagger$ are Bose annihilation and creation operators for the H⁻ bound state (two electrons bound to the proton) and H⁻ resonances (two electrons in an initially localized decaying state). They commute with $\hat{e}(x)$ and $\hat{e}^\dagger(x)$, as is the case for the positronium and electron operators[9-11]. The corresponding wave functions are denoted by $\phi_\alpha(x_1 x_2)$ and the set $\{\phi_\alpha\}$ can be chosen orthonormal; the quantum numbers α range over both the bound and resonance channels. The canonical transformation to the representation

(1) is effected by the unitary operator $\hat{U}$,

$$\hat{U} = \exp\left(\frac{\pi}{2}\hat{F}\right) \quad , \quad \hat{F} = \sum_{\alpha}\left(\hat{A}^{\dagger}_{\alpha}\hat{a}_{\alpha} - \hat{a}^{\dagger}_{\alpha}\hat{A}_{\alpha}\right) \quad ,$$

$$\hat{A}^{\dagger}_{\alpha} = 2^{-\frac{1}{2}}\int dx_1 dx_2 \ \phi_{\alpha}(x_1x_2)\hat{e}^{\dagger}(x_1)\hat{e}^{\dagger}(x_2) \qquad (2)$$

which should be compared with the operator $\hat{U}_{Ps}$, Eq.(16) of the positronium-hydrogen case[9].

The H^- bound and resonance energies (diagonal matrix elements) are

$$\epsilon_{\alpha} = \int \phi^{*}_{\alpha}(x_1x_2)H(x_1x_2)\phi_{\alpha}(x_1x_2) \ dx_1dx_2 \qquad (3)$$

with $H(x_1x_2)$ the Schrödinger Hamiltonian of two electrons in the field of the proton, assumed fixed at the origin:

$$H(x_1x_2) = H(x_1) + H(x_2) + \frac{1}{r_{12}}$$

$$H(x) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{1}{r} \quad . \qquad (4)$$

The corresponding off-diagonal matrix elements describing transitions between different resonance channels are

$$(\alpha|H|\beta) = \int \phi^{*}_{\alpha}(x_1x_2)H(x_1x_2)\phi_{\beta}(x_1x_2) \ dx_1dx_2 \quad . \qquad (5)$$

Note that there are no matrix elements connecting the H^- bound state ϕ_0 with the resonance channels ϕ_{α}, $\alpha \neq 0$, since the set $\{\phi_{\alpha}\}$ is *orthonormal and* ϕ_{α} satisfies the eigenvalue equation

$$H(x_1x_2)\phi_0(x_1x_2) = \epsilon_0\phi_0(x_1x_2) \quad . \tag{6}$$

The resonance wave functions ϕ_α do not satisfy an eigenvalue equation with the same Hamiltonian $H(x_1x_2)$. They can be determined, for example, by the complex stabilization method[12] or as discrete eigenstates, with complex eigenvalues, of a nonhermitian Hamiltonian derived by a related variational principle[13] or by the complex rotation method[14-16].

The matrix elements describing decay of the resonances are found to be

$$\begin{aligned}(x_1x_2|H|\alpha) &= H(x_1x_2)\phi_\alpha(x_1x_2) \\ &\quad - \int\Delta(x_1x_2,x_1'x_2')H(x_1'x_2')\phi_\alpha(x_1'x_2')\,dx_1'dx_2' \end{aligned} \tag{7}$$

where Δ is the bound state and resonance kernel

$$\Delta(x_1x_2,x_1'x_2') = \sum_\alpha \phi_\alpha(x_1x_2)\phi_\alpha^*(x_1'x_2') \quad . \tag{8}$$

The term involving Δ (which comes directly from the canonical transformation as in the positron-hydrogen case[9]) exactly cancels the term $H\phi_\alpha$ in the case $\alpha = 0$ (H^- bound state) when one takes account of (6) and orthonormality[17] of the ϕ_α. This corresponds to the physical property that the bound state ϕ_0 is stable (does not decay either into two free electrons or one free electron plus the bound hydrogenic electron). One expects a partial cancellation between the two terms in (7) also in the case $\alpha \neq 0$ (resonance channels), an advantage in numerical calculations.

The electron-electron scattering matrix elements in (1) are found to be

$$(x_1x_2|H|x_1'x_2') = \frac{1}{r_{12}}\delta(x_1 - x_1')\delta(x_2 - x_2')$$
$$- \left[H(x_1x_2) + H(x_1'x_2')\right]\Delta(x_1x_2,x_1'x_2')$$
$$+ \int\Delta(x_1x_2,xy)H(xy)\Delta(xy,x_1'x_2')\,dxdy \quad . \qquad (9)$$

As in the case of the matrix element (7), the "renormalization terms" in (9) are expected to partially cancel the leading bare Coulomb term, facilitating numerical calculations. Such an effect has been noted in calculations[10,11] of positron-hydrogen scattering cross sections.

Eqs. (1)-(9) of the present work should be compared with Eqs. (1)-(30) for the positron-hydrogen case[9]. The physical interpretation is almost the same, but there are two important differences: (a) the wave functions ϕ_α here are localized about the proton whereas the positonium wave functions used in the previous work have wave vector labels as well as internal quantum numbers; (b) electron exchange effects are included in the Hamiltonian (1) whereas no such exchange effect occurs in positron-hydrogen scattering.

We conclude with a brief discussion of the subsidiary condition necessary and sufficient for unitary equivalence of the Fock-representation Hamiltonian (1) and the standard Fock Hamiltonian, which has no explicit reference to the bound and resonance H^- channels. By a derivation paralleling that for the positron-hydrogen case[18] one finds that the required subsidary condition takes the form

$$\hat{N}'_- | \rangle = 0 \tag{10}$$

where $| \rangle$ is the Fock-Tani state vector and the operator $\hat{N}'_-$ is

$$\hat{N}'_- = \frac{1}{2}\int dx_1 dx_2 dx'_1 dx'_2 \ \hat{e}^\dagger(x_1)\hat{e}^\dagger(x_2)\Delta(x_1x_2,x'_1x'_2)\hat{e}(x'_2)\hat{e}(x'_1) \tag{11}$$

with $\hat{N}_-$ the number operator for H^- bound or resonance states in Fock-Tani representation:

$$\hat{N}_- = \sum_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha \quad . \tag{12}$$

The expression (11) for $\hat{N}'_-$ is exact on the two-electron subspace, as is the expression (1) for the Hamiltonian. The proof that (10) is satisfied by the asymptotic initial and final states for electron-hydrogen scattering proceeds as in the positron-hydrogen case[18]. The essential properties used are that (a) one electron in the initial or final state is bound to the proton whereas the other is free, and (b) the kernel Δ of Eq. (8) is localized about the proton, decaying to zero as any of its position arguments recede to infinity. This latter property is satisfied provided that all resonance wave functions included in the sum (8) are localized linear combinations of scattering states, the usual physical interpretation of a resonance.

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Footnotes

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17. Actually, the only properties of the ϕ_α that need to be used in this argument are that ϕ_0 is an energy eigenstate [Eq. (5)] and is normalized, and that the ϕ_α with $\alpha \neq 0$ are orthogonal to ϕ_0. The latter property can be regarded as a consequence of the fact that resonance wave functions are localized superpositions of scattering states, which are orthogonal to the bound state ϕ_0.

18. See Sec. 6 and Appendix E of reference 9.

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