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Fock-Tani Hamiltonian for reactions involving two-electron atoms

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The Fock-Tani Hamiltonian is found for scattering processes involving up to two ions and two electrons. Possible bound-state species include one or two electrons bound to an ion fixed at the origin, and a one-electron projectile atom. A diagrammatic technique is illustrated that simplifies the algebra of the transformation. Coulomb- or plane-wave states are automatically generated by the same asymptotic Hamiltonian for all arrangement channels.

I. INTRODUCTION

Fock-Tani representation was introduced by Girardeau¹ as a means to extend field-theoretic techniques to include bound composites as well as their unbound constituents. The resulting representation¹⁻¹⁰ has resolved several outstanding formal problems in atomic scattering theory, as discussed previously.⁷⁻¹⁰ In practical terms, the improved convergence of the Fock-Tani perturbation series over the Born series (as measured⁴ by Weinberg's criterion¹¹) has produced excellent results⁷⁻¹⁰ in first-order calculations for charge transfer involving one-electron atoms. In particular, it may be seen⁷ that the *first-order* Fock-Tani differential cross section for $H^+ + H \rightarrow H + H^+$ is virtually identical to that of the *second-order* boundary-corrected Born approximation¹² (B2B) at 125 keV. The present paper provides the Hamiltonian upon which first- and second-order Fock-Tani calculations for two-electron atoms may be based.

The major drawback of Fock-Tani representation lies in the difficulty of transforming the Fock Hamiltonian into the Hilbert space that includes elementary bound-state operators. One source of that difficulty is the tedium of accounting for integrals and sums over dummy variables that append the second-quantized operators. But it is the contraction of these propagators that is the physical content of the transformation, not the integrals in which they reside. The present paper introduces a simplified form of the diagrammatic notation of Gilbert,¹³ which greatly simplifies the multiplication and contraction of field operators because all integrals, sums, and dummy variables are suppressed. This notation is introduced in Sec. II and utilized in Sec. III to find the Hamiltonian for systems involving two electrons. The initial stage of this transformation has been performed by Straton and Girardeau⁹ and equations (N) of that paper will be referred to herein by (N -I). Finally, in Sec. IV the asymptotic Hamiltonian is found to automatically generate states appropriate to whether or not there is a net Coulomb force between target and projectile.

II. THE DIAGRAM NOTATION

An algebraic second-quantized representation always includes integration over the position variables of free particles and summation over the energies of the bound states. But the integrations and summations, and even the arguments themselves, are incidental to the operator algebra of transforming from Fock to Fock-Tani representations. For this reason Gilbert¹³ introduced a diagrammatic notation in which a line represents a creation or annihilation operator, with implied integration or summation over the dummy arguments. Fleckinger,¹⁴ Kvasnička,¹⁵ and Brittin¹⁶ have also used diagrammatic representations for bound-state problems. For the present problem the very general notation of Gilbert is not needed. By distinguishing ions from electrons and ordering diagrams with the former uppermost, one may use a very simple set of diagram rules.

One first defines the correspondences between annihilation operators and propagator lines,

$$\begin{aligned}
 & \cdots \Leftrightarrow \text{nucleus fixed at the origin} \\
 & x \bullet \text{-----} \leftarrow \Leftrightarrow \text{projectile fermionic propagator} \Leftrightarrow \hat{a}(x) \\
 & y \bullet \text{-----} \leftarrow \Leftrightarrow \text{electron fermionic propagator} \Leftrightarrow \hat{e}(y) \\
 & \mu \text{-----} \leftarrow \Leftrightarrow (a^+ e^-) \text{ bosonic propagator} \Leftrightarrow \hat{a}_\mu \\
 & \lambda \text{-----} \leftarrow \Leftrightarrow (b^+ e^- e^-) \text{ bosonic propagator} \Leftrightarrow \hat{\beta}_\lambda \\
 & \nu \text{-----} \leftarrow \Leftrightarrow (b e) \text{ fermionic propagator} \Leftrightarrow \hat{e}_\nu,
 \end{aligned} \tag{1}$$

with an implied integral or sum over the argument, bound-state wave functions

$$\begin{aligned}
 & \mu \text{-----} \leftarrow x \Leftrightarrow (-1) \phi_\mu^*(xy) \\
 & \lambda \text{-----} \leftarrow y \Leftrightarrow -2^{-1/2} \psi_\lambda^*(yy') \\
 & \nu \text{-----} \leftarrow y \Leftrightarrow -u_\nu^*(y),
 \end{aligned} \tag{2}$$

where the minus signs keep the present notation consistent with Straton and Girardeau,⁹ and the Schrödinger operators

$$\begin{aligned} \text{---} \text{---} \text{---} & \Leftrightarrow V(x, y) = V_{ae}(xy) + W_{ae}(xy) \\ & = \frac{-Z_a}{|\mathbf{x} - \mathbf{y}|} - \frac{1}{m_b} \nabla_x \cdot \nabla_y \end{aligned}$$

$$\begin{aligned} \text{---} \text{---} \text{---} & \Leftrightarrow V_{eb}(y) + T_e(y) \\ & = \frac{-Z_b}{y} - \frac{1}{2\mu_e} \nabla_y^2 \end{aligned}$$

$$\begin{aligned} \text{---} \text{---} \text{---} & \Leftrightarrow T_a(x) + V_{ab}(x) \\ & = \frac{Z_a Z_b}{x} - \frac{1}{2\mu_a} \nabla_x^2 \end{aligned}$$

$$\begin{aligned} \begin{array}{c} y \\ \text{---} \\ y' \end{array} & \Leftrightarrow V(yy') = V_{ee}(yy') + W_{ee}(yy') \\ & = \frac{1}{|\mathbf{y} - \mathbf{y}'|} - \frac{1}{m_b} \nabla_{y'} \cdot \nabla_{y'} \end{aligned} \quad (3)$$

The inertial potentials W , sometimes referred to as "mass polarization terms,"¹⁷ and the external potentials V_{ex} are a result of the transformation to an accelerated frame of reference in which the ion b is constrained to remain at the origin, and is thus a nondynamical particle. The two-body reduced masses are¹⁷

$$\mu_j = \frac{m_j m_b}{m_j + m_b} \quad (4)$$

Closure relations for the three bound states are expressed diagrammatically by

$$\text{---} \text{---} \text{---} \Leftrightarrow \dot{\mu} \delta_{\mu\nu}$$

$$\text{---} \text{---} \text{---} \Leftrightarrow \frac{1}{2} \dot{\mu} \delta_{\mu\nu}$$

$$\text{---} \text{---} \text{---} \Leftrightarrow \dot{\mu}$$

$$\begin{aligned} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} & \Leftrightarrow -H_{ae}(xy) \phi_\mu(xy) \\ & = -E_\mu \phi_\mu(xy) \Leftrightarrow \text{---} \text{---} \text{---} \end{aligned} \quad (6)$$

Finally, crossed fermion lines give a factor of -1 so that

$$\text{---} \text{---} \text{---} = - \text{---} \text{---} \text{---} \quad (7)$$

Thus, for example, the Fock bound-state annihilation operators are

$$\text{---} \text{---} \text{---} \Leftrightarrow -\hat{A}_\mu = -\int dx dy \phi_\mu^*(xy) \hat{e}(y) \hat{a}(x)$$

$$\text{---} \text{---} \text{---} \Leftrightarrow -\hat{B}_\lambda = -2^{-1/2} \int dy dy' \psi_\lambda^*(yy') \hat{e}(y') \hat{e}(y)$$

$$\text{---} \text{---} \text{---} \Leftrightarrow -\hat{E}_v = -\int dy u_v^*(y) \hat{e}(y), \quad (8)$$

where $u(y)$ is the hydrogenic orbital involving the relative coordinate y , $\psi(yy')$ is the corresponding two-electron orbital, and $\phi(xy)$ is a traveling one-electron orbital.

The operation of multiplication is defined as performing all possible combinations of connecting propagators from the two diagrams being multiplied (a normal ordering expansion) and putting unconnected lines in normal order. For example, the commutator $[\hat{A}_\mu, \hat{A}_\nu^\dagger]$ is

$$\begin{aligned} \left[\text{---} \text{---} \text{---}, \text{---} \text{---} \text{---} \right] & = \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \\ & + \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} - \text{---} \text{---} \text{---} \Leftrightarrow \delta_{\mu\nu} + \hat{C}_{\mu\nu}^* \end{aligned} \quad (9)$$

and the operation of a Schrödinger Hamiltonian upon its eigenstate is expressed by

Note that the $\hat{C}_{\mu\nu}^a$ diagram is neglected because it is zero on the subspace in which there is only one ion of type a .

III. THE TRANSFORMATION

A. The A transformation

The transformation from the Fock space of unbound propagators to the Fock-Tani space that includes elementary composite propagators is most easily done in three steps using a unitary operator defined as a product of three transformations, each onto the subspace containing one new bound-state operator. The ordering of the transformations must be such that the operator constituents of the Fock bound states of the earlier transformations are not subsets of the constituents of the Fock bound states to be transformed later.² Thus the transformation $\hat{U}_E$ for the atom consisting of one electron bound to the origin must come last. Since the operator constituents of $\hat{A}_\mu^\dagger$ and of $\hat{B}_\lambda^\dagger$ are not proper subsets of one another, there is a post-prior ambiguity in the choice of ordering, $\hat{U}_A\hat{U}_B\hat{U}_E$ or $\hat{U}_B\hat{U}_A\hat{U}_E$.

The present Fock Hamiltonian, for two electrons, one projectile, and one ion fixed at the origin, is exactly the same Hamiltonian that Straton and Girardeau transformed.⁹ In Eq. (2) of their paper, which will be referred to as Eq. (2-I) herein, one must merely rename the two "ions" to be "electrons" and the "electron" to be the "projectile a ." The undifferentiated "fourth particle fixed at the origin" is chosen here to be of positive charge to bind the electrons.

Then the transformation $\hat{U}_A^{-1}\hat{H}_F\hat{U}_A$ has already been completed. One may merely quote Eqs. (41-I) through (63-I) after making the replacements $X \rightarrow y$, $\hat{A}_\mu^\dagger \rightarrow -\hat{A}_\mu^\dagger$, $\hat{a}_\mu^\dagger \rightarrow -\hat{a}_\mu^\dagger$, and $\hat{C}_{\mu\nu}^p \rightarrow \hat{C}_{\mu\nu}^e$. With this work already done it is sensible to choose to find the post form of the Fock-Tani Hamiltonian for two-electron atoms using

$$\hat{U} = \hat{U}_A\hat{U}_B\hat{U}_E. \quad (10)$$

The transformed Hamiltonian (41-I) to fourth order in bound-state wave functions, is

$$\begin{aligned} \hat{U}_A^{-1}\hat{H}_F\hat{U}_A = & \text{diagram 1} + \text{diagram 2} + \frac{1}{2} \text{diagram 3} \\ & + \text{diagram 4} + \text{diagram 5} + \text{diagram 6} \\ & + \text{diagram 7} + \text{diagram 8} + \text{diagram 9} + \text{diagram 10} + \text{diagram 11} \end{aligned} \quad (11)$$

The algebraic translation of all but the last diagram have been given in Straton and Girardeau⁹ and will not be repeated here. The first three diagrams are the first three in the Fock Hamiltonian (41-I) and correspond to (42-I) under the above replacements. The fourth and sixth diagrams are the two terms of (53-I). The fifth diagram is (44-I) including the external potentials that were left out of the reduced form (50-I). The seventh diagram

is (57-I), the eighth is (55-I) (with the ninth as its Hermitian conjugate), and the tenth is (62-I). Finally, the last diagram

$$\begin{aligned} & \text{diagram 12} = - \text{diagram 13} - \text{H.c.} - \text{diagram 14} - \text{H.c.} \\ & + \text{diagram 15} + \text{diagram 16} \\ & + \frac{3}{2} \text{diagram 17} + \text{H.c.} \\ & + \text{diagram 18} + \frac{1}{2} \text{diagram 19} + \text{H.c.} \\ & + \text{diagram 20} + \text{H.c.} + \text{diagram 21} + \text{H.c.} \\ & + \text{diagram 22} + \text{H.c.} + \text{diagram 23} + \text{H.c.} \\ & + \frac{1}{2} \text{diagram 24} + \text{H.c.} + \text{diagram 25} \end{aligned} \quad (12)$$

is a trinary reaction term that was not included in the Hamiltonian of Straton and Girardeau (41-I), but will contribute to binary reactions after the subsequent transformations.

B. The B transformation

Turning now to the second step in the product transformation (10), we find that on the two-electron subspace, the generator $\hat{F}_B$

$$\hat{F}_B = - \text{diagram 26} + \text{diagram 27}, \quad (13)$$

of the unitary operator

$$\hat{U}_B = e^{(\pi/2)\hat{F}_B}, \quad (14)$$

is simpler than the generator

$$\hat{F}_A = - \text{diagram} + \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} \quad (15)$$

that appears in the unitary operator of the A transformation,

$$\hat{U}_A = e^{(\pi/2) \hat{F}_A} . \quad (16)$$

This is because the bound-state kernel terms $\hat{C}_{\lambda B, \tau B}$ arising from $[\hat{B}_\lambda, \hat{B}_\tau^\dagger] \equiv \delta_{\lambda\tau} + \hat{C}_{\lambda B, \tau B}$ would give terms in the generator¹⁸ annihilating three (bound or free) electrons, and thus give no contribution on the two-electron subspace.

The transformed Hamiltonian

$$\hat{H}_B = \hat{U}_B^{-1} \hat{H}_A \hat{U}_B \quad (17)$$

may be found by solving the equation of motion

$$\frac{dO(t)}{dt} = [O(t), \hat{F}_s] , \quad (18)$$

where

$$O(t) \equiv \hat{U}_s^{-1} O \hat{U}_s = e^{-t\hat{F}_s} O e^{t\hat{F}_s} \quad (19)$$

is any of the operators $\beta_\lambda(t)$, $\hat{B}_\lambda(t)$, and $\hat{e}(y, t)$ if $s = B$.

Then, on the two-electron subspace

$$\frac{d}{dt} \text{diagram}(t) = - \text{diagram} \quad (20)$$

and

$$\frac{d}{dt} \text{diagram}(t) = \text{diagram}(t) , \quad (21)$$

which clearly have the solution

$$\text{diagram}(t) = \text{diagram} \cos t - \text{diagram} \sin t \quad (22)$$

and

$$\text{diagram}(t) = \text{diagram} \cos t + \text{diagram} \sin t \quad (23)$$

satisfying the initial condition $\hat{\beta}_\lambda(0) = \hat{\beta}_\lambda$ and $B(0) = B$. Then (22) substituted into the equation for $\hat{e}(y, t)$ gives

$$\begin{aligned} \frac{d}{dt} y \text{---} \text{diagram}(t) &= - \left\{ y \text{---} \text{diagram}(t) + \text{diagram}(t) + \text{diagram}(t) \right\} + \text{diagram}(t) \\ &- \left\{ \text{diagram}(t) + \text{diagram}(t) \right\} = -2 \text{diagram}(t) \end{aligned}$$

$$+ O(\text{diagram}) = -2 \text{diagram} \cos t - 2 \text{diagram} \sin t , \quad (24)$$

where we have used the symmetry of the wave function to obtain the factor of 2. Integrating and using $\hat{e}(y, 0) = \hat{e}(y)$ gives

$$\begin{aligned} y \text{---} \text{diagram}(t) &= y \text{---} \text{diagram} - 2 \text{diagram} \sin t \\ &- 2 \text{diagram} (1 - \cos t) . \end{aligned} \quad (25)$$

Finally, setting $t = \pi/2$, the transformed electron annihilation operator is

$$\begin{aligned} \hat{U}_B^{-1} y \text{---} \text{diagram} \hat{U}_B &= y \text{---} \text{diagram} - 2 \text{diagram} \\ &- 2 \text{diagram} . \end{aligned} \quad (26)$$

Note that this transformation is exact (true to all orders in bound-state wave functions) on the two-electron subspace. Then the transformation of $\hat{H}_A$ consists of replacing all electron field operators by (26), performing all possible contractions of lines, and neglecting terms that annihilate three or more electrons. The resulting Hamiltonian will not be displayed here since it will be contained in the final Hamiltonian.

C. The E transformation

The final stage of the product transformation (10) closely follows that of the previous section. Since the Fock operators for one electron bound to the origin anti-commute, $\{\hat{E}_\nu, \hat{E}_\tau^\dagger\} = \delta_{\nu\tau}$, there are no bound-state kernel terms, $C_{\nu E, \tau E}$, that enter the generator,¹⁸ so

$$\hat{F}_E = - \text{diagram} + \text{diagram} . \quad (27)$$

Thus the last transformation of the electron propagators is identical to the B transformation (26), but with the E bound states.

The final post Fock-Tani Hamiltonian on the two-electron, one-projectile subspace in a coordinate system with a fourth particle fixed at the origin to bind the electrons is

$$\hat{U}^{-1} \hat{H}_F \hat{U} = \hat{U}_E^{-1} \hat{H}_B \hat{U}_E = H_0 + V_{01} + V_{02} + V_{11} + V_{12}, \quad (28)$$

where

$$\begin{aligned} H_0 = & \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} \\ & + \text{diagram 5} + \text{diagram 6} + 4 \text{diagram 7} \text{ monopole} \\ & + \text{diagram 8} \text{ monopole} + \text{diagram 9} \text{ monopole} \\ & + \text{diagram 10} \text{ monopole} + \text{diagram 11} \text{ monopole} \\ & + \text{diagram 12} \text{ monopole} + \text{diagram 13} \\ & + \text{diagram 14} \text{ monopole} + \text{diagram 15} \text{ monopole}, \quad (29) \end{aligned}$$

$$V_{01} = \text{diagram 16}, \quad (30)$$

$$\begin{aligned} V_{02} = & \text{diagram 17} + \text{diagram 18} + \text{H.c.} \\ & + 2 \text{diagram 19}, \quad (31) \end{aligned}$$

$$\begin{aligned} V_{11} = & \text{diagram 20} + \text{diagram 21} + \text{H.c.} \\ & \text{diagram 22} + \text{diagram 23} + \text{H.c.} \\ & \text{diagram 24} + \text{diagram 25} + \text{H.c.}, \quad (32) \end{aligned}$$

and

$$\begin{aligned} V_{12} = & \text{diagram 26} + \text{diagram 27} + \text{H.c.} \\ & + \text{diagram 28} + \text{diagram 29} + \text{H.c.} \\ & + \text{diagram 30} + \text{diagram 31} + \text{H.c.} \\ & + \text{diagram 32} + \text{H.c.} + \text{diagram 33} \\ & + \text{diagram 34} + \text{H.c.} + \text{diagram 35} + \text{H.c.} \\ & + \text{diagram 36} + \text{diagram 37} + \text{H.c.} \quad (33) \end{aligned}$$

The matrix elements are given in terms of the matrix elements of the previous sections. In V_{02} the renormalized (orthogonalized) matrix element for electron-electron scattering is

$$\begin{aligned} \text{diagram 38} = & \text{diagram 39} - 2 \text{diagram 40} \\ & - \text{H.c.} + 2 \text{diagram 41}, \quad (34) \end{aligned}$$

where

$$\text{diagram 42} = \frac{1}{2} \text{diagram 43} + \text{diagram 44}. \quad (35)$$

The renormalized matrix element for creating a one-electron bound state in the presence of a free electron is given in terms of (35),

$$\text{diagram 45} = -2 \text{diagram 46} + 2 \text{diagram 47}. \quad (36)$$

Note that the monopole part of the elastic scattering term for one bound and one free electron, the contribution of the third term of (42-I) to the last term of (31), has been moved to the twelfth term in asymptotic Hamiltonian (29). The nonphysical states involving $\hat{e}_\nu \hat{e}_\tau$ (or $\hat{e}_\nu^\dagger \hat{e}_\tau^\dagger$) are neglected.

In V_{11} the renormalized projectile-electron scattering matrix element is

$$\begin{aligned} \text{Diagram E} &= \text{Diagram O} - \text{Diagram with wavy line} - \text{H.c.} \\ &+ \text{Diagram with wavy line}, \end{aligned} \quad (37)$$

where in the first term of (37) the monopole part of the first term of (45-I) has been moved to the last term in the asymptotic Hamiltonian. The renormalized matrix element for formation of an (a, e) bound state in the field of the nuclear fixed at the origin is

$$\text{Diagram E} = \text{Diagram O} - \text{Diagram with wavy line}. \quad (38)$$

The (in)elastic scattering matrix element for the (a, e) bound state from the ion fixed at the origin, the fourth term of (32), is unchanged from (53-I) except that the monopole part of the second term in (53-I) has been moved to the tenth term in the asymptotic Hamiltonian. Likewise, the seventh term of V_{11} , corresponding to (in)elastic scattering of a projectile from the electron bound to the origin, has the monopole part of the first term in (45-I) moved to the fourteenth term in the asymptotic Hamiltonian. The matrix element for binding an electron to the origin in the presence of the projectile is

$$\text{Diagram O} = - \text{Diagram with wavy line} + \text{Diagram with wavy line} \quad (39)$$

and the last two terms of (32) represent charge transfer.

V_{12} contains the matrix for scattering two electrons and one projectile ion (of different species) from the ion fixed at the origin,

$$\begin{aligned} \text{Diagram E} &= \text{Diagram B} - \text{Diagram with wavy line} - \text{H.c.} \\ &- \text{Diagram with wavy line} - \text{H.c.} + \text{Diagram with wavy line} \\ &+ \text{Diagram with wavy line} + \text{Diagram with wavy line} + \text{H.c.} \end{aligned} \quad (40)$$

where

$$\text{Diagram B} = \text{Diagram O} - 2 \text{Diagram with wavy line} - \text{H.c.}$$

$$+ 4 \text{Diagram with wavy line} - 2 \text{Diagram with wavy line} - \text{H.c.}$$

$$+ 4 \text{Diagram with wavy line}. \quad (41)$$

This will be needed to find the Fock-Tani Hamiltonian for three-electron atoms. Likewise, there is a renormalized matrix element for formation of the (a, e) bound state in the presence of a free electron and the ion fixed at the origin,

$$\begin{aligned} \text{Diagram E} &= \text{Diagram O} - \text{Diagram with wavy line} \\ &- \text{Diagram with wavy line} - \text{Diagram with wavy line} + \text{Diagram with wavy line} \\ &+ \text{Diagram with wavy line}, \end{aligned} \quad (42)$$

where

$$\text{Diagram O} = \text{Diagram with wavy line} + \text{Diagram with wavy line}, \quad (43)$$

and an (a, e) scattering matrix element in the presence of a free electron and the charge at the origin,

$$\begin{aligned} \text{Diagram E} &= \text{Diagram O} - \text{Diagram with wavy line} - \text{H.c.} \\ &+ \text{Diagram with wavy line}. \end{aligned} \quad (44)$$

V_{12} also contains a renormalized term describing the double ionization of the two-electron bound state,

$$\begin{aligned}
 & \text{Diagram with } E = \text{Diagram 1} - \text{Diagram 2} \\
 & - \text{Diagram 3}, \quad (45)
 \end{aligned}$$

where

$$\begin{aligned}
 & \text{Diagram 1} = -2 \text{Diagram 2} + 4 \text{Diagram 3} \\
 & - 2 \text{Diagram 4} + 4 \text{Diagram 5}, \quad (46)
 \end{aligned}$$

and a renormalized transfer-ionization matrix element

$$\text{Diagram with } E = \text{Diagram 1} - \text{Diagram 2}, \quad (47)$$

where

$$\text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3}. \quad (48)$$

There is a matrix element for binding an electron to the origin in the presence of a free electron and projectile,

$$\begin{aligned}
 & \text{Diagram 1} = - \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4} + \text{Diagram 5} \\
 & - \text{Diagram 6} - \text{Diagram 7}, \quad (49)
 \end{aligned}$$

a scattering matrix for that bound state,

$$\begin{aligned}
 & \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} \\
 & - \text{Diagram 4} - \text{H. c.} \quad (50)
 \end{aligned}$$

a matrix for charge transfer in the presence of a free electron,

$$\begin{aligned}
 & \text{Diagram 1} = - \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4} - \text{Diagram 5}, \quad (51)
 \end{aligned}$$

and a term representing single ionization of the doubly-bound state in the presence of the projectile,

$$\text{Diagram 1} = \text{Diagram 2} - \text{Diagram 3}. \quad (52)$$

Single electron transfer between the two-electron atom and the projectile is given explicitly in the last two terms of V_{12} , (33).

Note that the seventh term in V_{12} (33), the scattering matrix of a projectile from a two-electron atom, is shown with a term subtracted,

$$\begin{aligned}
 & \text{Diagram 1} = 4 \text{Diagram 2} - 4 \text{Diagram 3} \\
 & + 4 \text{Diagram 4}. \quad (53)
 \end{aligned}$$

This monopole term in the elastic Coulomb scattering of the projectile from the two bound electrons is instead shifted to the seventh term in the asymptotic Hamiltonian H_0 (29). Likewise, the elastic part of the third to last term in (33), representing the scattering of one species of one-electron atom from another species of one-electron atom, has the monopole part of (58-I) shifted to the eighth and ninth terms in the asymptotic Hamiltonian.

IV. THE ASYMPTOTIC HAMILTONIAN—AN ELASTIC SCATTERING

The Fock-Tani Hamiltonian developed herein is appropriate for two-electron, one-projectile (ion) problems in which one or both electrons may be bound to a ion fixed at the origin and one electron may be bound to the projectile. Physically, one may have either Coulomb- or plane-wave asymptotic states, depending on the net charge of the bound states, and the asymptotic Hamiltonian has been chosen to automatically generate the appropriate type of wave. Consider first an initial state consisting of two electrons bound to the origin and a projectile,

simultaneously. This leads to the additional benefit for elastic scattering that the singular terms $\sim 1/R$ in the interaction potentials are automatically and consistently removed.²¹

V. CONCLUSIONS

The post form of the Fock-Tani Hamiltonian for two electrons, one projectile ion, and a ion fixed at the origin has been calculated using a diagrammatic notation. The resulting terms in the interaction potential have visually obvious physical interpretations such as (in)elastic scattering, single and double ionization, transfer-ionization, transfer-excitation, ionization-excitation, and charge transfer. Because the same

asymptotic Hamiltonian may be used for all these arrangement channels, appropriate wave functions for Coulomb- or plane-wave boundary conditions are automatically generated.

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