Pramāṇa, Vol. 6, No. 5, 1976, pp. 312–322. © Printed in India.

Feynman diagram method for atomic collisions

T PRADHAN* and AVINASH KHARE
Institute of Physics, Bhubaneswar 751007

MS received 1 December 1975; after revision 5 January 1976

Abstract. Feynman diagram method of treating atomic collision problems in perturbation theory is presented and matrix elements are calculated for a number of processes. The result for the resonant charge transfer in hydrogen is identical to the well known OBK value. However, in processes like collisional ionisation, the results are different from those obtained by conventional methods.

Keywords. Electron exchange; ion exchange; vertex function; collisional ionisation; photo-effect charge transfer.

1. Introduction

Feynman diagram method has proved to be very useful in a variety of problems in relativistic as well as non-relativistic physics. Apart from its indispensability in relativistic particle physics (Akhiezer and Beretetskii 1965), it has been found to be a very successful tool in handling many-body problems in nuclear, solid state (Fetter and Walecka 1971) and atomic physics (Kelley 1974). However, no attempt seems to have been made to apply this method to atomic collision problems. While exploring such possibilities the authors have found that in problems such as charge exchange processes the diagrammatic method not only gives an elegant physical picture of the phenomena but at the same time makes the calculation simple. The lowest order diagram consists of an electron exchange quite similar to the photon exchange in elastic scattering of charged particles. For the resonant charge transfer in hydrogen proton collision one obtains the familiar OBK amplitude (Brinkman and Kramers 1930); there is no diagram corresponding to the JS amplitude (Jackson and Schiff 1953*a*) in the lowest order. Another charge transfer mechanism operates in exchange scattering of electrons by hydrogen which can be represented by a Feynman diagram with a proton exchange. The success of the diagrammatic method in these processes has prompted us to apply it to a host of other atomic collision processes. Principal among these are the photo-electric effect and its inverse (the radiative recombination), ionisation of atoms by electron and ionic impact. Detailed calculation of the amplitude of these processes are presented in this paper.

The theory of charge exchange in positive ion-atom collision relevant to Feynman diagram method is presented in section 2 where amplitudes of other typical rearrangement processes of experimental interest have also been evaluated. Section 3 is

*On leave of absence from Saha Institute of Nuclear Physics, Calcutta 700009.

devoted to the calculation of photo-electric effect and its inverse process of radiative recombination where relativistic and Coulomb effects have been ignored for the sake of simplicity. In section 4, calculation of matrix element for ionisation of atoms by electron and ionic impact is presented. Section 5 is devoted to discussions.

2. Charge transfer collisions

We consider the process

$$A^+ + B \to A + B^+$$

where A^+ is a positive singly ionized atom which picks up an electron from the atom B after collision. In other words, exchange of an electron between B and A^+ characterises the collision. This exchange is, " literally " expressed by the Feynman diagram of figure 1.

The momenta of various particles indicated in the diagram refer to the centre of mass system. The rules for writing down the matrix elements being quite standard (Bhasin *et al* 1965) need not be repeated here. Using these rules, we obtain

$$M = \Gamma(\boldsymbol{K}_f,\ \omega_f;\ \boldsymbol{K}_f - \boldsymbol{K}_i,\ \omega)\ \triangle_F(\boldsymbol{K}_f - \boldsymbol{K}_i,\ \omega,\ m) \times \Gamma(\boldsymbol{K}_i,\ \omega_i;\ \boldsymbol{K}_f - \boldsymbol{K}_i,\ \omega) \tag{1}$$

where

$$S_{fi} = \delta_{fi} - (2\pi)^4\,\delta^{(3)}(\boldsymbol{P}_i - \boldsymbol{P}_f)\,\delta(E_i - E_f)\,M,$$

$$\omega_f = \boldsymbol{K}_f^2/2M_{B^+},\ \omega_i = \boldsymbol{K}_i^2/2M_{A^+},\ \omega = \Omega_i - \omega_f = \Omega_f - \omega_i,$$

$$\Omega_i = \boldsymbol{K}_i^2/2M_B - \epsilon_B,\ \Omega_f = \frac{\boldsymbol{K}_f^2}{2M_A} - \epsilon_A,$$

ϵ_A, ϵ_B being binding energy of the electron in atoms ' A ' and ' B ' respectively. $\Gamma(\boldsymbol{p}_1, \omega_1; \boldsymbol{p}_2, \omega_2)$ is the vertex function representing the interaction of particles 1 and 2 and the bound state composed of these particles and $\triangle_F(\boldsymbol{p}, \omega, m)$ is the propagator for the electron. The vertex function $\Gamma(\boldsymbol{p}_1, \omega_1; \boldsymbol{p}_2, \omega_2)$ is related to the Fourier transform

$$g_{12}\left(\frac{m_2\boldsymbol{p}_1 - m_1\boldsymbol{p}_2}{m_1 + m_2}\right)$$

of the Schrödinger wave-function of the bound state formed by particles 1 and 2 as follows (see Appendix):

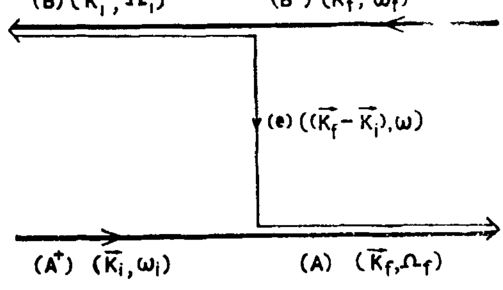


Figure 1. Feynman diagram for charge transfer process $A^+ + B \to A + B^+$.

$$\Gamma(\boldsymbol{p}_1\ \omega_1;\ \boldsymbol{p}_2,\ \omega_2) = g_{12}\left(\frac{m_2\boldsymbol{p}_1 - m_1\boldsymbol{p}_2}{m_1 + m_2}\right)\left[\left(\frac{\boldsymbol{p}_2^2}{2m_2} - \omega_2\right) - \left(\frac{\boldsymbol{p}_1^2}{2m_1} - \omega_1\right)\right] \tag{2}$$

The non-relativistic propagator can be written as

$$\triangle_F(\boldsymbol{p},\ \omega,\ m) = \frac{1}{\boldsymbol{p}^2/2m - \omega - i\eta}. \tag{3}$$

Substituting eqs. (2) and (3) in eq. (1) and taking into account the fact that particles A^+ and B^+ are on the mass-shell *i.e.*, $\boldsymbol{p}^2/2m = \omega$ we get

$$M = g_{B^+e}(a\boldsymbol{K}_i - \boldsymbol{K}_f)\, g_{A^+e}(b\boldsymbol{K}_f - \boldsymbol{K}_i)\left[\frac{(\boldsymbol{K}_f - \boldsymbol{K}_i)^2}{2m} - \omega\right], \tag{4}$$

where

$$a = M_{B^+}/M_B \qquad b = M_{A^+}/M_A,$$

The general formula eq. (4) can now be applied to the particular cases of

(*a*) $H^+ + H(1s) \to H(1s) + H^+$,

(*b*) $e^+ + (e^+e^-)_{1s} \to (e^+e^-)_{1s} + e^+$,

(*c*) $H^+ + (\mu^+e^-)_{1s} \to H(1s) + \mu^+$.

For the process (*a*)

$$M = g^{1s}_{H^+e}\left(\frac{M}{m+M}\boldsymbol{K}_i - \boldsymbol{K}_f\right) g^{1s}_{H^+e}\left(\frac{M}{m+M}\boldsymbol{K}_f - \boldsymbol{K}_i\right)$$
$$\times \left[(\boldsymbol{K}_f - \boldsymbol{K}_i)^2/2m - \boldsymbol{K}_f^2/2(M+m) + \frac{\boldsymbol{K}_i^2}{2M} + \epsilon\right], \tag{5}$$

where ϵ is the binding energy of the hydrogen atom ground state and M is the mass of the proton. Using the fact that $\boldsymbol{K}_i^2 = \boldsymbol{K}_f^2 = (K^2)$ which follows from over-all energy-momentum conservation and

$$g^{1s}_{H^+e}(\boldsymbol{p}) = \frac{8\pi^{1/2}s^{5/2}}{(s^2 + \boldsymbol{p}^2)^2}, \quad s = a_0^{-1},$$

a_0 being Bohr radius for ground state,

Eq. (5) simplifies to

$$M = \frac{32\pi s^5}{m}\,\frac{1}{[s^2 + K^2(\beta^2 + 4\sin^2\theta/2)]^3}, \tag{6}$$

with $\beta = m/M$ and $\cos\theta = \boldsymbol{K}_f \cdot \boldsymbol{K}_i/K^2$ which is readily seen to be the OBK amplitude. It is worth pointing out that figure 1 being the only possible Feynman diagram for the charge transfer process in the lowest order, OBK amplitude (Brinkman and Kramers 1930) constitutes the entire matrix element. There being no other diagram we conclude that JS amplitude (Jackson and Schiff 1953 *a*) is not obtainable from diagrammatic formalism. It seems therefore that Wick's contention (Jackson and Schiff 1953 *b*) that proton-proton potential should not contribute to the capture amplitude is borne out by Feynman diagram formalism. In view of the absence of the JS term, one may say that diagram method suffers from the drawback that in the lowest order there is no agreement with experiment. This is mainly due to ignoring the long-range Coulomb interaction between the bound electron and the colliding proton, which may be regarded as an initial state (or final state) interaction. The successful method of taking this effect into account is the Impulse Approximation initiated by one of us (TP) (Pradhan 1957) and refined by several others (Mcdowell and Coleman 1970).

For the process (*b*) the matrix element is simpler on account of equality of masses of all the particles involved. We find

$$M = \overset{1s}{g}_{e^+e^-}(\tfrac{1}{2} K_i - K_f)\, \overset{1s}{g}_{e^+e^-}(\tfrac{1}{2} K_f - K_i) \times \frac{1}{2m}[s_p^2 + \tfrac{1}{4}K^2(1 + 8\sin^2\theta/2)], \tag{7}$$

where s_p is the inverse Bohr radius of positronium. It is to be noted that we are using non-relativistic dynamics and as such ignoring spins of electron and positron. Using the formula

$$\overset{1s}{g}_{e^+e^-}(p) = \frac{8\pi^{1/2}\, s_p^{5/2}}{(s_p^2 + p^2)^2},$$

and the relation $K_i^2 = K_f^2 = K^2$ in eq. (7) we obtain

$$M = \frac{32\pi s_p^5}{m} \frac{1}{[s_p^2 + \frac{K^2}{4}(1 + 8\sin^2\theta/2)]^3} \tag{8}$$

which is identical to the OBK amplitude for the process under consideration.

For the process (*C*), the matrix element works out to

$$M = \frac{32\pi s^5}{m} \frac{1}{\left[s^2 + K^2\left(\frac{m^2}{Mm_\mu} + 4\sin^2\theta/2)\right)\right]^3} \tag{9}$$

where $K^2 = K_i^2 \neq K_f^2$ and $\cos\theta = K_f \cdot K_i / |K_f|K_i|$

As in the two previous cases, this is also identical to the corresponding OBK amplitude.

The mechanism for all the charge transfer processes considered so far is electron exchange. It may be worthwhile to consider a process which occurs through ionic exchange. In electron scattering by atoms, apart from the direct scattering of the electron the process where the incident electron is captured and the atomic electron ejected must be considered.* This latter process

$$e + A - A + e$$

can be represented by the Feynman diagram given in figure 2.

It is clear from the diagram that the mechanism for this process is through the exchange of the ion A^+. The matrix element for this diagram is

---

* This latter process is the only mechanism for inelastic electron scattering.

$$e + \text{He}(1'S) \rightarrow \text{He}(2^3P) + e$$

by Helium. The direct and exchange amplitudes can be measured individually by spin analysis of the scattered beam in experiments using polarised electrons on atoms.

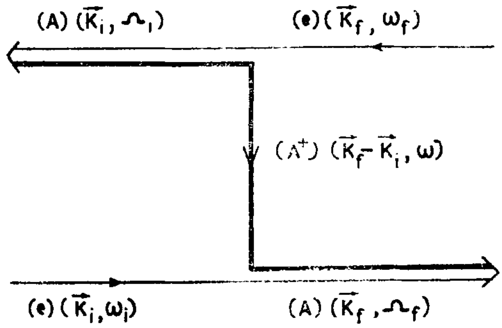


Figure 2. Feynman diagram for electron-atom scattering $e + A \rightarrow A + e$ through ion exchange.

$$M = \Gamma(K_f, \omega_f; K_f - K_i, \omega) \triangle_F (K_f - K_i) \omega, M_{A^+}) \\ \Gamma(K_f - K_i, \omega; K_i, \omega_i) \tag{10}$$

For the particular case of electron scattering by hydrogen where the exchanged particle is a proton this works out to

$$M = \frac{32\pi s^5}{m} \frac{1}{[s^2 + K^2(1 + 4\beta \sin^2 \theta/2)]^3}, \beta = m/M \tag{11}$$

which is somewhat different from the corresponding expression obtained by using the Born-Oppenheimer approximation (Mott and Massey 1965).

3. Photo-electric effect

We shall consider the processes of atomic K-shell photo-electric effect $h\nu + A \rightarrow A^+ + e$ and its inverse, the radiative recombination $A^+ + e \rightarrow h\nu + A$, in the non-relativistic approximation and ignore Coulomb effects. There are two diagrams for each of these processes in the lowest order. For the photo-effect these are represented by figures 3 *a* and 3 *b*.

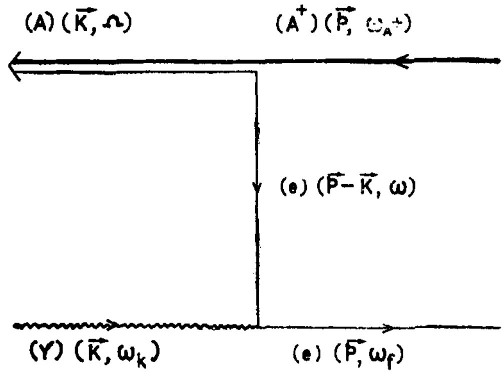
The matrix elements for these diagrams can be written as

$$M_a = \Gamma(p, \omega_{A^+}; p - K, \omega) \triangle_F (p - K, \omega; m) \\ \frac{1}{m} \gamma_i (p - K; p) a_i . (K), \tag{12 a}$$

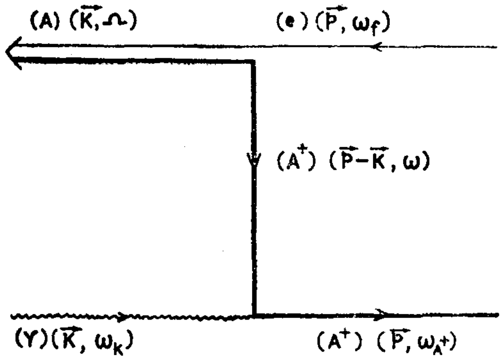
$$M_b = \Gamma(p, \omega_f; p - K, \omega) \triangle_F (p - K, \omega; M_{A^+}) \\ \frac{1}{M_{A^+}} \gamma_i (p - K; p) a_i . (K), \tag{12 b}$$

where $\gamma_i (p - K, p)$ is the charged particle-photon vertex and $a_i (K)$ is the polarisation vector of the incident photon. The vertex $\gamma_i (p - K, p)$ is given by (Heitler 1954)

$$\vec{\gamma}(p - K, p) = e \sqrt{\frac{2\pi \hbar^2 c^2}{k}} p \tag{13}$$



(3 *a*)



(3 *b*)

Figure 3 *a*. Feynman diagram for photo-electric effect $h\nu + A \rightarrow e + A^+$ through electron exchange.

Figure 3 *b*. Diagram for photo-electric effect through ionic exchange.

Substituting formulas (2) and (3) for Γ and $\triangle_F$ respectively and formula (13) for $\vec{\gamma}$ in eqs. 12 *a* and 12 *b* we get

$$M_a = \frac{8\pi e\hbar c\ \sqrt{2S^5Z^5/k}\ p\cdot a}{m\left[Z^2 s^2 + \left(p - \frac{M_{A^+}}{M_A}\ K\right)^2\right]^2} \qquad (14\,a)$$

$$M_b = \frac{8\pi e\hbar c\ \sqrt{2s^5Z^5/K}\ p\cdot a}{M_{A^+}\left[Z^2 s^2 + \left(p - \frac{m}{M_A} K\right)^2\right]^2} \qquad (14\,b)$$

The matrix element M_a is identical to the standard Born approximation result (Heitler 1954). The matrix element M_b for the second diagram is smaller than M_a by a factor of m/M_{A^+} and consequently very small and can therefore be neglected. It is a recoil effect and represents the extent to which the ion A^+ can be " pushed " by the photon.

The inverse process of radiative recombination can be represented by diagrams which are identical to those of figure 3 except that incoming and outgoing particles are interchanged. Thus the matrix elements are the same as those of the photo-electric effect.

4. Collisional ionisation

We shall consider the ionisation of atoms by electron impact

$$A + e \rightarrow A^{+} + e' + e,$$

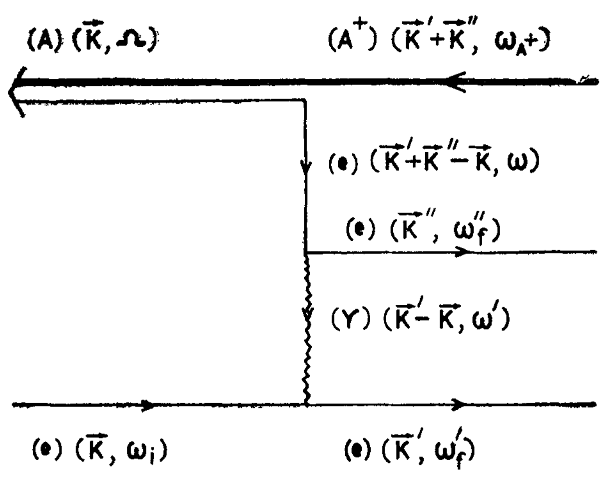
as well as heavy ion impact

$$A + Z \rightarrow A^{+} + Z + e$$

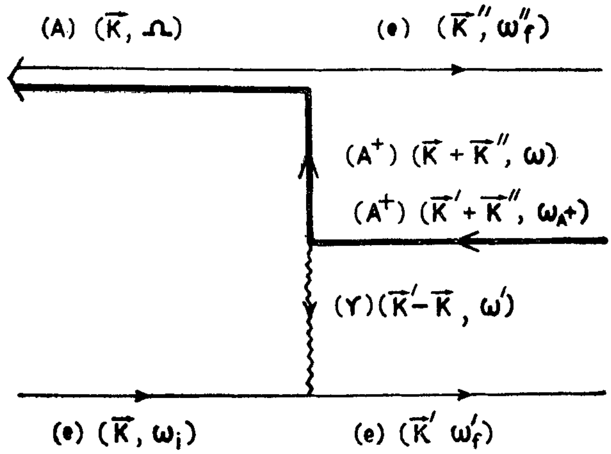
There are two Feynman diagrams for each of these processes. Figures 4*a* and 4*b* represent ionisation of an atom by electron impact and figures 5 *a* and 5 *b* represent ionisation by heavy ion impact.

The matrix elements for the ionisation by electron impact work out to be

$$M_{a} = g_{A^{+}e}\left(K + K'' - \frac{M_{A^{+}}}{M_{A}}K\right)\frac{4\pi e^{2}}{|K - K'|^{2}} \tag{15 a}$$



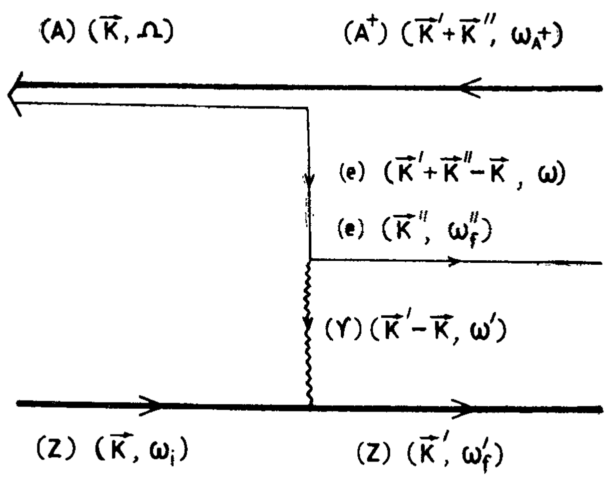
(4 *a*)



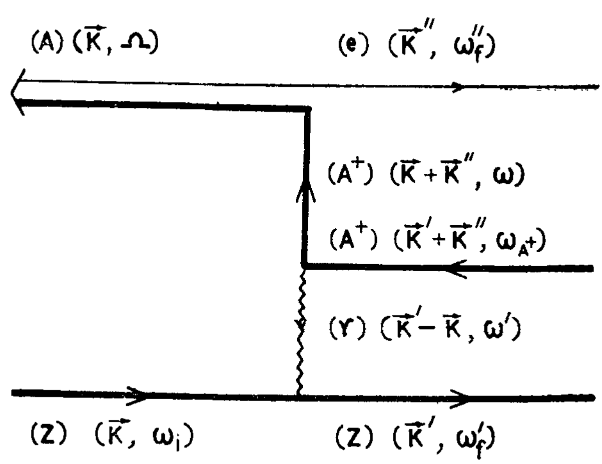
(4 *b*)

Figure 4 *a*. Feynman diagram for ionisation of atom by electron impact $e + A \rightarrow A^{+} + e' + e$ through electron exchange.

Figure 4 *b*. Diagram for ionisation by electron impact through ionic exchange.



(5 *a*)



(5 *b*)

Figure 5 *a*. Feynman diagram for ionisation of atom by ionic impact $A + Z \rightarrow A^+ + e + Z$ through electron exchange.

Figure 5 *b*. Diagram for ionisation of atom by ionic impact through ionic exchange.

$$M_b = g_{A^+e}\left(K'' + \frac{m}{M_A}K\right)\frac{4\pi e^2 F(|K - K'|^2)}{|K - K'|^2} \qquad (15\ b)$$

where F is the form factor of ion A^+. The matrix elements for ionisation by ionic impact represented by figures 5 *a* and 5 *b* can be written as

$$M_a = g_{A^+e}\left(\mathrm{K}' + K'' - \frac{M_{A^+}}{M_A}K\right)\frac{4\pi e^2 Z f(|K' - K|^2)}{|K' - K|^2}, \qquad (16\ a)$$

$$M_b = g_{A^+e}\left(K'' + \frac{M_A}{m}\mathrm{K}\right)\frac{4\pi e^2 Z F(|K' - K|^2) f(K' - K|)^2}{|K' - K|^2}, \qquad (16\ b)$$

where f is the form factor of the ion. The amplitudes (15 *b*) and (16 *b*) representing diagrams (4 *b*) and (5 *b*) are smaller in magnitude compared to those of (15 *a*) and (16 *a*) respectively on account of the extra factor $F(|K' - K|^2)$. These diagrams do not seem to have been considered in earlier treatments of the problem.

5. Discussion and conclusions

The calculations presented in this paper are convincing enough for adoption of Feynman diagram technique for atomic collision processes. There are a large number of complicated atomic and molecular reactions which can be represented by very simple Feynman diagrams involving exchange of either an electron or an ion or an atom. One has only to know the appropriate wave-functions representing the vertex functions occurring in the diagram to work out the complete matrix element. It is our hope that the diagram technique will prove to be a very handy tool for calculation of atomic and molecular collision processes in physical, chemical, biological and astrophysical problems.

Appendix

Here we derive the relation

$$\Gamma(p_1, \omega_1; p_2, \omega_2) = g_{12}\left(\frac{m_2 p_1 - m_1 p_2}{m_1 + m_2}\right) \left[\left(\frac{P_2^2}{2m_2} - \omega_2\right) - \left(\frac{P_1^2}{2m_1} - \omega_1\right)\right] \tag{A1}$$

between the vertex function Γ and the Fourier transform g_{12} of the Schrödinger wave function of the bound state formed by particles 1 and 2. For the very special case of $m_1 = m_2$ the relation has been mentioned in the paper of Pradhan and Tripathy (Pradhan and Tripathy 1969). However, the detailed steps have been omitted and general case of unequal mass particles has not been considered. We have thought it to be important enough to obtain the relation between Γ and g for the unequal mass case.

The Bethe-Salpeter amplitude for a two particle system is defined by (Schweber 1962)

$$\beta^{(2)}_{P, E, \alpha}(X_1, t_1; X_2, t_2) = \langle O \mid (\psi(x_1, t_1)\,\psi(x_2, t_2))_+ \mid 2, P, E, \alpha \rangle \tag{A2}$$

Its Fourier transform

$$\psi(P_1, \omega_1; P_2, \omega_2) = \int \beta^{(2)}_{P, E, \alpha}(X_1, t_1; X_2, t_2) \exp\left[-\frac{i}{\hbar}(P_1 \cdot X_1 + P_2 \cdot X_2 - \omega_1 t_1 - \omega_2 t_2)\right] d^3 X_1\, d^3 X_2\, dt_1 dt_2 \tag{A3}$$

is related to the vertex function by the equation

$$\psi(P_1, \omega_1; P_2, \omega_2) = i(2\pi)^4 \delta^{(3)}(P - P_1 - P_2)\, \delta(E - \omega_1 - \omega_2)\, \Delta_F(P_1, \omega_1, m_1)\, \Delta_F(P_2, \omega_2, m_2)\, \Gamma(P_1, \omega_1; P_2, \omega_2), \tag{A4}$$

where P and E are the C.M. momentum and energy respectively and Δ_F' s are the propagators for the particles 1 and 2. Separating the C.M. motion from the relative motion in the manner

$$\beta^{(2)}_{P,E,\alpha}(X_1, t_1; X_2, t_2) = b^{(2)}_{P,E,\alpha}(\vec{\gamma}, t)\exp\left[\frac{i}{\hbar}(P\cdot X - ET)\right], \tag{A5}$$

where

$$X = \frac{m_1 X_2 + m_2 X_1}{m_1 + m_2}, \quad T = \frac{m_1 t_2 + m_2 t_1}{m_1 + m_2},$$

$$\vec{\gamma} = X_1 - X_2, \quad t = t_1 - t_2, \tag{A6}$$

we have

$$\psi(P_1, \omega_1; P_2, \omega_2)$$

$$= \int b^{(2)}_{P,E,\alpha}(\vec{\gamma}, t)\exp\left[\frac{i}{\hbar}\left\{(P - P_1 - P_2)\cdot X - (E - \omega_1 - \omega_2)\,T + \frac{(m_1 p_2 - m_2 p_1)}{m_1 + m_2}\cdot\vec{\gamma} - \frac{(m_1\omega_2 - m_2\omega_1)}{m_1 + m_2}\,t\right\}\right] d^3x\, d^3\gamma\, dT dt, \tag{A7}$$

which, after integration over X and T becomes

$$\psi(P_1, \omega_1; P_2, \omega_2) = (2\pi)^4\,\delta^{(3)}(P - P_1 - P_2)$$

$$\delta(E - \omega_1 - \omega_2)\int b^{(2)}_{P,E,\alpha}(\vec{\gamma}, t)\exp\left[\frac{i}{\hbar}\left\{\frac{(m_1 P_2 - m_2 P_1)\cdot\vec{\gamma}}{m_1 + m_2} - \frac{(m_1\omega_2 - m_2\omega_1)}{m_1 + m_2}\,t\right\}\right] d^3\vec{\gamma}\, dt. \tag{A8}$$

It can be shown that for $P = 0$, $b^{(2)}(\vec{\gamma}, t)$ is related to the Fourier transform g_{12} of the Schrödinger wave-function*

$$f(X_1, X_2) = \langle 0 \mid \psi(x_1)(x_2) \mid 2, P = 0, E, \alpha\rangle, \tag{A9}$$

by the equation

$$b^{(1)}_{E,\alpha}(\vec{\gamma}, t) = \int \frac{d^3q}{(2\pi)^3}\left[\theta(t)\exp\left[\frac{i}{\hbar}(q.r - E_q t)\right] + \theta(-t)\exp\left[-\frac{i}{\hbar}(q\cdot\vec{\gamma} - E_q t)\right] g_{12}(q)\right] \tag{A10}$$

Using eq. (A 10) in eq. (A8) it is straightforward to verify that

$$\psi(P_1, \omega_1; P_2, \omega_2) = i(2\pi)^4\,\delta^{(3)}(P - P_1 - P_2)\,\delta(E - \omega_1 - \omega_2)$$

$$g_{12}\left(\frac{m_2 p_1 - m_1 p_2}{m_1 + m_2}\right)\left[\frac{1}{p_1^2/2m_1 - \omega_1 - i\eta} - \frac{1}{p_2^2/2m_2 - \omega_2 - i\eta}\right] \tag{A11}$$

Comparing eqs. (A4) and (A11) we obtain the desired relation (A1) between Γ and g_{12}.

---

* It should be noted that whereas Bethe-Salpeter amplitude is the matrix element of *time ordered product* of two field operators, the Schrödinger amplitude is the *ordinary product* of such operators.

References

Akhiezer A I and Beretetskii V B 1965 *Quantum Electrodynamics* (Interscience)
Bhasin V S, Shrenk G L and Mitra A N 1965 *Phys. Rev.* **137B** 398
Brinkman H C and Kramers H A 1930 *Proc. Acad. Sci. Amsterdam* **33** 973
Fetter A L and Walecka J D 1971 *Quantum Theory of Many Particle Systems* (Mcgraw-Hill, N.Y.)
Heitler W 1954 *The Quantum Theory of Radiation* Third Edition (Clarendon Press, Oxford)
Jackson J D and Schiff H 1953 *a* *Phys. Rev.* **89** 559
Jackson J D and Schiff H 1953 *b* "Note added in Proof" to the paper in *Phys. Rev.* **89** 559
Kelley H P 1974 *Phys. Rev.* **136** B 896
Mcdowell M R C and Coleman J P 1970 *Introduction to the Theory of Ion-Atom Collisions* (North Holland, Amsterdam)
Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions* Third Edition (Clarendon Press, Oxford) p 508
Pradhan T 1957 *Phys. Rev.* **105** 1250
Pradhan T and Tripathy D N 1969 *Nuovo Cimento* **62B** 317
Schweber S S 1962 *Ann. Phys.* **20** 61