[24]D. R. Sweetman, Proc. Phys. Soc. Lond. A **256**, 416 (1960).
[25]L. I. Pivovar, V. M. Tubaev, and M. T. Novikov, Zh. Eksp. Teor. Fiz. **40**, 34 (1961) [Sov. Phys.-JETP **13**, 23 (1961)].
[26]K. H. Berkner, S. N. Kaplan, R. V. Pyle, and J. W. Stearns, Phys. Rev. **146**, 9 (1966).
[27]K. G. Williams, in *Abstracts of the Sixth International Conference on the Physics of Electronic and Atomic Collisions* (MIT Press, Cambridge, Mass., 1969), p. 735.
[28]See, for example, R. D. Evans, *The Atomic Nucleus* (McGraw-Hill, New York, 1955), p. 835.

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Charge Transfer in Proton-Hydrogen Collisions by the Faddeev Approach

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An approximate form of the Faddeev equations has been applied to the charge-transfer process in proton-hydrogen collisions. The effect of coupling with the direct channel has been taken into account. This formalism satisfies the unitarity condition below the breakup threshold. Results for the ground-state capture cross section have been obtained with and without the inclusion of the effect of proton-proton interactions. The experimental findings for the capture cross section in the energy range 1–150 keV lie in between our two sets of results. At high incident energies our results with and without the proton-proton interaction have approached the Jackson–Schiff and Brinkman–Kramers cross sections, respectively. The differential cross sections for the capture in the forward direction have been compared with the corresponding results of other theorists. Results for the elastic cross section have also been obtained.

I. INTRODUCTION

The problem of electron transfer in the proton-hydrogen (H^+, H) system has drawn the special attention of many theorists since this is one of the simplest type of rearrangement collisions. Several experimental investigations[1] have also been carried out on this problem. Brinkman and Kramers (BK)[2] have investigated this problem in the first-order Born approximation, neglecting the proton-proton interaction. The neglect of this interaction is justifiable since the ion-nucleus interaction can be removed by Canonical transformation (cf. Wick's comment in Ref. 3). Jackson and Schiff (JS)[3] and Bates and Dalgarno, [4] who have reconsidered the problem after many years, have shown that the effect of the proton-proton interaction when taken in the first Born approximation reduces the cross section considerably in better agreement with experiment. Unexpectedly, this reduction does not become vanishingly small even at high energies. In the high-energy limit, the JS cross section approaches the BK cross section multiplied by 0.661. These results have encouraged further investigations into the actual nature of the cross section. One may also visualize the problem in an impact-parameter treatment. The proton-proton interaction in this formalism affects the transition amplitude by introducing a phase factor, and thus the transition probability cannot be affected. Sil[5] has developed a variational method which has been applied to the problem in the impact-parameter formalism. He has concluded that when the Schrödinger equation is solved exactly the proton-proton interaction would not contribute to the capture cross section. Dalgarno and Yadav[6] have made calculations for the capture cross section using the perturbed-stationary-states method of Bates, Massey, and Stewart. [7] Further work by Drisko, [8] who has included the proton-proton interaction, has shown that the electron-transfer cross section obtained by taking higher-order Born series up to the third-order term does not converge to the BK results. Prodhan and Tripathy[9] have also obtained similar results using the impulse approximation. The work of McCarrol and Salin[10] has also reached a similar conclusion. Geltman[11] has suggested a formalism to study the electron-transfer problem by including the proton-proton interaction in the unperturbed part of the problem. For this inclusion, the plane wave in the final state is replaced by a Coulomb wave. Their results for the capture cross section lie between the corresponding BK and JS values for all energies. In the high-energy limit, their value of the cross section approaches 0.8 times the BK value. Gallaher and Wilets[12] have used a Sturmian basis in their close-coupling approximation for the low-incident-energy region and have obtained good agreement with the experimental findings. In their investigations on the proton-hydrogen collision, Cheshire, Gallaher, and Taylor[13] have also used the close-coupling method. They have retained $1s$, $2s$, $2p$ hydrogenic states and three orthogonal pseudostates are then added.

The (H^+, H) collision is a three-body problem. Therefore it is reasonable that it should be studied by the sophisticated and elegant Faddeev formalism. In this paper, an approximate form of the Faddeev equations[14] has been applied to investigate this problem. This method can include the effect of couplings to all physical states and the unitarity is preserved below the breakup threshold. This formalism has been applied to electron-hydrogen scattering by Sloan and Moore[15] and Sil and Ghosh.[16] The positron-hydrogen collision problem has also been studied by the same method by Banerjee *et al.*[17] It may be mentioned that Chen and Kramer (CK)[18] have investigated this problem through the first-order Faddeev–Watson multiple-scattering approximation.[19] The electron-transfer cross-section results of CK lie inbetween the corresponding BK and JS values and are very close to the results of Geltman in the intermediate energies. Asymptotically, the CK values approach the JS values from above. Recently Shastry *et al.*[20] have reconsidered the same problem retaining the first-order terms in the Faddeev expansion.

II. THEORY

We consider the following direct and rearrangement channels:

$$H^+(1)+H(2,3)\rightarrow H^+(1)+H(2,3), \tag{2.1a}$$

$$H^+(1)+H(2,3)\rightarrow H^+(3)+H(1,2), \tag{2.1b}$$

respectively. In the initial state for both processes, particles 2 (electron) and 3 (proton) form a bound state and particle 1 (proton) is free. In the direct process [Eq. (2.1a)] the final state remains unchanged. In the rearrangement channel [Eq. (2.1b)] the final state, after the collision, represents a bound state (1, 2) with 3 as the outgoing particle.

Following Sloan and Moore,[15] the on-shell three-body transition amplitudes may be written

$$\langle\beta\vec{k}'n'|Y|\alpha\vec{k}n\rangle=\langle\beta\vec{k}'n'|Y^{(1)}|\alpha\vec{k}n\rangle-i\pi\sum_{\nu}\sum_{n''=1}^{N_\nu}\int d\vec{k}''\,\langle\beta\vec{k}'n'|Y^{(1)}|\nu\vec{k}''n''\rangle\,\delta(E-E'')\,\langle\nu\vec{k}''n''|Y|\alpha\vec{k}n\rangle \tag{2.2}$$

(the notations are the same as used by the above authors), where α and β denote channels with the initial and final momentum K and K'. Here we have neglected the excitations of the target atom and two values of ν are possible since the proton-proton bound state is not possible. The operator $Y^{(1)}_{\beta\alpha}$ is a multiple-scattering series of the two-body operator $T^{(1)}_{\beta\alpha}$ and takes the form

$$Y^{(1)}_{\beta\alpha}=V_\beta G_0\left((1-\delta_{\beta\alpha})(S-H_0)+\sum_{\beta\neq\nu\neq\alpha}T^{(1)}_\nu+\sum\sum_{\beta\neq\nu\neq\delta\neq\alpha}T^{(1)}_\nu G_0 T^{(1)}_\delta+\cdots\right)G_0V_\alpha\,. \tag{2.3}$$

We retain only the first-order terms in (2.3), and from the high-energy consideration we may write

$$Y^{(1)}_{11}\simeq V_{12}+V_{13}\,,\quad Y^{(1)}_{13}\simeq V_{12}+V_{13}\,,$$

$$Y^{(1)}_{31}\simeq V_{23}+V_{13}\,,\quad Y^{(1)}_{33}\simeq V_{23}+V_{13}\,,$$

Accordingly, the matrix elements of $Y^{(1)}$ become Born or Born–Oppenheimer transition amplitudes. We retain only the 1s state in the summation over n'' in Eq. (2.2). Therefore, Eqs. (2.2) reduce to two coupled equations,

$$\begin{aligned}\langle\vec{k}'1s|Y_{11}|\vec{k}1s\rangle&=\langle\vec{k}'1s|Y^{(1)}_{11}|\vec{k}1s\rangle-i\pi[\int d\vec{k}''\,\langle\vec{k}'1s|Y^{(1)}_{11}|\vec{k}''1s\rangle\,\delta(E-E'')\,\langle\vec{k}''1s|Y_{11}|\vec{k}'1s\rangle\\&\quad+\int d\vec{k}''\,\langle\vec{k}'1s|Y^{(1)}_{13}|\vec{k}''1s\rangle\,\delta(E-E'')\,\langle\vec{k}''1s|Y_{31}|\vec{k}'1s\rangle],\\\langle\vec{k}'1s|Y_{31}|\vec{k}1s\rangle&=\langle\vec{k}'1s|Y^{(1)}_{31}|\vec{k}1s\rangle-i\pi[\int d\vec{k}''\,\langle\vec{k}'1s|Y^{(1)}_{31}|\vec{k}''1s\rangle\,\delta(E-E'')\,\langle\vec{k}''1s|Y_{11}|\vec{k}1s\rangle\\&\quad+\int d\vec{k}''\,\langle\vec{k}'1s|Y^{(1)}_{33}|\vec{k}''1s\rangle\,\delta(E-E'')\,\langle\vec{k}''1s|Y_{31}|\vec{k}1s\rangle\,.\end{aligned} \tag{2.4}$$

Now the matrix elements of the two-body operators have been expressed as

$$\langle\vec{k}'1s|Y^{(1)}_{\beta\alpha}|\vec{k}1s\rangle=-(1/4\pi^2)f^B_{\beta\alpha}(\hat{K}'\cdot\hat{K}). \tag{2.4'}$$

Similarly, the expressions for the three-body amplitudes are

$$\langle\vec{k}'1s|Y_{\beta\alpha}|\vec{k}1s\rangle=-\frac{1}{4\pi^2}f_{\beta\alpha}(\hat{K}'\cdot\hat{K}). \tag{2.4''}$$

With the help of (2.4′) and (2.4″), we can write Eq. (2.4) as

$$f_{11}(1s,\,1s)(\hat{k}'\cdot\hat{k})=f^{B}_{11}(1s,\,1s)(\hat{k}'\cdot\hat{k})+\frac{ik}{4\pi}\left\{\iint\left[f^{B}_{11}(1s,\,1s)(\hat{k}'\cdot\hat{k}'')f_{11}(1s,\,1s)(\hat{k}''\cdot\hat{k})\right.\right.$$
$$\left.\left.+f^{B}_{13}(1s,\,1s)(\hat{k}'\cdot\hat{k}'')f_{31}(1s,\,1s)(\hat{k}''\cdot\hat{k})\right]\sin\theta''\,d\theta''\,d\varphi''\right\},$$
$$f_{31}(1s,\,1s)(\hat{k}'\cdot\hat{k})=f^{B}_{31}(1s,\,1s)(\hat{k}'\cdot\hat{k})+\frac{ik}{4\pi}\left\{\iint\left[f^{B}_{31}(1s,\,1s)(\hat{k}'\cdot\hat{k}'')f_{11}(1s,\,1s)(\hat{k}''\cdot\hat{k})\right.\right.$$
$$\left.\left.+f^{B}_{33}(1s,\,1s)(\hat{k}'\cdot\hat{k}'')f_{31}(1s,\,1s)(\hat{k}''\cdot\hat{k})\right]\sin\theta''\,d\theta''\,d\varphi''\right\}. \tag{2.5}$$

Equations (2.5) can be expressed as

$$F^{+}=g^{+}+\frac{ik}{4\pi}\int g^{+}(\theta,\,\theta'',\,\varphi'')F^{+}(\theta'')\sin\theta''\,d\theta''\,d\varphi'',$$
$$F^{-}=g^{-}+\frac{ik}{4\pi}\int g^{-}(\theta,\,\theta'',\,\varphi'')F^{-}(\theta'')\sin\theta''\,d\theta''\,d\varphi'', \tag{2.6}$$

where

$$F^{\pm}=f_{11}\pm f_{31},$$
$$g^{\pm}=f^{B}_{11}\pm f^{B}_{31}.$$

Thus we see that the F^{+} and F^{-} are decoupled. We have calculated the three-body transition matrix elements with both BK and JS as inputs. The expressions for BK and JS amplitudes are taken from Brinkman and Kramers[2] and Jackson and Schiff,[3] respectively.

III. RESULTS AND DISCUSSION

We have solved numerically the two uncoupled integral equations (2.6). We have obtained two sets of results for the direct and the rearrangement collision amplitudes, one with BK as input (BK_{pr}; pr stands for the present results) and the other with JS as input (JS_{pr}). In the case of BK_{pr} we have performed the φ'' integration analytically and in the other case the φ'' integration has been performed numerically. Thus we are left with one-dimensional integral equations. These resulting integral equations have been solved by using the Gaussian-quadrature method and the convergence of the results has been tested by increasing the number of Gaussian points. The BK and JS cross sections have been calculated as a check of the program. We have calculated the total cross sections for the elastic and rearrangement processes, the incident energy varying from 1 keV to 2 MeV. We have also calculated the differential cross sections in the forward direction.

In Fig. 1 we have shown our BK_{pr} and JS_{pr} curves for the ground-state charge-transfer cross section and compared them with the recent experimental findings.[1] All the experimental points lie between the JS_{pr} and BK_{pr} curves in the energy range 1–150 keV. From 1 keV to about 50 keV, the BK_{pr} values are in close agreement with the experimental findings due to Fite *et al.*, whereas from 60 keV and above, JS_{pr} curves are closer to the experimental findings of Ryding and Gilbody. It may be mentioned that the curves due to Wilets and Gallaher,[12] McCarroll,[21] Ferguson,[22] and McElroy,[23] which are all very close to McClure's experimental findings, also lie between our two results. It is too early to comment as to which one of the inputs is more physical. It will be interesting to study the influence of the coupling to higher excited states and the effects of virtual excitations.

In Table I, we have presented our two sets of results for the total cross section along with the corresponding BK and JS values for the incident

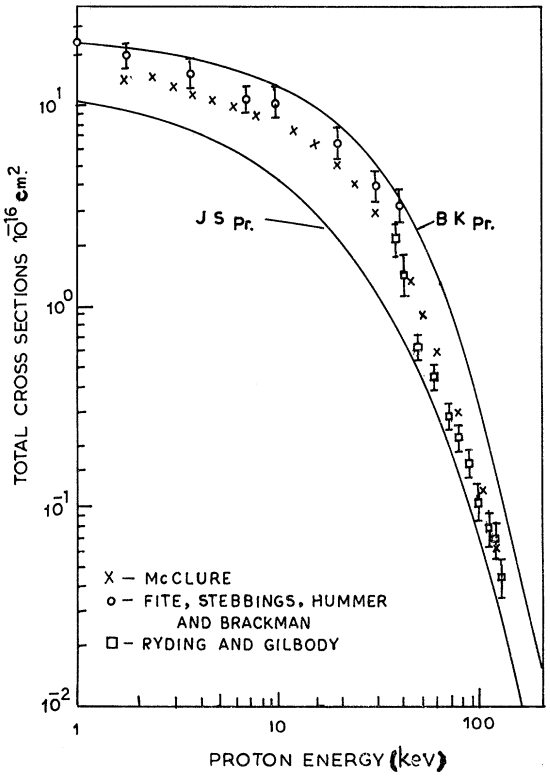

FIG. 1. Present calculations of the ground-state charge-transfer cross section, BK_{pr} and JS_{pr}, are compared with the experimental results of McClure (Ref. 1), Fite *et al.* (Ref. 1), and Ryding and Gilbody (Ref. 1) in the energy range 1–150 keV.

TABLE I. Charge-exchange cross section[a] for the ground state in units of πa_0^2.

Energy (keV)	BK	BK_{pr}	Sil[b]	JS	JS_{pr}
1	1217.365	23.517	18.636	144.019	11.907
2	579.413	21.242	15.911	69.024	10.149
3			14.314		
5	200.483	17.591	12.383	24.373	7.345
10	79.432	13.979	10.012	9.974	4.869
15	42.397	11.302		5.489	3.405
20	25.701	9.119		3.426	2.451
30	11.481	5.853		1.615	1.350
50	3.367	2.400		0.511	0.489
100	0.399	0.351		0.733(−1)	0.734(−1)
200	0.263(−1)	0.243(−1)		0.598(−2)	0.602(−2)
400	0.102(−2)	0.962(−3)		0.291(−3)	0.289(−3)
800	0.270(−4)	0.257(−4)		0.943(−5)	0.930(−5)
1000	0.793(−5)	0.757(−5)		0.293(−5)	0.288(−5)
2000	0.156(−6)	0.151(−6)		0.674(−7)	0.663(−7)

[a]The number in parentheses in each entry is the exponent of 10 by which the cross-section value should be multiplied.

[b]Reference 5.

energy range 1 keV to 2 MeV, as well as the results obtained by Sil[5] for the range 1–10 keV. From 1 to 10 keV, results obtained by Sil are inbetween our two sets of results. From the table it is apparent that BK and JS values are too high in the low-energy region. Noticeable differences between the JS and the JS_{pr} values have been found up to 0.76 keV; the values are almost identical from 100 keV and above. The difference between BK and BK_{pr} values, however, exists up to about 800 keV.

In Fig. 2 we have given our two curves and the curve of CK for the total capture cross section. The CK[18] curve lies inbetween our BK_{pr} and JS_{pr}

TABLE II. Total cross sections for the elastic scattering of protons by hydrogen atoms in units of πa_0^2.

Energy (keV)	Present BK as input	Present JS as input	FBA
1	58.539	16.858	58.214
2	43.660	11.322	29.107
5	25.655	5.653	11.642
10	13.674	2.835	5.821
15	7.949	1.824	3.881
20	4.825	1.357	2.910
30	2.022	0.955	1.940
50	0.699	0.699	1.164
100	0.385	0.417	0.582
200	0.236	0.238	0.291
400	0.129	0.129	0.145
800	0.067	0.067	0.072
1000	0.055	0.055	0.058
2000	0.028	0.028	0.029

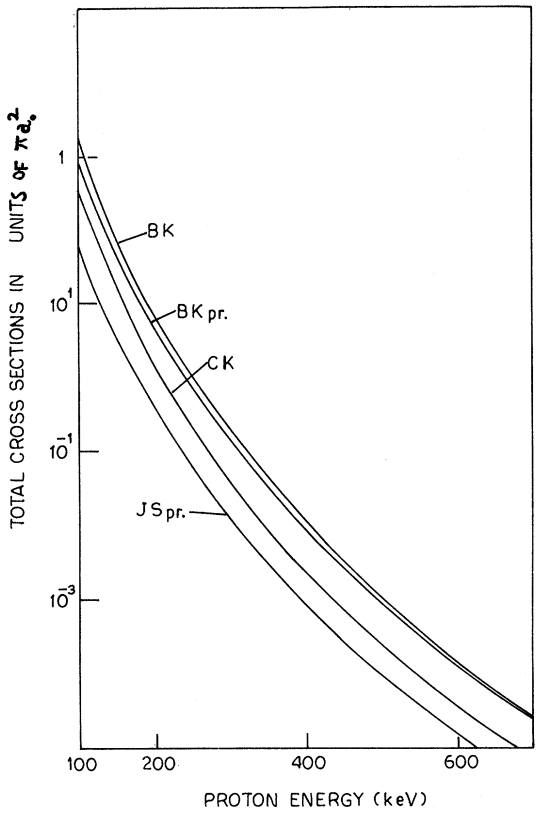

FIG. 2. Total capture cross-section results BK_{pr} and JS_{pr} are compared with CK and BK curves for the energy range 100–700 keV.

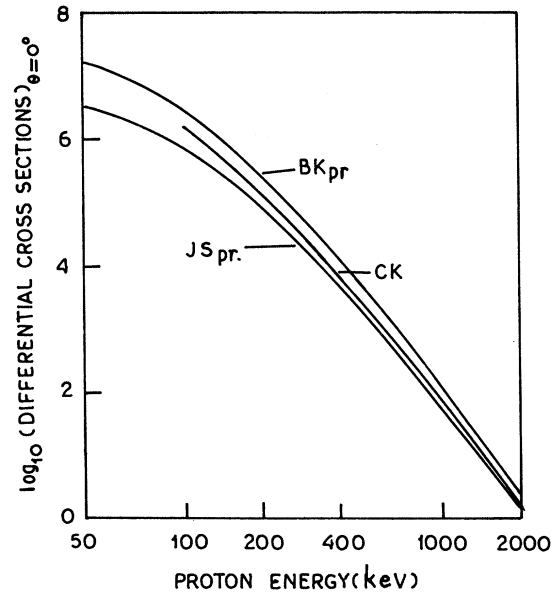

FIG. 3. Results of forward-direction differential cross sections are compared with the corresponding CK results from 50 keV to 2 MeV (in units of πa_0^2).

curves. It may be mentioned that the values due to Geltman[11] which are slightly greater than the CK results are closer to our BK_{pr} values. The cross-section results obtained by Shastry *et al.*,[20] which are in good agreement with CK results, also lie inbetween our two sets of results. There is no difference between the JS and JS_{pr} curves from 100 keV and above. Similar features have been obtained for the charge-transfer cross section for (e, H) scattering investigated by Banerjee *et al.*[17]

In Fig. 3 we have given our two curves for the differential cross section at $\theta = 0^\circ$ scattering angle along with the corresponding CK curve. Here we also find that the CK curve lies inbetween our two curves. The CK curve approaches the JS_{pr} curve from above at high energies.

We have also calculated the total cross sections for the elastic scattering of a proton by a hydrogen atom which are presented in Table II along with the first Born-approximation (FBA) results. The effect of couplings on the rearrangement channel has been taken into account. When BK is taken as input our results are greater than the FBA results from 1 to 30 keV. Above this energy, our values are less than FBA. Our results with JS as input are always less than FBA. At 1 keV our result is about 3.5 times less than FBA. With the increase of energy, the difference decreases. From 200 keV to MeV, our two results are more or less the same. At the highest energy, i.e., at 2 MeV, our two results differ from FBA by about 3%. A similar feature has also been noticed for the same process by Sinfailam and Chen.[24] For $(e^+\text{-H})$ scattering, Sil and his collaborators[16,17] have obtained similar differences between their results and the corresponding results of FBA.

[1]G. W. McClure, Phys. Rev. **148,** 47 (1966); W. L. Fite, R. T. Brackmann, and W. R. Snow, Phys. Rev. **112,** 1161 (1958); W. L. Fite, R. F. Stebbings, D. G. Hummer, and R. T. Brackmann, Phys. Rev. **119,** 663 (1960); W. L. Fite, A. C. H. Smith, and R. F. Stebbings, Proc. R. Soc. A **268,** 527 (1962); G. Ryding and H. B. Gilbody, in *Abstracts of the Proceedings of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec,* 1965, edited by L. Kerwin and W. Fite (Science Bookcrafters, Hastings-on-Hudson, New York, 1965).

[2]H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33,** 973 (1930).

[3]J. D. Jackson and H. Schiff, Phys. Rev. **89,** 359 (1953).

[4]D. R. Bates and A. Dalgarno, Proc. Phys. Soc. Lond. A **65,** 919 (1952).

[5]N. C. Sil, Proc. Phys. Soc. Lond. **75,** 194 (1960).

[6]A. Dalgarno and H. N. Yadav, Proc. Phys. Soc. Lond. A **66,** 173 (1953).

[7]D. R. Bates, H. S. W. Massey, and A. L. Stewart, Proc. R. Soc. A **216,** 437 (1953).

[8]D. R. Drisko, Ph.D. thesis (Carnegie Institute of Technology, 1955) (unpublished).

[9]T. Pradhan and D. N. Tripathy, Phys. Rev. **130,** 2317 (1963).

[10]R. McCarrol and A. Salin, Proc. R. Soc. A **300,** 202 (1967).

[11]S. Geltman, J. Phys. B **4,** 1288 (1971).

[12]D. F. Gallaher and L. Wilets, Phys. Rev. **169,** 139 (1968).

[13]I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B **3,** 813 (1970).

[14]L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39,** 1459 (1960) [Sov. Phys.-JETP **12,** 1014 (1961)].

[15]I. H. Sloan and E. J. Moore, J. Phys. B **1,** 414 (1968).

[16]N. C. Sil and A. S. Ghosh, Phys. Rev. A **5,** 2122 (1972).

[17]G. Banerji, A. S. Ghosh, and N. C. Sil, Phys. Rev. A 7, 571 (1973).

[18]J. C. Y. Chen and P. J. Kramer, Phys. Rev. A **5,** 1207 (1972).

[19]J. C. Y. Chen and C. J. Joachain, Physica (Utr.) **53,** 333 (1971).

[20]C. S. Shastry, A. K. Rajagopal, and J. Callaway, Phys. Rev. A **6,** 268 (1972).

[21]R. McCarroll, Proc. R. Soc. A **264,** 547 (1961).

[22]A. F. Ferguson, Proc. R. Soc. A **264,** 540 (1961).

[23]M. B. McElroy, Proc. R. Soc. A **272,** 542 (1963).

[24]A. L. Sinfailam and J. C. Y. Chen, Phys. Rev. A **5,** 1218 (1972).