

Transform for calculating scattering amplitudes. II. Numerical results for the Yukawa potential

C. M. Rosenthal

Department of Chemistry, Drexel University, Philadelphia, Pennsylvania 19104

(Received 21 October 1974)

Numerical evaluation of high-order terms in the Born series for an attractive Yukawa potential is accomplished with a transform described in an earlier paper. Born terms through order five are computed at high energy and through order seven at low energy. These are resummed using a variational functional for the T -matrix elements suggested by Rabitz and Conn to give good agreement with the existing numerical study of Walters.

I. INTRODUCTION

In an earlier paper¹ a transform of the free-particle Green's function was obtained which led to an inhomogeneous line-integral equation for potential scattering amplitudes. This equation has been iterated numerically for an attractive Yukawa potential at high and low energies, thus generating at the high (low) energy the first five (seven) terms in the Born series. These terms have been resummed using the variational approach of Rabitz and Conn² to give good agreement with the direct numerical studies of Walters.³

II. REVIEW OF TRANSFORM APPROACH

In the first paper of this series the function

$$F(k, s) = \frac{-V_0}{2\pi} \int e^{-i\hat{k}_f \cdot \vec{r}} \frac{e^{-sr}}{r} \psi_+(\vec{r}) d\vec{r}$$

was shown to satisfy the inhomogeneous line-integral equation

$$F(k, s) = F_0(k, s) - \frac{V_0}{k} \int_0^k \frac{F(\tau, s_0 + s') d\tau}{s'} \quad (1)$$

[e.g., (12) of paper I], with

$$F_0(k, s) = \frac{-V_0}{2\pi} \int e^{-i\hat{k}_f \cdot \vec{r}} \frac{e^{-sr}}{r} e^{i\hat{k}_i \cdot \vec{r}} d\vec{r} \\ = \frac{-2V_0}{s^2 + k^2 + k_0^2 - 2kk_0 \cos x} ,$$

$$E = \frac{1}{2}k_0^2, \quad \cos x = \hat{k}_f \cdot \hat{k}_i, \quad \vec{k}_i = k_0 \hat{k}_i .$$

$F_0(k_0, s_0)$ is equal to the first Born term for elastic scattering off $V_0(e^{-s_0/r})$, and $F(k_0, s_0)$ is the complete elastic scattering amplitude off $V_0(e^{-s_0/r})$. The variable s' which occurs in Eq. (1) is a particular function of s , k , and τ , namely, $s'^2 = \sigma\tau - \tau^2 - k_0^2$, with $\sigma = (s^2 + k^2 + k_0^2)/k$; in order for (1) to be valid the branch of s' must be so chosen that $s' = -ik_0$ when $\tau = 0$ and s' must have a positive real

part when $\tau = k$. This uniquely determines how the branch cuts must be drawn in the complex τ plane.

III. ITERATIVE SOLUTION OF EQ. (1)

As Eq. (1) involves the integral of a function of two variables over a curve in the space of its variables, it is best described as an inhomogeneous line-integral equation. Iterating the equation (or expanding in powers of V_0 , the potential strength) generates the sequence of equations

$$F_n(k, s) = -\frac{1}{k} \int_0^k \frac{F_{n-1}(\tau, s_0 + s') d\tau}{s'} . \quad (2)$$

The solutions of these equations evaluated at the points (k_0, s_0) are the terms in the Born series for the T matrix,

$$T(\vec{k}_f, \vec{k}_i) = \sum_{n=1}^{\infty} V_0^{(n)} T^{(n)}(\vec{k}_f, \vec{k}_i) , \quad (3)$$

$$T^{(n)}(k_f, k_i) = F_{n-1}(k_0, s_0) .$$

As Eq. (2) involves only a one-dimensional integration, it is well suited for numerical evaluation. The computation requires knowledge of the previous iterate along the line $(\tau, s_0 + s'(\sigma, \tau))$ for $0 \leq \tau \leq k$. Once a quadrature scheme has been decided upon, the calculation proceeds as follows. For each n , we need $F_{n-1}(k_0, s_0)$. Thus F_{n-1} is needed along the line

$$(\tau_{n-1}, s_0 + s'(\sigma_{n-1}, \tau_{n-1})), \quad 0 \leq \tau_{n-1} \leq k_0$$

with $\sigma_n = (s_0^2 + 2k_0^2)/k_0$. This in turn requires F_{n-2} along the line

$$(\tau_{n-2}, s_0 + s'(\sigma_{n-1}, \tau_{n-2})), \quad 0 \leq \tau_{n-2} \leq \tau_{n-1}$$

$$\sigma_{n-1} = \frac{s_{n-1}^2 + \tau_{n-1}^2 + k_0^2}{\tau_{n-1}} ,$$

with $s_{n-1} = s_0 + s'(\sigma_n, \tau_{n-1})$. Likewise, this requires F_{n-3} along the line

$$(\tau_{n-3}, s_0 + s'(\sigma_{n-2}, \tau_{n-3})), \quad 0 \leq \tau_{n-3} \leq \tau_{n-2}$$

$$\sigma_{n-2} = \frac{s_{n-2}^2 + \tau_{n-2}^2 + k_0^2}{\tau_{n-2}},$$

with $s_{n-2} = s_0 + s'(\sigma_{n-1}, \tau_{n-2})$. Continuing this backward recurrence, we ultimately require F_0 at a set of points N^n in number, where N is the number of quadrature points used in the numerical integration scheme. Note also that although σ_n is real, σ_{n-1} will be complex for some values of τ_{n-1} , because $s'(\sigma_n, \tau_{n-1})$ is complex for some values of τ_{n-1} . Recalling that Eq. (1) was obtained by choosing the branch of $s'^2(\sigma, \tau) = \sigma\tau - \tau^2 - k_0^2$ in such a manner that $s'(\sigma, 0) = -ik_0$ and $\text{Res}'(\sigma, k) > 0$, we see that $s'(\sigma_m, \tau_{m-1})$ must also be such that $s'(\sigma_m, 0) = -ik_0$ and $\text{Res}'(\sigma_m, \tau_m) > 0$ for all $0 \leq m \leq n-1$; otherwise the assumed integral expression for $F_m(\tau_m, s_0 + s'(\sigma_{m+1}, \tau_m))$ would not be valid. This means that one must either carefully choose the branch of s' at each stage of the recurrence procedure or, what is equivalent, augment the energy by an infinitesimal positive imaginary $i\epsilon$, and take the principal root of $s^2(\sigma_m, \tau_{m-1})$. Appendix A shows that this does indeed give rise to the correct branch.

IV. QUADRATURE SCHEME

In Sec. III an iterative scheme for the evaluation of $F_n(k_0, s_0)$ was described which depended upon a numerical quadrature of Eq. (2). To carry out this quadrature, we first observe that $s'(\sigma_m, \tau_{m-1})$ which occurs in the denominator of the integrand represents a possible singularity. The roots of s' occur at $\tau_{m-1} = \frac{1}{2}\sigma_m + \rho_m$ and $\frac{1}{2}\sigma_m - \rho_m$, with $\rho_m^2 = \frac{1}{4}\sigma_m^2 - k_0^2$. Letting $x_1 + iy_1$ denote the root which has its real part closest to the origin, and $x_2 + iy_2$ the other root, we note that both x_1 and x_2 must either be simultaneously positive or negative (i.e., one root cannot lie in the right half-plane and the other in the left half-plane). This may be easily checked by examining the two equations $x_1x_2 - y_1y_2 = k_0^2$, $x_1y_2 + x_2y_1 = 0$. Furthermore, y_1 and y_2 must either have opposite signs or both be 0. Also, the two roots cannot coalesce. For this to occur ρ_m must equal zero, which cannot occur if σ_m has an imaginary part ($\rho_m^2 = \frac{1}{4}\sigma_m^2 - k_0^2$), and also cannot occur if σ_m is pure real. For σ_m real, we must have s_m real; if s_m is real then $\sigma_m \geq 2(s_m^2 + k_0^2)^{1/2}$, so that $\rho_m \geq s_m \geq s_0 > 0$. Thus, as the roots cannot coalesce the possible singularities in the integrand are still integrable singularities. The quadrature scheme employed makes use of this fact in the following way. If $x_1 > 0$, break the integration region up into two pieces $0 \leq \tau_{m-1} \leq x_1$ and $x_1 \leq \tau_{m-1} \leq \tau_m$. (The second region is unnecessary if $\tau_m \leq x_1$.) In the first region use a new integration variable $x = (x_1 - \tau_{m-1})^{1/2}$, in the

second $x = (\tau_{m-1} - x_1)^{1/2}$; if $x_1 < 0$, only a single region is necessary, along with the substitution $x = (\tau_{m-1} - x_1)^{1/2}$. In both cases the integrand expressed in terms of the new variable is well behaved at the point $x = 0$ ($\tau_{m-1} = x_1$) for all values of y_1 , including the case $y_1 = 0$. [As the integration in Eq. (2) proceeds along the real axis, the singularity in s' occurs only when $y_1 = 0$, but the substitutions described here ensure that the integrand is uniformly bounded and continuous expressed as a function of the new variable x , and thus readily approximated by a quadrature for all values of y_1 .] The only other point we have to worry about is $\tau_{m-1} = x_2$. Appendix B shows that this point does not give rise to any difficulty in the quadrature.

It is clear then that after changing to the new integration variable x , ordinary Gauss-Legendre quadrature should do very well, as each interval is of finite length and the integrand is continuous and bounded throughout. For the numerical results reported below, a minimal number of points (four) was used in each quadrature step. As a check on the procedure and to see whether four quadrature points were sufficient the numerical results were compared with the analytic iteration of Eq. (2) once [see paper I and references therein]; the agreement was essentially exact.

V. NUMERICAL RESULTS

Tables I–III present the numerical results for the calculations described in the previous sections;

TABLE I. Terms in the Born series for scattering off $-1.1825 e^{-r}/r$.

k_0	n	$T^{(n)}(0)$	$T^{(n)}(\frac{1}{2}\pi)$	$T^{(n)}(\pi)$
1.816	1	-2.000 00 ^a	-0.263 30	-0.140 93
		0.000 00 ^b	0.000 00	0.000 00
1.816	2	0.140 93	$0.548\ 09 \times 10^{-1}$	$0.340\ 71 \times 10^{-1}$
		0.511 86	0.270 21	0.192 30
1.816	3	0.173 09	0.144 10	0.125 37
		-0.125 40	$-0.904\ 45 \times 10^{-1}$	$-0.721\ 79 \times 10^{-1}$
1.816	4	$-0.828\ 64 \times 10^{-1}$	$-0.744\ 57 \times 10^{-1}$	$-0.680\ 68 \times 10^{-1}$
		$-0.492\ 15 \times 10^{-1}$	$-0.488\ 83 \times 10^{-1}$	$-0.480\ 07 \times 10^{-1}$
1.816	5	$-0.455\ 71 \times 10^{-2}$	$-0.555\ 85 \times 10^{-2}$	$-0.635\ 69 \times 10^{-2}$
		$0.448\ 55 \times 10^{-2}$	$0.436\ 13 \times 10^{-1}$	$0.424\ 54 \times 10^{-1}$
0.663	1	-2.000 00	-1.064 31	-0.725 09
		0.000 00	0.000 00	0.000 00
0.663	2	0.725 08	0.621 77	0.544 50
		0.961 47	0.880 66	0.814 38
0.663	3	0.126 95	0.139 88	0.151 23
		-0.978 45	-0.955 13	-0.933 12
0.663	4	-0.644 17	-0.645 36	-0.646 43
		0.565 23	0.559 19	0.553 26
0.663	5	0.753 75	0.753 62	0.753 48
		$-0.139\ 24 \times 10^{-1}$	$-0.124\ 34 \times 10^{-1}$	$-0.109\ 56 \times 10^{-1}$
0.663	6	-0.519 64	-0.519 51	-0.519 38
		-0.416 04	-0.416 39	-0.416 74
0.663	7	0.121 51	0.121 45	0.121 40
		0.576 06	0.576 13	0.576 21

^aReal part.

^bImaginary part.

TABLE II. Computed scattering amplitudes.

$k_0 = 1.816$	$T(0)$	$T(\frac{1}{2}\pi)$	$T(\pi)$
Born sum	2.1244	0.0170	-0.1114
$[\sum_1^5 (V_0)^n T^{(n)}]$	0.7231	0.3310	0.1962
[2, 3] Padé approximant	2.1865	0.0796	-0.0482
Walters calculation	0.7387	0.3474	0.2123
	2.182	0.079	-0.05
	0.739	0.3478	0.2134
$k_0 = 0.663$			
Born sum	0.1667	-1.1076	-1.6373
$[\sum_1^5 (V_0)^n T^{(n)}]$	4.0997	3.9328	3.7888
Born sum	-1.6468	-2.9207	-3.4499
$[\sum_1^7 (V_0)^n T^{(n)}]$	1.0998	0.9318	0.7865
[2, 3] Padé approximant	1.1589	-0.1106	-0.6424
Walters calculation	1.6818	1.5123	1.3606
	1.1580	-0.1156	-0.6555
[3, 4] Padé approximant	1.7148	1.5190	1.3571
Walters calculation	1.116	-0.142	-0.651
	1.671	1.5041	1.3584

V_0 was set to -1.1825 in order to facilitate comparison with the study of Walters³; two incident energies $k_0 = 1.816$ and $k_0 = 0.663$ were selected and the terms in the Born series were calculated at three angles ($\theta = 0, \frac{1}{2}\pi$, and π) through order five at the larger energy and seven at the smaller. These terms are listed in Table I. When summed

up using Eq. (3), we get an approximation to the scattering amplitude. Table II shows that the agreement between these Born sums and Walters's calculation at $k_0 = 1.816$ is fair and at $k_0 = 0.663$ poor. That is not at all surprising, since the Born series is not expected to converge at low energies. On the other hand, using the variational approach of Rabitz and Conn² for the T matrix one may use the computed terms in the Born series at each energy and each angle to generate a variational approximation to the scattering amplitude. Writing

$$T_{\text{trial}} = x_1 T^{(1)} + x_2 T^{(2)} + \dots + x_N T^{(N)},$$

and requiring that the functional

$$I_{ba} = \langle b | V | a \rangle + \langle b | V G_0 T_{\text{trial}} | a \rangle + \langle b | T_{\text{trial}} G_0 V | a \rangle - \langle b | T_{\text{trial}} G_0 T_{\text{trial}} | a \rangle + \langle b | T_{\text{trial}} G_0 V G_0 T_{\text{trial}} | a \rangle$$

be stationary with respect to variations in the parameters (x_1, \dots, x_N) gives rise to an optimum T_{trial} that is equal to the $[N, N+1]$ Padé approximant to the scattering amplitude. The coefficients of this approximant are easily obtained from the first $2N+1$ terms in the Born series. Those coefficients are listed in Table III, and the corresponding variational approximations to the scattering amplitudes are listed in Table II for compari-

TABLE III. Coefficients in Padé approximants.

n	$T_{\text{var}} = [\sum_1^{N+1} (V_0)^n P_n] / [1 + \sum_1^N (V_0)^n Q_n]$					
	$P_n(0)$	$P_n(\frac{1}{2}\pi)$	$P_n(\pi)$	$Q_n(0)$	$Q_n(\frac{1}{2}\pi)$	$Q_n(\pi)$
$k_0 = 1.816 \quad N = 2$						
1	-2.000 00	-0.263 31	-0.140 93	0.288 92	0.294 59	0.350 74
	0.000 00	0.000 00	0.000 00	0.554 85	0.625 22	0.698 92
2	-0.436 92	$-0.227 58 \times 10^{-1}$	$-0.153 59 \times 10^{-1}$	$-0.375 96 \times 10^{-1}$	$-0.694 66 \times 10^{-1}$	$-0.956 35 \times 10^{-1}$
	-0.597 84	0.105 58	$0.938 04 \times 10^{-1}$	$0.613 98 \times 10^{-1}$	$0.767 29 \times 10^{-1}$	0.120 09
3	$0.499 51 \times 10^{-2}$	$0.959 34 \times 10^{-2}$	$0.163 89 \times 10^{-1}$			
	$-0.221 10 \times 10^{-1}$	$0.321 96 \times 10^{-2}$	$0.215 92 \times 10^{-2}$			
$k_0 = 0.663 \quad N = 2$						
1	-2.000 00	-1.064 32	-0.725 09	0.895 11	0.846 80	0.845 57
	0.000 00	0.000 00	0.000 00	0.684 12	0.748 63	0.683 62
2	-1.065 15	-0.279 50	$-0.686 07 \times 10^{-1}$	$0.789 22 \times 10^{-1}$	$0.914 78 \times 10^{-2}$	$0.446 08 \times 10^{-1}$
	-0.406 77	$0.838 73 \times 10^{-1}$	0.318 69	0.203 92	0.220 09	0.176 38
3	$-0.396 32 \times 10^{-1}$	$-0.263 18 \times 10^{-2}$	$0.225 77 \times 10^{-1}$			
	$-0.296 15 \times 10^{-1}$	$0.218 41 \times 10^{-1}$	$-0.166 96 \times 10^{-3}$			
$k_0 = 0.663 \quad N = 3$						
1	-2.000 00	-1.064 32	-0.725 09	1.922 29	2.459 38	2.339 90
	0.000 00	0.000 00	0.000 00	0.996 93	1.188 87	0.512 06
2	-3.119 49	-1.995 79	-1.115 21	0.775 30	1.059 14	1.441 15
	-1.032 39	-0.384 68	0.443 09	1.116 46	1.779 86	1.057 41
3	-0.988 35	-0.505 22	$-0.366 50 \times 10^{-1}$	$0.246 26 \times 10^{-1}$	$-0.605 31 \times 10^{-1}$	0.105 02
	-0.736 50	$0.556 07 \times 10^{-1}$	0.484 54	0.216 04	0.354 46	0.269 45
4	$-0.314 97 \times 10^{-1}$	$-0.102 91 \times 10^{-1}$	$0.326 88 \times 10^{-1}$			
	$-0.313 09 \times 10^{-1}$	$0.386 03 \times 10^{-1}$	$0.132 22 \times 10^{-2}$			

son with the Born series and the Walters calculation. This time agreement with the Walters calculation is excellent at the high energy and good at the low energy. Furthermore, the calculated amplitudes at the low energy are seen to be very stable on going from the [2, 3] to the [3, 4] Padé approximant.

VI. CONCLUSIONS

A practical scheme for computing accurate high-order terms in the Born series for potential scattering has been illustrated with an attractive Yukawa potential. When resummed using a variational procedure these terms give excellent agreement with existing calculations. The Born terms themselves will be analyzed in a later study to see what information they provide about the nature and position of the singularity which determines the radius of convergence of the Born series.

APPENDIX A: BRANCH $s'(\sigma_m, \tau_{m-1})$

We demonstrate here that replacing k_0^2 by $k_0^2 + i\epsilon$ and selecting the principal branch of

$$s'^2(\sigma_m, \tau_{m-1}) = \sigma_m \tau_{m-1} - \tau_{m-1}^2 - (k_0^2 + i\epsilon)$$

leads to

$$s'(\sigma_m, 0) = -ik_0, \quad \text{Res}'(\sigma_m, \tau_m) > 0.$$

Suppose that k_0^2 has been replaced by $k_0^2 + i\epsilon$, then

$$\sigma_m = (s_m^2 + \tau_m^2 + k_0^2 + i\epsilon) / \tau_m$$

and

$$\begin{aligned} s'^2(\sigma_m, \tau_{m-1}) &= \sigma_m \tau_{m-1} - \tau_{m-1}^2 - k_0^2 - i\epsilon \\ &= \left(\frac{s_m^2 + \tau_m^2 + k_0^2}{\tau_m} \right) \tau_{m-1} - \tau_{m-1}^2 \\ &\quad - k_0^2 - i\epsilon \left(1 - \frac{\tau_{m-1}}{\tau_m} \right), \end{aligned}$$

thus choosing the principal branch of the square root certainly gives $s'(\sigma_m, 0) = -ik_0$. Furthermore, we can show that s_m must lie in the lower right quadrant of the complex plane. To see this note that $s'(\sigma_n, \tau_{n-1})$ is either negative pure imaginary or non-negative real, and $s'(\sigma_n, k_0) = s_0$. [Recall that $\sigma_n = (s_0^2 + 2k_0^2)/k_0$.] Thus $\text{Res}_{n-1} \geq s_0 > 0$ and

$\text{Im}s_{n-1} \leq 0$. Thus taking the principal branch of $s'^2(\sigma_{n-1}, \tau_{n-2})$, we see that either (a) if $\text{Im}s_{n-1} < 0$, then $\text{Im}s'^2(\sigma_{n-1}, \tau_{n-2}) < 0$, so that $\text{Res}'(\sigma_{n-1}, \tau_{n-2}) > 0$ and $\text{Im}s'(\sigma_{n-1}, \tau_{n-2}) < 0$ for all $0 \leq \tau_{n-2} \leq \tau_{n-1}$; or (b) if $\text{Im}s_{n-1} = 0$, then $\text{Im}s'(\sigma_{n-1}, \tau_{n-2}) < 0$ for $0 \leq \tau_{n-2} < \tau_{n-1}$, so that again $\text{Res}'(\sigma_{n-1}, \tau_{n-2}) > 0$, $\text{Im}s'(\sigma_{n-1}, \tau_{n-2}) < 0$, and at the point $\tau_{n-2} = \tau_{n-1}$, $s'^2 = s_{n-1}^2 = \text{Re}(s_{n-1})^2 \geq s_0^2$ (because $\text{Im}s_{n-1}$ is assumed equal to zero). This ensures $s'(\sigma_{n-1}, \tau_{n-2}) = \text{Res}_{n-1} \geq s_0$. Thus in all cases $s'(\sigma_{n-1}, \tau_{n-2})$ lies in the lower right quadrant, so that $\text{Res}_{n-2} \geq s_0$ and $\text{Im}s_{n-2} \leq 0$. Clearly one may proceed inductively to show that $\text{Res}_m \geq s_0 > 0$ and $\text{Im}s_m \leq 0$ for all $0 \leq m \leq n-1$; arguing as above this ensures that $s'(\sigma_m, 0) = -ik_0$; $\text{Res}'(\sigma_m, \tau_m) > 0$ for $1 < m < n$.

APPENDIX B: SECOND SINGULARITY OF

$$s'^2 = \sigma_m \tau_{m-1} - \tau_{m-2}^2 - k_0^2$$

Note that $|y_2| = |(x_2/x_1)y_1|$ so that the second singularity is further away from the real axis than the first (recall that x_2 and x_1 were labeled so that $|x_2| > |x_1|$). Again there is no difficulty if $|y_2| > 0$; the integration proceeds along the real axis. Let us examine the case $y_2 = 0$ more closely. $y_2 = 0$ implies $y_1 = 0$ implies σ_m real implies s_m real. We must determine whether the variable τ_{m-1} ever gets out as far as x_2 . The answer is no:

$$\sigma_m = (s_m^2 + \tau_m^2 + k_0^2) / \tau_m \geq 2(s_m^2 + k_0^2)^{1/2}$$

so that

$$x_2 = \frac{1}{2}\sigma_m + \rho_m \geq (s_m^2 + k_0^2)^{1/2} + s_m > k_0 + s_0,$$

because s_m real and $\text{Res}_m > s_0$. Thus $x_2 > k_0 + s_0 > \tau_m$. Thus the integrand is bounded and continuous at the point τ_m , the end point of the integration, as well as at x_1 for the case $y_1 = y_2 = 0$. For small but nonzero y_2 we must examine $1/[(\tau_{m-1} - x_2)^2 + y_2^2]^{1/2}$ in the range $0 \leq \tau_{m-1} \leq \tau_m$ and show that it is uniformly bounded. For $\text{Im}\sigma_m = 0$, we have seen this term is at most $1/s_0$; as both y_2 and x_2 vary continuously with $\text{Im}\sigma_m$ there must exist an interval $0 \leq |\text{Im}\sigma_m| \leq \delta$ in which

$$1/[(\tau_{m-1} - x_2)^2 + y_2^2]^{1/2} > 1/2s_0.$$

For $|\text{Im}\sigma_m| > \delta$, there is also no problem. Recall that x_2 was the root with a real part of largest absolute value, and also that $x_2 = \text{Re}(\frac{1}{2}\sigma_m \pm \rho_m)$; if σ_m lies in the lower right-hand quadrant σ_m^2 lies in the lower left-hand quadrant, so that ρ_m lies in the lower right-hand quadrant and the plus sign

is appropriate. That also means

$$y_2 = \text{Im}(\frac{1}{2}\sigma_m + \rho_m) \geq \text{Im}\frac{1}{2}\sigma_m \geq \frac{1}{2}\delta .$$

If σ_m lies in the lower left quadrant, then σ_m^2 lies

in the upper half-plane; ρ_m lies in the upper right quadrant, so the minus sign is appropriate for x_2 .
Thus

$$|y_2| = |\text{Im}(\frac{1}{2}\sigma_m - \rho_m)| \geq |\text{Im}\frac{1}{2}\sigma_m| > \frac{1}{2}\delta .$$

¹C. M. Rosenthal, Phys. Rev. A 9, 273 (1974).

²H. A. Rabitz and R. Conn, Phys. Rev. A 7, 577 (1973).

³H. R. J. Walters, J. Phys. B 4, 437 (1971).