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A. TEMKIN

Y. HAHN

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GODDARD SPACE FLIGHT CENTER

GREENBELT, MARYLAND

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A. Temkin
Theoretical Studies Branch
National Aeronautice and Space Administration
Goddard Space Flight Center
Greenbelt, Maryland 20771

Y. Hahn
Department of Physics
University of Connecticut
Storrs, Connecticut 06268

ABSTRACT

The problem of the threshold law for electron-atom impact ionization is reconsidered as an extrapolation of inelastic cross sections through the ionization threshold. The cross sections are evaluated from a distorted wave matrix element, the final state of which describes the scattering from the N^{th} excited state of the target atom. The actual calculation is carried for the e-H system, and a model is introduced in which the r_{12}^{-1} repulsion is replaced by $(r_1+r_2)^{-1}$. This model is shown to preserve the essential properties of the problem while at the same time reducing the dimensionability of the Schrodinger equation. Nevertheless, the scattering equation is still very complex. It is dominated by the optical potential which is expanded in terms of eigen-spectrum of QHQ. It is shown by actual calculation that the lower

eigenvalues of this spectrum descend below the relevant inelastic thresholds; it follows rigorously that the optical potential contains repulsive terms. Analytical solutions of the final state wave function are obtained with several approximations of the optical potential: (o) omission of the optical potential (1) inclusion of the lowest term and dominant pole term (2) a closure approximation which depends on an effective energy $\bar{\mathcal{E}}_N$ for each threshold energy E_N. The threshold law in all these cases is obtained. In the closure approximation the law depends on the sign and N dependence of $E_N - \bar{\mathcal{E}}_N$, however it cannot be excluded that the difference in an oscillating function of N. In that case the derivative of the yield curve is an oscillating (but non-negative) function of the available energy E. A form of such a threshold law is suggested.

I. INTRODUCTION

In previous papers[1,2] we have begun to consider the impact ionization problem from a completely quantum mechanical point of view. The touchstone of our understanding of that problem is the threshold law, and it is to that specific problem that we return.

The insight that we tried to gain was by a study of the doubly excited (i.e. auto-detaching) states of the electron-atom system associated with ever higher principal quantum numbers of the target atom. The actual extrapolation procedure that was used, however, was through a summation of inelastic cross sections to such higher states, in which the final state wave function was taken as being of the form as the doubly excited state which minimized the energy.

As reasonable as this procedure would appear, it is at best speculative, because the doubly excited states actually enter the equation for the final state scattering functions as specific terms in the optical potential. For each scattering function there are an infinity of optical potential terms plus direct potentials, not to mention coupling terms between various excited states that must in principle be considered. In the light of this complexity it is naive to expect that the final state scattering function is simply of the form of the lowed lying doubly excited state.

Thus we here consider the scattering problem itself. First we define a model which we believe contains all the essentials of the electron-hydrogen ionization problem and yet greatly

reduces the mathematical complexity: we replace the electron-electron repulsion $\frac{2}{r_{12}}$ (in rydberg units which we use throughout) by $2/(r_1+r_2)$:

$$\frac{2}{r_{12}} \rightarrow \frac{2}{r_1+r_2} \tag{1.1}$$

and thereby reduce the S-wave Schrodinger equation to a two-dimensional partial differential equation[3]. As a result the excited spectrum of target states contain only s-states and loses the ℓ degeneracy associated with the complete hydrogenic spectrum. Nevertheless the long range dipole potential which the scattering particle sees is retained in the model. These and other characteristics will become clear as we go along.

In Section II we consider the scattering problem starting from a general close coupling expansion. We show that because of the nature of the spectrum of $Q_N H Q_N$ that for N large the optical potential starts to contain repulsive terms even when all the coupling is included. This is our most important rigorous observation. We shall also argue (Section II) that for purposes of evaluating inelastic scattering matrix elements, we can neglect the coupling terms, i.e. in effect we are considering a distorted wave approximation and that is our most important approximation.

The direct potential (Hpp) problem is considered in Section III. Here we can introduce some benign approximations which allow analytic solutions to be given, which are nevertheless essential for a cogent analysis of what happens in the limit

$N \to \infty$. Basically these are the zero energy solutions in a Coulomb and in a dipole potential.

The optical potential is examined in Section IV. We consider three approximations: a lowest term approximation; an effective intermediate state (dominant pole) approximation; and an effective energy or closure approximation. In Section V the threshold law for these various approximations is worked out, and some discussion of the results is given including comparison with other recent approaches to the problem based on Wannier[4].

II. A MODEL OF THE ELECTRON-HYDROGEN INTERACTION AND THE SCATTERING PROBLEM

We consider the Schrodinger equation (rydberg units throughout)

$$H\Psi_N = E\Psi_N \tag{2.1}$$

for model corresponding to (1.1). The Hamiltonian is given by

$$H = -\frac{1}{r_1}\frac{\partial^2}{\partial r_1^2} r_1 - \frac{1}{r_2}\frac{\partial^2}{\partial r_2^2} r_2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_1 + r_2}$$

and we expand the solution in two parts

$$\Psi_N = \underset{N-N}{P\Psi} + Q_N \Psi_N \tag{2.3}$$

corresponding to open channels,

$$P\Psi_N = \sum_{n=1}^{N} \frac{u_n(r_1)}{r_1} \varphi_n(r_2) + (1 \rightleftarrows 2) \tag{2.4}$$

and closed channels

$$Q\Psi_N = \left(\sum_n + \int\right) \frac{u_n(r_1)}{r_1} \varphi_n(r_2) + (1 \rightleftarrows 2) \tag{2.5}$$

for a total energy E where

$$E_N \leq E \leq E_{N+1} \tag{2.6}$$

with E_N being the energy of N^{th} excited state of hydrogen

$$E_N = -\frac{1}{N^2} \tag{2.7}$$

[We consider for the present only singlet solutions giving rise to only the + sign in (2.4) and (2.5).] The functions $u_n(r)$ are to be determined; the target states $\phi_n(r)$ are S eigenstates of the

of the hydrogen atom:

$$\phi_n(r) = \frac{1}{r} R_n(r) \tag{2.8}$$

As is by now well known, an equation equivalent to the Schrodinger equation can be derived[5] for the open channel wave function $P\,\underline{\Psi}_N$

$$[P\ HP + \mathcal{V}_{opt}^{Q} - E]\ P\underline{\Psi}_N = 0, \tag{2.9}$$

where the Q-part of the optical potential is given by

$$\mathcal{V}_{opt}^{Q} = P\ HQ\ \frac{1}{E - Q\ HQ}\ Q\ HP \tag{2.10a}$$

For use in Appendix C we define the Q-space Green's function in the above equation.

$$G^{Q} = \frac{Q}{E - Q\ HQ} \tag{2.10b}$$

Explicit forms for P and Q can be given as simple generalizations of the formulas for N=1[6]

$$Q = Q_1\ Q_2\ , \tag{2.11a}$$

where

$$Q_i = 1 - \sum_{n=1}^{N} \phi_n(i) \rangle\langle \phi_n(i)\ , \tag{2.11b}$$

and as usual

$$P = 1 - Q\ . \tag{2.12}$$

However we shall not need them, as our functions will be constructed to be manifestly in P or Q space.

In this and many other contexts it is most convenient to expand the optical potential in terms of the eigenfunctions of $Q\ HQ$:

$$Q\,HQ\,\Phi_{N\nu} = \mathcal{E}_{N\nu}\Phi_{N\nu}, \tag{2.13}$$

where the eigenfunctions $\Phi_{N\nu}$ are understood to be in Q space:

$$Q\,\Phi_{N\nu} = \Phi_{N\nu} \tag{2.14}$$

Using (2.13) we obtain the spectral representation of the (Q-part of) the optical potential

$$V_{opt}^{Q} = \frac{\langle P_N HQ\Phi_{N\nu}\rangle\langle Q\Phi_{N\nu} HP_N\rangle}{E - \mathcal{E}_{N\nu}} \tag{2.15}$$

The expansion (2.15) is not only useful, but it manifests many features of interest. For example in scattering from low lying states the fact that the numerator of (2.15) is positive definite taken together with the fact that the lowest states of QHQ are just slightly below the next inelastic threshold (=> $E-\mathcal{E}_{N\nu}<0$ for $E\simeq E_N$) implies that the optical potential is negative definite (i.e. attractive) and this is the basis for lower bound principles for the scattering phase shifts[6,7].

However, this is a situation that only obtains for low-lying N as Table I shows. There we have computed

$$\mathcal{E}_N = \langle\Phi_N H\Phi_N\rangle = \frac{2}{N^2} + \langle\Phi_{N\nu}\frac{2}{r_1+r_2}\Phi_{N\nu}\rangle \tag{2.16}$$

for

$$\Phi_N = \varphi_N(r_1)\,\varphi_N(r_2) \tag{2.17}$$

and we see that $\mathcal{E}_N < E_{N-1}, E_{N-2}, E_{N-\mu}$ whenever $\mu\simeq\frac{1}{9}N$.

In other words the lowest eigen value associated with higher N' states can descend below the N^{th} threshold, and when this happens the contribution of those terms to the optical potential

is repulsive. This does not prove that the effect of the whole optical potential will be repulsive, but it does suggest that it may be repulsive, and that in any event its effect will have to be considered very carefully.

On the right hand side of Table I we have given similar results for the full interaction, $V=2/r_{12}$, in which case Φ_N refers to a configuration interaction wave function[1]

$$\Phi_N^{(j)} = \sum_{\ell=0}^{N-1} C_{N\ell}^{(j)} \phi_{N\ell}(r_1)\phi_{N\ell}(r_2)P_\ell(\cos\theta_{12})$$

and the linear combination giving the lowest energy is given (j=1). Details of this calculation are given in Ref. 1. The point of showing those results is to demonstrate that the lowering of QHQ eigenvalues below lower N states is a property of the full e-H problem and not simply of the model. Indeed the Table shows that the model is remarkably accurate.

Finally it should be realized that in the model (and correspondingly in the complete interaction case) there are many other linear independent functions in Q space, for example

$$\Phi_{N,N+1} = \frac{2^{-1/2}}{r_1 r_2}\left[R_N(r_1)R_{N+1}(r_2) + (1 \rightleftarrows 2)\right],$$

which have similar type of spectral properties going over finally to the purely dipole type states (labelled $\psi_D^{(N)}$ in Ref. 1) in which the outer electron sees the induced dipole moment from the inner electron and the nucleus. Here too, there are an infinity of states but that spectrum probably always remains between E_{N-1} and E_N.

III. THE DIRECT POTENTIAL PROBLEM

The Hpp problem, i.e.,

$$[P\,HP - E_N]P\Psi_N = o \tag{3.1}$$

is itself a complicated problem by virtue both of the coupling between different open channels as well as the exchange terms associated with $P\Psi_N$. The latter, however, involve the same type of integral terms as those coming from the optical potential without involving the small energy denominators. Thus they are negligible in this context (although it should be recalled that they are essential even for qualitative purposes in low energy elastic scattering from the ground state to give the right nodal structure to the scattered orbital).

The coupling terms in (3.1) involve terms of the form $V_{nm}(r_1)U_m(r_1)$ and assuming n and m are of the order of N then $V_{n\,m} \lesssim \frac{(n-m)}{N^3}$ for all values of r. In perturbation theory these potentials are to be divided by the energy differences which are also of the order $\sim\frac{(n-m)}{N^3}$. But the energy differences are of both signs, thus it is not unreasonable to assume that a kind of random phase phenomenon will ensue in which the various terms will have a cancelling effect on each other. Furthermore, it must be recalled that the physical distance between the various N shells, $\langle N/r/N\rangle - \langle N+1/r/N+1\rangle \propto N$, actually increases with N. Finally it should be realized that the wave function we are attempting to calculate is to be used in an integral expression for the inelastic amplitude. This is consistent with the philosophy of the

distorted wave approximation that the integral expression corrects to some extent for the inadequacies of the approximations of the wave functions that one puts into it. None of these arguments, however, is intended to imply that the omission has been rigorously justified.

The Hpp equation becomes in this approximation

$$\left[\frac{d^2}{dr^2} - V_{N,N}^{(r)} + k_N^2\right] u_N(r) = o \tag{3.2}$$

where

$$k_N^2 = E - E_N \tag{3.3}$$

and

$$V_{N,N}^{(r)} = \langle R_N(r_2) | \frac{-2}{r_1} + \frac{2}{r_2+r} | R_N(r_2) \rangle \tag{3.4}$$

$$= \frac{-2}{r_1} + v_{NN}(r) \tag{3.5}$$

Little v_{NN} is then the diagonal element of the electron-electron repulsion and it alone survives in off-diagonal elements

$$V_{NM}(r) = v_{NM}(r) = \langle \varphi_N(r_2) | \frac{2}{r_2+r} | \varphi_M \rangle \Big|_{N \neq M} . \tag{3.6}$$

Although the potentials in their entirety are complicated their effect in our application can be simply approximated by (N=M)

$$V_{N,N}(r) \cong \begin{cases} -\frac{2}{r} & r < r_0 \\ -\frac{b_N}{r^2} & r > r_0 \end{cases} \tag{3.7}$$

where r_o is the mean radius of the N^{th} state

$$r_o = \langle N|\mathbb{r}|N\rangle = \frac{3}{2} N^2, \tag{3.8}$$

and b_N the dipole moment :

$$-\frac{2}{r} + \frac{2}{r+r_2} \xrightarrow[r>r_2]{} \frac{b_N}{-r^2} + O(r^{-3}) \tag{3.9}$$

where

$$b_N = 2r_o = 3N^2. \tag{3.10}$$

The approximation of $V_{N,N}$ enables a solution of (3.7) to be analytically determined:

$$u_N^{(0)}(r) = \begin{cases} \left(\frac{r}{2}\right)^{1/2} J_1(\sqrt{8r}) & r < r_0 \\ r^{1/2}\left[A \sin(\alpha_N \ln r) + B \cos(\alpha_N \ln r)\right] & r > r_0 \end{cases} \tag{3.11a}$$

where

$$\alpha_N = \sqrt{b_N - \frac{1}{4}} \tag{3.12}$$

for $k_N = 0$ corresponding to the usual procedure of multiplying the solution by a k_N dependent normalization factor to properly take care of both the k_N dependence and the normalization to a plane wave at infinity (see below).

On matching function and derivative at $r=r_o$ and using the well known asymptotic form[8] of J_1, one obtains to leading order (for $r \gg 1$)

$$u_N^{(0)}(r) \simeq \begin{cases} \frac{r^{1/4}}{\sqrt{2\pi}(2)^{1/2}} \cos\left(\sqrt{8r} - \frac{3\pi}{4}\right) & r < r_0 \\ \frac{r^{1/2}}{\sqrt{2\pi}(2r_0)^{1/2}} \cos\left(\alpha_N \ln\left(\frac{r}{r_0}\right) + \sqrt{8r_0} - \frac{3\pi}{4}\right) & r > r_0 \end{cases} \tag{3.11b}$$

IV. APPROXIMATIONS OF THE OPTICAL POTENTIAL

We consider here three approximations of the optical potential.

(i) The first includes only the lowest energy term coming from the

$$\bar{\Phi}_{N+1} = \mathcal{Q}\,\Phi_{N+1} = \varphi_{N+1}^{(r_1)}\,\varphi_{N+1}^{(r_2)} \tag{4.1}$$

Substitution of this into (2.15) gives rise to an integro-differential equation.

$$\left[\frac{d^2}{dr^2} - V_{N,N}(r)\right] u_N(r) - \frac{R_{N+1}(r)\, V_{N,N+1}(r) \langle \varphi_{N+1}\, V_{N,N+1} \frac{u_N}{r} \rangle}{E - \mathcal{E}_{N+1}} = 0 \tag{4.2}$$

In this case because we have a separable kernel, the solution is given by

$$u_N(r) = u_N^{(0)}(r) + C\, u_N^{(1)}(r) \tag{4.3}$$

where $U_N^{(o)}(r)$ is the homogeneous solution Eq. (3.11), $U_N^{(1)}$ is a solution of the homogeneous eq.

$$\left[\frac{d^2}{dr^2} - V_{N,N}(r)\right] u_N^{(1)}(r) = -V_{N,N+1}(r)\, R_{N+1}(r) \tag{4.4}$$

and C can be solved for to be

$$C = \frac{-K^{(o)}}{E - \mathcal{E}_{N+1} + K^{(1)}}, \tag{4.5}$$

with

$$K^{(o)} = \int_0^\infty R_{N+1}(r)\, V_{N,N+1}(r)\, u_N^{(0)}(r)\, dr \tag{4.6}$$

and

$$K^{(1)} = \int_0^\infty R_{N+1}(r)\, V_{N,N+1}(r)\, u_N^{(1)}(r)\, dr \tag{4.7}$$

The coupling potential $V_{N,N+1}$, Eq. 3.6) is also a complicated function which can simply be approximated:

$$V_{N,N+1}(r) \cong 0.8\, N^{-2}\left[1 + 2(r/r_0)\right]^{-2} \qquad (4.8)$$

In Figure 1 we plot $N^2 V_{N,N+1}$ vs. r for two values of N exactly calculated from (3.6) together with the approximation (4.8). ——>

——> The convergence as a function of N can be appreciated by our pointing out that the difference between N=10 and N=11 results would be indistinguishable on the graph. The fit of (4.8) is not perfect around $r/r_0 \approx .5$, however, our results below are not affected. A better fit can be obtained with

$$V_{N,N+1} \cong \sqrt{2}\, N^{-2}\left[2\sqrt{1.633 + (r/r_0)} - \sqrt{1.266 + (r/r_0)} + \sqrt{r/r_0}\right]$$

The solution of the $U_N^{(1)}$ equation, (4.4), is effected with a Green's function technique

$$U_N^{(1)}(r) = \int_0^\infty G(r,r')\left[-R_{N+1}(r')\, V_{N,N+1}(r')\right] dr' \qquad (4.9)$$

where the Green's function is

$$G(r,r') = (-2\Pi)\, U_N^{(0)}(r_<)\, v_N^{(0)}(r_>), \qquad (4.10)$$

and v_N is (any) irregular solution of the homogeneous equation. We choose the complementary form of (3.11) whose asymptotic form is

$$v_N^{(0)}(r) \cong \begin{cases} \dfrac{r^{1/4}}{\sqrt{2\pi}(2)^{1/2}} \sin\left(\sqrt{8r} - \dfrac{3\pi}{4}\right) & r < r_0 \\[2ex] \dfrac{r^{1/2}}{\sqrt{2\pi}(2r_0)^{1/2}} \sin\left[\alpha_N \ln\left(\dfrac{r}{r_0}\right) + \sqrt{8r_0} - \dfrac{3\pi}{4}\right] & r > r_0 \end{cases} \qquad (4.11)$$

The details of the quadrature involved in (4.8) are given in Appendix A. The result is ($r<r_o$)

$$U_N^{(1)} = U_N^{(o)}(r)\,II(r) + v_N^{(o)}(r)\,I(r) \tag{4.12}$$

where I(r) and II(r) are given in (A.7) and (A.10).

The evaluation of the N dependence of $K^{(o)}$ is exceedingly simple. One finds

$$K^{(o)} \propto \frac{1}{N^{1/2}} \tag{4.13}$$

The N dependence of $K^{(1)}$ is derived in Appendix B:

$$K^{(1)} \propto \frac{C_1 + C_2 \sin(2\sqrt{12}\,N\pi)}{N^2} \tag{4.14}$$

In order finally to evaluate C of Eq. (4.5) and thus $U_N(r)$ of (4.2) we need to know the energy differences $E - \mathcal{E}_{N+1}$. The total energy, as was indicated, is taken as that energy to excite the N^{th} level

$$E \to E_N = -\frac{1}{N^2}\,, \tag{4.15}$$

and from Table I we find that $\mathcal{E}_{N+1}$ can be well fit by

$$\mathcal{E}_{N+1} \simeq -\frac{1.27}{(N+1)^2} \tag{4.16}$$

To lowest order therefore

$$E_{N+1} - \mathcal{E}_{N+1} \simeq \frac{.27}{N^2} + O\left(\frac{1}{N^3}\right) \tag{4.17}$$

The function $U_N(r)$ in the region $r \sim r_o$ is dominated by the term $v_N^{(o)}(r)\,I(r)$ by noting that for $r \sim r_o$

$$I(r) \propto \frac{1}{N^{1/2}} \tag{4.18}$$

as opposed to $II(r) \propto N^{-3/2}$ [using (A.11) and (A.12)]. Thus putting these behaviors together we find

$$\lim_{N\to\infty} u_N(r)\Big|_{r\cong r_0} \approx \beta_1(N)\, v_N^{(0)}(r) \tag{4.19}$$

where

$$\beta_1(N) \equiv \frac{CN}{1-B\sin(2\sqrt{12N}\pi)} \tag{4.20}$$

The above is the essence of the $P\underline{\psi}_N$ contribution to the wave function, however the total wave function includes a contribution $Q\underline{\psi}_{-N}$. This may be derived from $P\underline{\psi}_N$ using the relation

$$Q\underline{\psi} = \frac{1}{E-QHQ}\, QHP\underline{\psi} \tag{4.21}$$

Eq. (4.21) is the first step in deriving the optical potential[5] equation (2.9) from the Schrodinger equation (2.1). For the one term approximation that we are here considering, (4.21) reduces to

$$Q\Psi = \langle \underline{\Phi}_{N+1} \Big| \frac{2}{r_1+r_2} \Big| \frac{u_N(r_1)}{r_1}\varphi_N(r_2)\rangle\, \underline{\Phi}_{N+1}\,(E-\mathcal{E}_{N+1})^{-1} \tag{4.21b}$$

where Φ_{N+1} is given in (4.1). The integral reduces to

$$\langle \underline{\Phi}_{N+1} \Big| \frac{2}{r_1+r_2} \Big| \frac{u_N(r_1)}{r_1}\varphi_N(r_2)\rangle = \int_0^\infty \bar{R}_{N+1}(r)\, V_{N,N+1}(r)\, u_N(r)\, dr, \tag{4.22}$$

and using (4.19) for $U_N(r)$ reduces this to a form involving $K^{(0)}$ and $K^{(1)}$. One finds in fact

$$Q\Psi = \beta_1(N)\, \underline{\Phi}_{N+1} \tag{4.23a}$$

where

$$\beta_1(N) = N^2\left[K^{(0)} + \sqrt{N}\,\beta_1(N)\,K^{(1)}\right] \tag{4.23}$$

which upon substitution reduces to

$$q_1(N) = N^{3/2}\left[\frac{C_1 - C_2 \sin(2\sqrt{12}\,N\pi)}{B_1 - B_2 \sin(2\sqrt{12}\,N\pi)}\right] \tag{4.24}$$

where the C's and B's are constants which can in principle be determined.

The threshold law is derived for this as well other approximations of the optical potential in the next section.

(ii) The second approximation we shall consider is motivated by the observation the optical potential (2.15) is (formally) dominated by states $\mathcal{E}_{N\nu} = E$ (dominant pole approximation). The actual states for which

$$\mathcal{E}_{N+\mu} = E_N \tag{4.25}$$

are readily deduced from (4.15) and (4.16) to be

$$\mu = .12\ N \tag{4.26}$$

[Cf. below Eq. (2.17)]. In other words we consider an optical potential based on one intermediate state

$$\Phi_{N+\mu} = \frac{1}{r_1 r_2} R_{N+\mu}(r_1) R_{N+\mu}(r_2) \tag{4.27}$$

Because the energy denominator vanishes (to order N^2) in this case, $p_2(N)$ may be simply gotten by putting $E = \mathcal{E}$ in (4.5). Then using (4.19) we see that

$$p_2(N) = \frac{1}{\sqrt{N}} \frac{K^{(0)}}{K^{(1)}} \propto \frac{N}{C_1 + C_2 \sin(2\sqrt{12}\,N\pi)} \tag{4.28a}$$

On the other hand $q_2(N)$ must be evaluated more carefully, because the expression (4.21) is indeterminate. One finds

$$q_2(N) \propto \frac{K^{(0)}}{K^{(11)}} \propto \frac{N^{3/2}}{C_1 + C_2 \sin(2\sqrt{12}\,N)} \qquad (4.28b)$$

The relation (4.19) for $U_N(r)$ applies in this case also.

(iii) Finally we consider a closure approximation; the intermediate energies in (2.15) are replaced by a mean energy so that

$$\mathcal{V}_{op}^{Q} \to \frac{1}{E-\bar{\mathcal{E}}_N} \sum_{\nu} P\,HQ\Phi_{N\nu}\rangle\langle Q\Phi_{N\nu}HP = \frac{1}{E-\bar{\mathcal{E}}_N} PHQ^2HP$$

$$= \frac{1}{E-\bar{\mathcal{E}}_N} PH(Q)HP \qquad (4.29)$$

$$\doteq \frac{1}{E-\bar{\mathcal{E}}_N} PV(1-P)VP\ ,$$

since $[P, H_0] = 0 = PQ$.

In the uncoupled approximation, P reduces to

$$P \to \varphi_N \rangle\langle \varphi_N$$

The optical potential $\mathcal{V}_{op}^{Q}$ of (2.10) becomes

$$\mathcal{V}_{op}^{Q} = \frac{1}{E-\bar{\mathcal{E}}_N} [PV^2P-(PVP)^2]\,, \qquad (4.30)$$

where

$$V = -\frac{2}{r_1} + \frac{2}{r_1+r_2} \qquad (4.31)$$

Based on an approximation similar to that used to derive the form (3.7) for V_{NN}, we can show (Appendix C)

$$\langle R_N(r_2) \mid V^2 \mid R_N(r_2) \rangle \simeq \begin{cases} 4/r_1 & r_1 < r_0 \\ 10N^4/r_1^4 & r_1 > r_0 \end{cases} \quad (4.32)$$

Therefore, with use of (3.7) for V_{NN}, (4.30) becomes

$$V_{op}^{Q} \simeq \begin{cases} 0 & r_1 < r_0 \\ \dfrac{N^4}{E - \bar{E}_N} \dfrac{1}{r_1^4} & r_1 > r_c \end{cases} \quad (4.33)$$

The N-dependence of $\bar{E}_N$ may be estimated variationally (Appendix C) to give

$$\bar{E}_N \propto \frac{1}{N^2} \quad (4.34)$$

Our approximations are not sufficiently accurate for either the sign or the N-dependence of the energy difference $E_N - \bar{E}_N$ occurring in (4.33) to be determined. The best we can do is to limit the difference by

$$|E_N - \bar{E}_N| \leq O(\frac{1}{N^2}) \quad (4.35)$$

This gives rise to an effective local potential for the scattering function

$$[\frac{d^2}{dr^2} + V_c(r)]\, u_N(r) = 0 \quad (4.36)$$

where

$$V_c(r) = \begin{cases} 2/r & r < r_0 \\ \dfrac{-N^4}{(E_N - \bar{E}_N) r^4} & r_0 < r < r_\beta \\ b_N/r^2 & r > r_\beta \end{cases} \quad (4.37)$$

In (4.37) we have made the assumption that the optical potential in fact exceeds the dipole potential in some finite region (i.e. $r_\beta > r_o$), where r_β may be determined by the condition

$$N^4 / |(E_N - \bar{E}_N) r_\beta^4| = b_N / r_\beta^2 \qquad (4.38)$$

which leads to

$$r_\beta = \frac{N}{\sqrt{3|E_N - \bar{E}_N|}} \qquad (4.39)$$

If (4.39) does not lead to $r_\beta > r_o$, then the equation and solution revert back to $U_N^{(o)}$ of Eq. (3.11b).

The solutions of (4.36) must again be determined by matching and one finds to lowest order $r < r_o$

$$U_N^{(\beta)}(r) = U_N^{(o)}(r) \qquad (4.40a)$$

and for $r_o < r < r_\beta$

$$U_N^{(\beta)}(r) \cong \begin{cases} \dfrac{r}{\sqrt{2\pi(2)^{1/2}}} \dfrac{\cos\left[\sqrt{8 r_o} + \beta\left(\frac{1}{r} - \frac{1}{r_o}\right) - \frac{3\pi}{4}\right]}{r_o^{3/4}} & E_N - \bar{E}_N > 0 \\ \dfrac{r}{\sqrt{2\pi(2)^{1/2}}} \dfrac{\cos\left(\sqrt{8 r_o} - \frac{3\pi}{4}\right) \cosh\left[\beta\left(\frac{1}{r} - \frac{1}{r_o}\right)\right]}{r_o^{3/4}} & E_N - \bar{E}_N < 0 \end{cases} \qquad (4.40b)$$

where

$$\beta^2 = \frac{N^4}{|E_N - \bar{E}_N|} \qquad (4.41)$$

The solutions for $r > r_\beta$ go into the general form of the dipole potential given in the lower part of Eq. (3.11a). The coefficients are again determined by matching, but we shall not consider them further.

V. THRESHOLD LAWS

Threshold laws are calculated from the expression[1]

$$\mathcal{Y} = \int_0^E k_N |\eta|^2 |M.E.|^2 N^3 d\omega_N \tag{5.1}$$

$\mathcal{Y}$ is the yield as a function of the available energy E after ionization. M.E. is a matrix element

$$M.E. = \langle \Psi_N | V | \Phi_{initial} \rangle \tag{5.2}$$

which causes the transition from the unperturbed initial state

$$\Phi_{initial} = (\sin kr_1/kr_1)\, \varphi_{N=1}(r_2) \tag{5.3}$$

to a final state Ψ_N the calculation of which we have discussed in the previous sections. The quantity η is a normalization constant which adjusts the U_N to be a plane wave at $r_1 \to \infty$. η was evaluated in the appendix of Ref. 1

$$\eta = \frac{(r_m \alpha_N / k_N)^{1/2}}{|u_N(r_m)| \sqrt{\alpha_N^2 + (r_m \mathcal{R}(r_m) - 1/2)^2}} \tag{5.4}$$

It should be noted the factor $\alpha_N^{1/2}$ was omitted in Ref. 1. (We are indebted to A.K. Bhatia for finding the error[9].) From (3.12) we see that

$$\lim_{N\to\infty} \alpha_N = \sqrt{3}\, N \tag{5.5}$$

and in (5.4)

$$\mathcal{R}(r_m) \equiv u_N'(r_m)/u_N(r_m), \tag{5.6}$$

where r_m a matching radius beyond which only the dipole potential b_N/r^2 and the outgoing energy k_N^2 enter the equation for U_N. The point is that the k_N dependence of U_N is completely absorbed in η and the calculation for U_N are done at $k_N=0$.

In order to arrive at the ionization region we have assumed an analytic continuation of the inner electron's energy from $E_N = \frac{-1}{N^2}$ [Eq. (2.7)] to $\omega_N = +\frac{1}{N^2}$

$$E_N \to \omega_N = \frac{1}{N^2} \tag{5.7}$$

This continuation is motivated by the well-known fact that a Coulomb wave for negative energy becomes a positive energy solution by changing $N \to -i/\omega_N$, in the confluent hypergeometric function[8].

The threshold laws are then derived from (5.1) wherein from (5.4) the explicit k_N dependence cancels out, and the remaining part of the integrand is converted to a function of ω_N via (5.7), so that integration gives the E dependence of $\mathcal{L}$ which is what we are seeking.

To gain confidence in the analytic continuation - let us consider as an example, the homogeneous solution of the Hpp problem, i.e. $U_N^{(o)}$ given in Eq. (3.11b). Here the matching radius is naturally taken as r_o:

$$r_m = r_o \tag{5.8}$$

so that to leading order

$$\frac{d\,U_N^{(o)}}{dr} = \frac{\sqrt{2}}{r_o^{1/4}} \frac{\sin(\sqrt{8 r_o} - 3\pi/4)}{\sqrt{2\pi(2)^{1/2}}}$$

and

$$\mathcal{L}_0(r_o) = \frac{\sqrt{2}}{r_o^{1/2}} \tan\left(\sqrt{8 r_o} - \frac{3\pi}{4}\right)$$

Thus using (5.5) and (5.8) for the N-dependence of r_o and α_N we find

$$\eta \propto \frac{(r_o \alpha_N / k_N)^{1/2}}{r_o^{1/4} \cos(\sqrt{8 r_o} - \frac{3\pi}{4}) \alpha_N \sqrt{1 + \tan^2(\sqrt{8 r_o} - \frac{3\pi}{4})}}$$

or finally,

$$\eta \propto \frac{r_o^{1/4}}{\sqrt{k_N}\, \alpha_N^{1/2}} \propto \frac{1}{\sqrt{k_N}}$$

What is nice is that the oscillating factors in the denominator cancel away; we shall find this to be essentially always the case as regards η.

The remaining piece of the integrand is the matrix element which in this approximation is

$$M_o \equiv \left\langle \frac{u_N^{(o)}(r_1)}{r_1} \varphi_N(r_2) \,|\, V \,|\, \Phi_{initial} \right\rangle \qquad (5.9a)$$

In Appendix D we show

$$M_o \propto N^{-3/2} \qquad (5.9b)$$

With M.E. being M_o in this case and substituting for η, we find

$$\mathcal{L}_o \propto \int_0^E k_N \left[\frac{1}{\sqrt{k_N}} \frac{1}{N^{3/2}} \right]^2 N^3 \, d\nu_N \propto \int_0^E d\nu_N$$

or

$$\mathcal{L}_o \propto E \qquad (5.10)$$

A linear law is precisely what we expect in this approximation in which the potential felt by the outer electron is purely Coulombic on the inside and attractive dipole on the outside. For it is now well known that the latter also causes a finite inelastic cross section at threshold[10], and this is guaranteed in our formulation by the normalization constant η. (The subscript on $\mathcal{L}$ will attempt

to specify the particular approximation used.)

We next consider the lowest term and dominant pole approximations of the optical potential. In these cases the matrix element contains a part from Q-space (the term multiplied by $q_i(N)$ below) in addition to the P-space contribution:

$$M.E.=[1+N^{-3/2}q_i(N)]M_o+p_i(N)M_1. \tag{5.11}$$

The index i=1,2 specifies the two approximations. M_1 is the part of matrix element coming from the irregular solution part of U_N:

$$M_1=\langle \frac{U_N^{(1)}(r_1)}{r_1}\phi_N(r_2)|V|\phi_{initial}\rangle \tag{5.12}$$

$U_N^{(1)}(r)$ is given in (4.12). Although M_1 is more difficult to calculate exactly we have shown in Appendix D that

$$M_1 \leq \frac{1}{N^3} \tag{5.12b}$$

From (4.20) and (4.28a) we see that $p_1(N)$ and $p_2(N)$ are essentially proportional to N thus $p_i(N)M_1$ is smaller than the M_o term of (5.11). Concerning the evaluation of η the dominant term of U_N is dominated by $p_i(N)$ [Eq. 4.19] which one power N larger than in the $U_N^{(o)}$ case. On the other hand the logarithmic derivative is the same

$$f_1(r_o) \simeq \sqrt{2}\, r_o^{-1/2} \cot(\sqrt{8}r_o - 3\pi/4) \tag{5.13}$$

aside from the interchange of sine and cosine factors. The same interchange is true for $U_N^{(1)}$ vs. $U_N^{(o)}$; therefore the oscillating factors continue to cancel out and we are left with

$$\eta_1 \propto \frac{1}{k_N^{1/2} N} \left|1 - B\sin\left(2\sqrt{12N}\right)\right| \tag{5.14}$$

In comparison with η this normalization constant is dominated by the N in the denominator which causes the threshold to be contain an extra power of $E^{1/2}$

$$2_1 \propto \int_0^E w\left[1 - B\sin\left(2\sqrt{\frac{12}{w}}\right)\right]^2 dw$$

which to leading order is

$$2_1 \propto E^2 \tag{5.15}$$

This result is at first sight very unexpected. However, from the point of view of the lowest optical potential term approximation, wherein we have shown that this term is rigorously repulsive, the result is seen to be reasonable consequence of the repulsive optical potential term retained. In the dominant pole approximation, in which the term selected is at the border line between attraction and repulsion, the physical origin of the result is not clear. This is particularly true because the shift, $K^{(1)}$ of Eq. (4.14), is also very likely to be an oscillating function of N. [We have, together with Dr. Bhatia, numerical solutions of the exact lowest term eqs. up to N≃9 which indicates that this is the case.] The lesson to be learned is whether we understand or not the optical potential can be expected to have a profound effect on the threshold law.

We finally consider the closure approximations. Here we have the possibility of many results in view of our ignorance of the

sign and the exact N-dependence of $E_N - \bar{\mathcal{E}}_N$ even within the confines of (4.35). We shall subdivide these into attractive and repulsive cases, both with the assumption that the β^2/r^4 potential is stronger than the b_N/r^2 in the region $r_o<r<r_\beta$ [i.e. $r_\beta>r_o$ from (4.31)].

In the attractive case we find, using the upper solution of (4.40),

$$\eta \propto N/(\sqrt{\bar{\kappa}_N}\, r_\beta^{1/2}) \tag{5.16}$$

Furthermore we have shown in Appendix D that the N dependence of the matrix element is not altered by the contribution of $U_N^{(\beta)}$ from $r_o<r<r_\beta$ providing $E_N - \bar{\mathcal{E}}_N \propto N^{-2}$.

$$M.E. \propto M_o \propto N^{-3/2} \tag{5.17}$$

Thus substituting gives

$$\mathcal{Q}_1 \propto \int_0^E \frac{N'^2}{r_\beta}\, d\omega_N \tag{5.18}$$

And now considering, as implied above,

$$E_N - \bar{\mathcal{E}}_N \propto -\frac{1}{N^2}, \tag{5.19}$$

which implies from (4.39)

$$r_\beta \propto N^2, \tag{5.20}$$

gives using (5.7) in (5.18):

$$\mathcal{Q}_{1a} \propto E \tag{5.21}$$

Another conceivable alternative would be for example, $E_N - \bar{\mathcal{E}}_N \propto N^3$. For this case the matrix element would be dominated by

the $Q\Psi$ part of Ψ, as shown in Appendix D. The net effect would be to give an $E^{1/4}$ threshold which we shall not pursue further.

Penultimately we consider the repulsive closure approximations corresponding to $U_N^{(\beta)}$ of (4.40b). Here the normalization constant turns out to be

$$\eta_2 \propto \frac{N}{\sqrt{r_N}\, r_\beta^{1/2} \left|\cos\left(\sqrt{8} r_0 - \frac{3\pi}{4}\right)\right| \cosh\left[\beta\left(\frac{1}{r_\beta} - \frac{1}{r_0}\right)\right]} \tag{5.22}$$

The cosh factor in the denominator which appears to dominate η_2 is however, cancelled by a similar factor in the transition matrix element (Appendix D)

$$M.E. \propto \frac{\cos\left(\sqrt{8} r_0 - \frac{3\pi}{4}\right) \ln r_\beta \cosh\left[\beta\left(\frac{1}{r_\beta} - \frac{1}{r_0}\right)\right]}{N^3} \tag{5.23}$$

Using $\frac{\beta}{r_0} \propto N^\gamma$, where $\gamma > 0$ in all cases, we are left with

$$\mathcal{L}_2 \propto \int_0^E \frac{(\ln r_\beta)^2}{r_\beta} w^{-1/2}\, dw$$

If now we restrict ourselves to quadratic dependence of r_β on N specified by (5.20) [albeit now in a repulsive sense], we find

$$\mathcal{L}_2 \propto E^{5/2} (\ln E)^2 \tag{5.25}$$

There is absolutely nothing at this time which prevents the effective optical potential, as contained in the energy difference $E_N - \bar{\xi}_N$ from being an oscillating function of N in sign. From (4.39) we see that $r_\beta \to \infty$ when $E_N - \bar{\xi}_N$ changes signs. Assuming the amplitude of these oscillations is $1/N^2$, we see from (5.18) that attractive portions give a linear rise whereas from (5.24) the repulsive portions are essentially flat. There are of course many analytical functions which can give this type of behavior - an example would be

$$\mathcal{Z}_3 \propto E[1-C\sin(\ln E)] \qquad (5.26)$$

where in order for the slope not to be negative we must have $C \leq 2^{-1/2}$.

A sketch of such a threshold law is given in Figure 2 for C=1/2. It can be seen that such a threshold is distinctly non-linear. In addition its oscillations about the line $\mathcal{Z}=E$ continue right down to origin.

V. DISCUSSION

We have not attempted to derive a unique threshold law. Our purpose in this paper has been to present what we believe is potentially useful and rather different approach to the problem. The approach naturally leads to the optical potential as the key element beyond the obvious potentials that the outermost (scattered) electron sees. We have been able to show rigorously that this optical potential contains repulsive terms, although we have not been able to determine whether the repulsion or attracti dominates in the potential as a whole. The repulsive approximations can lead to a considerable diminution even beyond a simple phase space dependence on E:

$$\mathcal{Q}_{\text{phase space}} \propto \int d^3k_1\, d^3k_2\, \delta(E - k_1^2 - k_2^2) \propto E^2 \qquad (1)$$

Conventional wisdom on the subject might have dictated that we delete those approximations which lead to a higher power than two however, we have included them because we know in other contexts that threshold barriers can have an overwhelming effect on threshold cross sections and we cannot exclude that situation here.

We have not discussed the salient recent work[11,12] which attempts to justify the Wannier law on the basis of a more consistent WKB approach. That work is significant but it is not rigorous. It can be shown in fact that the Wannier threshold law remains the same in that approach[4] when the r_{12}^{-1} interaction with that of our model $(r_1+r_2)^{-1}$. However, the most provocative of our results is the oscillating derivative threshold expressed

in (5.27). It is the possible existence of such a threshold law which makes a reliable calculation $\bar{\mathcal{E}}_N$ an attractive initial endeavor as part of the general problem of synthesing the optical potential in a definitive manner.

APPENDIX A: Evaluation of $u_N^{(1)}$

We wish to compute the function $u_N^{(1)}$ of (4.9) with $G(r,r')$ given by (4.10), $U_N^{(0)}$ by (3.11), $v_N^{(0)}$ by (4.11), $V_{N,N+1}$ by (4.8), and R_{N+1} by a similar asymptotic expansion:

$$R_N(r) \cong \begin{cases} \dfrac{(2r)^{1/4}}{\sqrt{\pi N^3}} \cos\left(\sqrt{8r} - \dfrac{3\pi}{4}\right) & r < 2r_0 \\ C_N e^{-r/N} r^N & r > 2r_0 \end{cases} \qquad (A.1)$$

C_N is the Nth (last) coefficient in the expansion of the R_N (which is rxR_{N0} in the notation of Bethe & Salpeter[8])

$$C_N = \frac{(-1)^{N-1} 2^N}{N^{3/2} N!\ N^{N-1}} \qquad (A.2)$$

It should first be noted that our approximation of $R_N(r)$ is not continuous at $r=2r_0$ and that the part for $r>2r_0$ is the very asumptotic form to be used only in showing that contributions to $u_N^{(1)}(r)$ from $r>2r_0$ are negligible. (Cf. Fig. 3).

It is to be emphasized that the rhs of (A.1) is divided into two regions at $r=2r_0$. The fit of R_N by the rhs of (A.1) is no longer accurate even for $r \simeq r_0$; the well-known but complicated WKB expressions[8] for R_N could be used between the classical turning points 0, $\frac{4}{3}r_0 = 2N^2$, particularly around $r \lesssim r_0$ and they are much more accurate that (A.1). However reference to Figure 3 shows that the exact function is somewhat larger than (A.1) around $r=r_0$ and oscillates more

slowly, it does continue to oscillate beyond $r=r_0$ but it ceases to oscillate and is much smaller than the rhs of (A.1) at $r=2r_0$. For this reason we believe, for integration purposes, these compensating effects are adequately accounted by simply continuing the rhs to $r=2r_0$.

From (4.9)

$$u_N^{(1)} = v_N^{(0)}(r)\, I(r) + u_N^{(0)}\, II(r) \qquad (A.3)$$

with

$$I(r) = 2\pi \int_0^r u_N^{(0)}(x)\, R_{N+1}(x)\, V_{N,N+1}(x)\, dx \qquad (A.4)$$

and

$$II(r) = 2\pi \int_r^\infty v_N^{(0)}(x)\, R_{N+1}(x)\, V_{N,N+1}(x)\, dx \qquad (A.5)$$

Assuming $r<r_0$ and using the equations stated above, we find

$$I(r) \propto \sqrt{N} \int_0^r \frac{x^{1/2}}{(r_0+2x)^2} \cos^2\left(\sqrt{8x} - \frac{3\pi}{4}\right) dx \qquad (A.6)$$

Replacing cosine square factor by its average value (1/2) gives

$$I(r) \propto \sqrt{N} \left\{ -\frac{\sqrt{r}}{r_0 + r} + \frac{1}{\sqrt{2r_0}} \tan^{-1}\sqrt{\frac{2r}{r_0}} \right\} \qquad (A.7)$$

For $r<r_0$ the factor II(r) contains two contributions. We shall show later that the contribution from $2r_0$ to ∞ is negligible, therefore we have contributions from r to r_0 and r_0 to $2r_0$.

The first is

$$II_<(r) \simeq \int_r^{r_0} v_N^{(0)}(x)\, R_{N+1}(x)\, V_{N,N+1}(x)\, dx \qquad (A.8)$$

Making similar approximations as above but retaining the sinusoidal factors, we get

$$\underset{<}{II}(r) \propto \frac{\sqrt{N}}{\xi r_0^2} \int_{\sqrt{r}}^{\sqrt{r_0}} y^2 \sin\left[2\left(\sqrt{8}y - \frac{3\pi}{4}\right)\right] dy \qquad (A.9)$$

The factor ξ is a number of the order $1 \leq \xi \leq 10$ to make up for the fact that the bound

$$r_0^{-2} > (r_0 + 2\chi)^{-2} > (3r_0)^{-2}$$

has also been used in deriving (A.9). Here the sinusoidal factor cannot be dropped because its mean value is zero, but (A.9) can be integrated to give

$$\underset{<}{II}(r) \propto \frac{\sqrt{N}}{r_0^2}\Big\{4\sqrt{8}\left[\sqrt{r_0}\cos\left(2\sqrt{8r_0}\right) - \sqrt{r}\cos\left(2\sqrt{8r}\right)\right] + \left[4/(8r_0) - 2\right]\sin\left(2\sqrt{8r_0}\right) - \left[4/(8r) - 2\right]\sin\left(2\sqrt{8r}\right)\Big\} \qquad (A.10)$$

The expressions (A.10) and (A.7) into (A.3) are to be used in Eq. (4.12). Note that the N dependence of II(r) dominated by the second term and that (for $r \neq r_0$) it is

$$\underset{<}{II}(r) \propto \frac{1}{N^{3/2}} \qquad (A.11)$$

We shall now show that the contribution to II(r) from $r_0 < r < 2r_0$ is of maximum order $N^{-3/2}$. Using the $r \geq r_0$ form of $v_N^{(0)}$ gives for II(r)^

$$\left| \int_{r_0}^{2r_0} v_N^{(0)} R_{N+1} V_{N,N+1}\, dr \right| \propto \left| \int_{r_0}^{2r_0} \frac{r^{1/2}}{r_0^{1/4}} \sin\left[\alpha_N \ln\left(\frac{r}{r_0}\right) + \sqrt{8r_0} - \frac{3\pi}{4}\right] \frac{r_0 R_N(r)}{(r_0 + 2r)^2}\, dr \right|$$

The potential $\frac{r_0}{(r_0+2r)^2}$ being bounded by $\frac{1}{r_0}$ and $R_{N+1}^{(r)}$, being bounded by setting the cosine factor equal to one:

$$R_{N+1} \leq (2r)^{1/4} / \sqrt{\pi N^3}$$

gives, aside from numerical factors,

$$\left| \int_{r_0}^{2r_0} \nu_N^{(e)} R_{N+1} V_{N,N+1} \, dr \right| \leq \frac{1}{\sqrt{N}} \left| \int_0^{\ln 2} e^{-\frac{1}{4}y} \sin[\sqrt{3}Ny + \text{const.}] \, dy \right|$$

where we have let $r = r_0 e^y$. We can extend the integral on the rhs to ∞, since the major contribution comes from y small. Thus

$$\left| \int_{r_0}^{2r_0} \nu_N^{(e)} R_{N+1} V_{N,N+1} \, dr \right| \leq \frac{1}{\sqrt{N}} \left| \int_0^{\infty} e^{-\frac{1}{4}y} \sin[\sqrt{3}Ny + \text{const.}] \, dy \right|$$

$$\leq \frac{1}{\sqrt{N}} \frac{\sqrt{3}N}{\frac{1}{16} + (\sqrt{3}N)^2} = O\left(\frac{1}{N^{3/2}}\right)$$

This is the same N dependence as $\Pi_<(r)$; we are left with

$$\lim_{N\to\infty} \Pi(r) = \Pi_<(r) = C\left(\frac{r}{N^{3/2}}\right)$$

We next show that the contribution to II(r) (and also for the similar contribution to I(r)) from $2r_o<\chi<\infty$ is truly negligible. Using (A.1), (4.8), (3.11) or(4.11), we find

$$\int_{2r_0}^{\infty} \begin{Bmatrix} u_N^{(c)} \\ v_N^{(s)} \end{Bmatrix} V_{N,N+1} R_{N+1}\, dr \simeq \frac{C_{N+1}}{r_0^{1/4}} N^2 \int_{2r_0}^{\infty} r^{1/2} \begin{Bmatrix} \sin \\ \cos \end{Bmatrix} \left[\alpha_N \ln\left(\frac{r}{r_0}\right) + \sqrt{8 r_0} - \frac{3\pi}{4}\right] \times \frac{e^{-r/N+1}}{r^2} r^{N+1}\, dr$$

Use of $r_o \propto N^2$ shows the rhs is bounded by

$$\leq N^{3/2} C_{N+1} \int_{2r_0}^{\infty} e^{-\frac{r}{N+1}} r^N dr$$

Below we drop factors N^ν where ν is any number independent of N

$$\doteq 2^N e^{-2r_0/N} 3^{N(N+1)} N^{2N+1}/(N!\,N^N)$$

which using Stirling's formula is

$$\propto e^{N(\log 6 - 2)} \simeq e^{-.21N}$$

or finally

$$\int_{2r_0}^{\infty} \begin{Bmatrix} u_N^{(c)} \\ v_N^{(s)} \end{Bmatrix} V_{N,N+1} R_{N+1}\, dr \leq e^{-.21N}$$

That is smaller than any inverse power of N.

APPENDIX B: Evaluation of $K^{(1)}$

From (4.7), (4.12) and the fits to $V_{N,N+1}$ and R_{N+1}, the main contribution comes from

$$K^{(1)} \propto N^{1/2} \int_0^{r_0} \frac{r^{1/4}\cos(\sqrt{8r} - \frac{3\pi}{4})}{(r_0+2r)^2} \left\{ u_N^{(0)} II(r) + v_N^{(0)} I(r) \right\} dr.$$

Consider the first term in curly brackets; using (A.12)

$$N^{1/2} \int_0^{r_0} \frac{r^{1/4}\cos(\sqrt{8r} - \frac{3\pi}{4})}{(r_0+2r)^2} u_N^{(0)}(r)\, II(r)\, dr \propto \frac{N^{1/2}}{N^{3/2}} \int_0^{r_0} \frac{[r^{1/4}\cos(\sqrt{8r} - \frac{3\pi}{4})]^2}{(r_0+2r)^2} dr$$

$$\propto \frac{1}{N} \int_0^{r_0} \frac{r^{1/2}\cos^2(\sqrt{8r} - \frac{3\pi}{4})}{(r_0+2r)^2} dr$$

which is to leading order is

$$\propto \frac{1}{N} \int_0^{r_0} \frac{r^{1/2}(1/2)}{(r_0+2r)^2} dr$$

$$\propto \frac{1}{N r_0^{1/2}} \int_0^1 f(\rho)\, d\rho \propto \frac{1}{N^2}$$

The other contribution to $K^{(1)}$ is

$$N^{1/2} \int_0^{r_0} \frac{r^{1/4}\cos(\sqrt{8r} - \frac{3\pi}{4})\, v_N^{(0)}(r)\, I(r)\, dr}{(r_0+2r)^2}$$

$$\propto N^{1/2} \int_0^{r_0} \frac{r^{1/2}\sin[2(\sqrt{8r} - \frac{3\pi}{4})]}{(r_0+2r)^2} \cdot N^{1/2} \left\{ \frac{-\sqrt{r}}{r_0+r} + \frac{1}{\sqrt{2r_0}} \tan^{-1}\sqrt{\frac{2r}{r_0}} \right\}$$

$$\propto \frac{N}{r_0} \int_0^1 \rho^{1/2} \cos(2\sqrt{8r_0}\sqrt{\rho}) f(\rho)\, d\rho$$

Now use Dwight[13], Eq. (416.17),

$$\cos a\rho = \frac{2a \sin a\pi}{\pi}\left\{\frac{1}{2a^2} + \frac{\cos\rho}{1^2-a^2} - \frac{\cos 2\rho}{2^2-a^2} + \cdots\right\},$$

and realize that the main contribution comes from first term. Thus find that the above contribution is

$$\propto \frac{N}{r_0}\sqrt{r_0}\,\frac{\sin(2\sqrt{8r_0}\,\pi)}{2(2\sqrt{8r_0})^2}\int_0' g(\rho)\,d\rho \propto \frac{\sin(2\sqrt{12}N\pi)}{N^2}$$

This is the order as the first term but of oscillating sign. The sum is

$$K^{(1)} \propto \frac{C_1 + C_2 \sin(2\sqrt{12}N\pi)}{N^2}$$

APPENDIX C: Closure Approximation and Evaluation of the Average Energy $\bar{E}_N$.

The closure approximation is introduced in (4.29) to simplify the Q-part of the optical potential $\mathcal{V}_{op}^{Q}$. We consider here in more detail the evaluation of the average energy $\bar{E}$ which appears as a parameter in that approximation.

(i) Since V assumes the form

$$V = -\frac{2}{r_1} + \frac{2}{r_1 + r_2} = -\frac{2r_2}{r_1(r_1+r_2)}$$

$$\rightarrow \begin{cases} -2r_2/r_1^2 & r_1 >> r_2 \\ -2/r_1 & r_1 << r_2 \end{cases} \qquad (C.1)$$

we simply set

$$\langle \varphi_N V^2 \varphi_N \rangle \simeq \begin{cases} (4/r_1^2)\int_0^\infty \varphi_N^2 dr_2 = 4/r_1^2 & r_1 < r_0 \\ \frac{4}{r_1^4}\int_0^\infty r_2^2 \varphi_N^2 dr \simeq \frac{10N^4}{r_1^4} & r_1 > r_0 \end{cases} \qquad (C.2)$$

and, from (3.7),

$$\langle \varphi_N V \varphi_N \rangle^2 \equiv (V_{N,N})^2 \simeq \begin{cases} 4/r_1^2 & r_1 < r_0 \\ b_N^2/r_1^4 = \frac{9N^4}{r_1^4} & r_1 > r_0 \end{cases} \qquad (C.3)$$

therefore, $\mathcal{V}_{op}^{Q}$ may be approximated as

$$\mathcal{V}_{op}^{Q} \simeq \begin{cases} 0 \quad \text{to order } O(\frac{1}{r_1}) & r_1 < r_0 \\ \frac{N^4}{E-\bar{E}}\,\frac{1}{r_1^4} & r_1 > r_0 \end{cases}$$

or

$$\mathcal{V}_{op}^{Q} = \left(\frac{N^4}{E-\bar{E}}\right)\frac{\theta(r_1 - r_0)}{r_1^4} \qquad (C.4)$$

where θ is the unit step function.

The approximations involved in (C.2) is essentially the same as that employed in the evaluation of V_{NN} and (C.3), so that $\mathcal{V}_{op}^{Q}$ is the form (C.4) is consistent with the P-part of the problem treated in Sec. III.

(ii) The evaluation of the average $\bar{\mathcal{E}}_N$ is carried out by a variational procedure developed earlier.[14] That is, we have replaced G^Q in (2.10b) by $G^Q_{C\ell}$:

$$G^{\varphi} \equiv \frac{\varphi}{\varphi(E-H)\varphi} \longrightarrow \frac{\varphi}{E-\bar{\mathcal{E}}} \equiv G^{\varphi}_{\ell} \tag{C.5}$$

On the other hand, we can introduce a separable form for G^Q with a set of variational functions $Q\phi$ and $Q\tilde{\phi}$, as

$$G^{\varphi} \simeq \frac{Q\phi\rangle\langle\varphi\tilde{\phi}}{\langle\varphi\tilde{\phi}[E-H]Q\phi\rangle} \equiv G^{\varphi}_{S} \tag{C.6}$$

It is to be emphasized here that the final state wave function we are trying to calculate corresponds to the elastic scattering from the N^{th} excited state at total energy E. Thus in the analysis below we will eventually put the initial and final state wave functions equal to each other. Consider first, however, the somewhat more general case $i \neq f$ where the transition element is given by

$$\mathcal{T}^{\varphi}_{fi} = \langle \chi_f \, G^{\varphi} \, \chi_i \rangle \tag{C.7}$$

with

$$\chi_i = \varphi V P \Psi_i^{P}$$
$$\chi_f = \varphi V P \Psi_f^{P} \tag{C.8}$$

We require that both (C.5) and (C.6) give the same $\mathcal{J}_{fi}^{Q}$

That is,

$$\langle \chi_f \, G_s^{Q} \, \chi_i \rangle \equiv \langle \chi_f \, (Q/E-\bar{\mathcal{E}}) \, \chi_i \rangle \qquad (C.9)$$

which gives then the connection between $\bar{\mathcal{E}}$ and $\langle Q\phi, \, Q\tilde{\phi} \rangle$.

Substituting for G^Q as given by (C.6) allows (C.9) to be solved for $\bar{\mathcal{E}}$ in the form:

$$\bar{\mathcal{E}} = E\left\{1 - \frac{\langle \chi_f \chi_i \rangle \langle Q\tilde{\phi}, Q\phi \rangle}{\langle \chi_f \, Q\phi \rangle \langle Q\tilde{\phi}, \chi_i \rangle}\right\} \qquad (C.10)$$

$$+\left\{\frac{\langle \chi_f \chi_i \rangle}{\langle \chi_f \, Q\phi \rangle \langle Q\tilde{\phi}, \chi_i \rangle} \langle Q\tilde{\phi}, [QHQ] Q\phi \rangle\right\}$$

Thus far, the trial functions $Q\phi$ and $Q\phi$ are left arbitrary, except the normalization (linear) parameter which was eliminated by writing G_s^Q in the normalization-independent form (C.6). Now, we choose these trial functions such that (C.10) assumes a simple form, i.e. let

$$Q\phi = \chi_i \qquad Q\tilde{\phi} = \chi_f \qquad (C.11)$$

Substitution of (C.11) into (C.10) immediately reduces to a form

$$\bar{\mathcal{E}} = \frac{\langle \chi_f \, QHQ \, \chi_i \rangle}{\langle \chi_f \chi_i \rangle} \equiv \frac{B}{D} \qquad (C.12)$$

where, using (C.8), we can write

$$B = \langle \chi_f \, Q H Q \, \chi_i \rangle = \langle P\underline{\Psi}_f^{P} \, PVQHQVP\underline{\Psi}_i^{P} \rangle \qquad (C.13)$$

$$D = \langle \chi_f \, \chi_i \rangle = \langle P\underline{\Psi}_f^{P} \, PVQVP\underline{\Psi}_i^{P} \rangle$$

We can explicity estimate the N-dependence of B and D for $\overline{\mathcal{E}}_N$ using the result of Sec. III for the case $P\Psi_i^P = P\Psi_f^P = \frac{U_N^{(0)}(r)\phi_N(r_2)}{r_1}$. Firstly, consider the constant D, which becomes (using Q=1-P) as in (C.4)

$$D = \int_0^\infty dr_1 \left[u_N^{(0)}(r_1)\right]^2 \langle \varphi_N, \left[V^2 - (V_{N,N})^2\right] \varphi_N \rangle$$

$$\cong \int_0^\infty dr_1 \left[u_N^{(0)}(r_1)\right]^2 \frac{N^4}{r_1^4}\, \theta(r_1 - r_0)$$

$$\cong N^4 \int_{r_0}^\infty dr_1 \left[u_N^{(0)}(r_1)\right]^2 r_1^{-4}$$

Using (3.11b) for $U_N^{(0)}$ (the part for $r>r_0$) and replacing the $\cos^2(\alpha_N \ln(r/r_0) - \sqrt{8}r_0 - 3\pi/4)$ by 1/2, we get for the integral

$$\int_{r_0}^\infty dr \left[u_N^{(0)}(r)\right]^2 r^{-4} \propto \frac{1}{\sqrt{r_0}} \int_{r_0}^\infty r^{-3} dr \propto \frac{1}{N^5}$$

Thus

$$D \propto N^4/N^5 \propto 1/N \tag{C.14}$$

The evaluation of B is longer and somewhat more involved. We have

$$B = \langle P\Psi^P\, PVQHQVP\Psi^P \rangle \tag{C.15}$$

where

$$P\Psi^P = U_N^{(0)}(1)\,\varphi_N(2)$$

$$U_N^{(0)}(1) = u_N^{(0)}(r_1)/r_1$$

$$H = h_1 + h_2 + v$$

$$P = \varphi_N(2)\times\varphi_N(2) \quad ; \quad Q = 1 - P$$

Thus using $h_2\phi_N(2)=E_N\phi_N(2)$ gives

$$\begin{aligned} QHQ &= Q(h_1+h_2+v)Q \\ &= Qh_1+Qh_2-E_NQ+QvQ \,, \end{aligned} \tag{C.16}$$

so that

$$B=\sum_{i=1}^{4} B_i \,,$$

where the four terms come directly from the substitution of (C.16) into (C.15). Consider first

$$B_1=\langle U_N^{(0)}\phi_N(2)VQh_1VU_N^{(0)}(1)\phi_N(2)\rangle$$

$$= \langle U_N^{(0)}(1)\,V_{NN}(1)\,h_1\,U_N^{(0)}(1)\rangle - \langle U_N^{(0)}(1)\,V_{NN}(1)\,h_1\,U_N^{(0)}(1)\rangle$$

$$= 0. \tag{C.17}$$

Here we have used the definition

$$V_{NN}(1) = \langle \varphi_N(2)\,V(1,2)\,\varphi_N(2)\rangle$$

One can also readily find that

$$\begin{aligned} B_2 + B_3 = {} & \langle U_N^{(0)}(1)\,\varphi_N(2)\,|\,Vh_2V\,|\,U_N^{(0)}(1)\,\varphi_N(2)\rangle \\ & - E_N\langle U_N^{(0)}(1)\,(V^2)_{NN}\,U_N^{(0)}(1)\rangle \end{aligned} \tag{C.18}$$

and

$$B_4 = \langle U_N^{(0)}(1)\left[(Vv-V)_{NN} - 2(Vv)_{NN} + (V_{NN})^2 v_{NN}\right]U_N^{(0)}(1)\rangle \tag{C.19}$$

where in our approximation

$$r \equiv \frac{2}{r_1 + r_2} \cong \begin{cases} 0 & r < r_0 \\ \frac{2}{r_1} - \frac{2r_2}{r_1^2} & r_1 > r_0 \end{cases} \qquad (C.20)$$

Each of these terms may be evaluated in a straightforward manner except for the first term of (C.18). In that case we use our approximation for V (but we neglect the cusp) before differentiating to find

$$\langle \bar{U}_N^{(0)}(1)\, \varphi_N(2)\, V h_2 V\, \bar{U}_N^{(0)}(1)\, \varphi_N(2) \rangle \qquad (C.21)$$

$$= E_N \langle \bar{U}_N^{(0)}(1) (V^2)_{NN} \bar{U}_N^{(0)}(1) \rangle + \frac{\text{const.}}{N^3} + O\left(\frac{\cos(2\sqrt{2}N)}{N^7}\right)$$

The first term of (C.21) cancels with the second term of (C.18). All the remaining terms are of order N^{-3}. Thus

$$B \propto \frac{1}{N^3} \qquad (C.22)$$

so that combining that with (C.14), we get finally

$$\bar{\mathcal{E}}_N = \frac{B}{D} \propto \frac{1/N^3}{1/N} \propto N^{-2}. \qquad (C.23)$$

APPENDIX D: Evaluation of Transition Matrix Elements

We want to find the N dependence of M.E. in the various approximations we have used. The PΨ part of M.E. is

$$(ME)_{P\Psi} \equiv \left\langle \frac{u_N(r_1)}{r_1}\varphi_N(r_2) \,\middle|\, V \,\middle|\, \Phi_{initial} \right\rangle \tag{D1}$$

$$\propto \int_0^\infty\int_0^\infty dr_1\, dr_2\; u_N(r_1)\, R_N(r_2)\left[-\frac{2}{r_1}+\frac{2}{r_1+r_2}\right]\sin kr_1\, R_1(r_2)$$

The first term of V gives zero by orthogonality and since $R_1(r_2) \propto r_2 e^{-r_2}$, the r_2 coordinate is confined to be close to origin; we can very accurately expand

$$\frac{2}{r_1+r_2} = \frac{2}{r_1} - \frac{2r_2}{r_1^2} \tag{D.2}$$

Thus

$$(ME)_{P\Psi} \propto \langle N|r_2|1\rangle \int_0^\infty dr_1\; u_N(r_1)\, r_1^{-2} \sin kr_1 . \tag{D3}$$

The lower limit on the integral can be extended to 0 (rather than r_2) because the integrand converges at the origin. If now we divide the integral into two regions,

$$\int_0^\infty dr\, u_N(r)\frac{1}{r^2}\sin kr = \int_0^{r_0} dr\, u_N(r)\frac{\sin kr}{r^2} + \int_{r_0}^\infty u_N(r)\frac{\sin kr}{r^2}\, dr \tag{D4}$$

we note that the first term is cut off by the oscillations in sinkr (which are independent of N). And because $(0<\gamma\leq 1)$,

$$u_N(r) \leq \left(\frac{r}{r_o^{3/4}}\right)^{\gamma} \cdot \text{sinusoidal function of } r;$$

the second integral always converges and is proportional to $N^{-(3/2)\gamma}$. Thus the second term in (D.4) is negligible compared to the first term. This is true whether $u_N(r)\big|_{r>r_o}$ is either the attractive $u_N^{(\beta)}$ of (4.40b) or simply $u_N^{(o)}(r>r_o)$ of (3.11b). Thus the N dependence of $(ME)_{p\Psi}$ is controlled by the first term of (D.4) and this in turn is determined by $\langle N|r_2|1\rangle$ which is, trivially,

$$\langle N|r_2|1\rangle \propto \frac{1}{N^{3/2}} . \tag{D.5}$$

M_o is a special case of $(ME)_{p\Psi}$ so that we have finally

$$M_o \propto (ME)_{p\Psi} \propto \Big|_{\text{attractive } r^{-4}}^{N^{-3/2}} \tag{D.6}$$

We must also consider the contribution from the $Q\Psi$ of the wave function. In the closure approximation (4.21a) reduces to

$$Q\underline{\Psi} = \frac{1}{E_N - \bar{\mathcal{E}}_N} Q V P \underline{\Psi} \tag{D.7}$$

Assuming

$$Q\underline{\Psi} = \theta_N(1)\varphi_{N+1}(2) \tag{D.8}$$

and using $P\underline{\Psi} = U_N(1)\varphi_N(2)$, $Q = 1 - \varphi_N\rangle\langle\varphi_N$, one can reduce (D.7) to

$$\theta(1) = \frac{V_{N,N+1}(r_1)\, U_N(1)}{E_N - \bar{\mathcal{E}}_N} \tag{D.9}$$

To calculate the Q-part of matrix element

$$(ME)_{Q\Psi} = \int Q\Psi V \Phi_{initial} \quad , \tag{D.10}$$

we bound the $r<r_o$ contribution by

$$V_{N,N+1} \propto \frac{N^2}{(r+r_o)^2} \leq \frac{N^2}{r_o^2} \propto \frac{1}{N^2} . \tag{D.11}$$

Thus

$$(ME)_{Q\Psi} = \frac{1}{E_N - \bar{E}_N} \int U_N(1) \varphi_N(2) V_{N,N+1} V \Phi_{initial}$$

$$\leq \frac{1}{N^2(E_N - \bar{E}_N)} \int P\Psi \; V\Phi$$

or finally

$$(ME)_{Q\Psi} \propto [N^2(E_N - \bar{E}_N)]^{-1} (ME)_{P\Psi} \tag{D.12}$$

Note that as long as $|E_N - \bar{E}_N| \propto N^{-2}$ that both the $P\Psi$ and $Q\Psi$ contributions to M.E. have the same N dependence. However if $|E_N - \bar{E}_N| < 0(\frac{1}{N^2})$ then the $Q\Psi$ contribution dominates.

We next consider the repulsive $\frac{\beta^2}{r^4}$ case which is now dominated by the contribution from r_o to r_β. Using (4.40c) in the second term of (D.4)

$$\int_{r_o}^{r_\beta} \frac{u_N(r) \sin kr \, dr}{r^2} \propto \frac{\cos(\sqrt{8}r_o - 3\pi/4)}{N^3} \int_{r_o}^{r_\beta} dr \, \frac{\cosh[\beta(\frac{1}{r} - \frac{1}{r_o})]}{r} \tag{D.13}$$

Integration by parts give

$$\int_{r_0}^{r_\beta} \frac{dr}{r} \cosh[\beta(r^{-1}-r_0^{-1})] = \ln r \cosh[\beta(r^{-1}-r_0^{-1})]\Big|_{r_c}^{r_\beta} + \int_{r_0}^{r_\beta} dr \frac{\ln r}{r^2} \sinh[\beta(r^{-1}-r_0^{-1})] \tag{D.14}$$

In the region $r>r_0$, $r^{-2}<<r^{-1}$ and since sinh is less than cosh throughout the interval, the second integral has higher inverse power of N dependence than the first term, so that we obtain in leading order

$$(ME)_{P\Psi}\Big|_{\text{repulsive } r^{-4}} \propto \frac{\cos(\sqrt{8}r_0 - 3\pi/4)}{N^3} \ln r_\beta \cosh\left[\beta\left(\frac{1}{r_\beta} - \frac{1}{r_0}\right)\right] \tag{D.15}$$

Finally, we consider the part of the matrix element coming from the $U_N^{(1)}$ which occurs in the lowest term and dominant pole approximations:

$$M_1 = \int_c^\infty \int_c^\infty u_N^{(1)}(r_1) R_N(r_2) \frac{2}{r_1+r_2} \sin kr_1 \, R_1(r_2) \, dr_1 \, dr_2 \tag{D.16}$$

where $U_N^{(1)}$ is given by (4.12). The functions I(r) and II(r) can be shown to be of the order of or bounded by

$$I(r) \longrightarrow \begin{cases} r^3/N^{7/2} & r \to 0 \\ N^{-1/2} & r \to r_0 \end{cases} \tag{D.17}$$

$$II(r) \propto N^{-3/2} \qquad 0 < r < r_0 \tag{D.18}$$

Thus the two contributions to M_1 are

$$M_{11} \propto \langle N|r_2|1\rangle \int v_N^{(0)}(r) I(r) \frac{2}{r^2} \sin kr \, dr$$

$$\propto \frac{1}{N^{3/2}} \int v_N^{(0)}(r) I(r) \frac{2}{r^2} \sin kr \, dr \qquad (D\,19)$$

and

$$M_{12} \propto N^{-3/2} \int u_N^{(0)}(r) II(r) \frac{2}{r^2} \sin kr \, dr.$$

Considering the latter first and using (D.18) :

$$M_{12} \propto N^{-3} \int_0^\infty \frac{u_N^{(0)}(r) \sin kr}{r^2} dr \qquad (D\,20)$$

The integrand is bounded at the origin, since both $u_N^{(0)}$ and $\sin(kr)$ vanish at r=o, and it is bounded at ∞ since $|u_N^{(0)}| \leq r^{1/2}$. Therefore,

$$M_{12} \propto N^{-3} \qquad (D\,21)$$

For M_{11} we have

$$M_{11} \propto \frac{1}{N^{3/2}} \int \frac{v_N^{(0)}(r) I(r)}{r^2} \sin kr \, dr \qquad (D\,22)$$

If we use $N^{-1/2}[1 - e^{-\left(\frac{r}{N}\right)^3}]$ to interpolate on I(r) from (D.17) and put all sinusoidal factors equal to 1, we can bound M_{11} by

$$M_{11} \leq \frac{1}{N^2} \int_0^{r_0} \frac{r^{1/4}}{r^2} \left[1 - e^{-\left(\frac{r}{N}\right)^3}\right] dr \qquad (D\,23)$$

The term in square brackets forces the contribution from the lower limit of the integral to be 0 ; thus the major contribution comes from the upper limit, so that we are left with

$$M_{11} \leq \frac{1}{N^2}\left[\int^{r_0} \frac{dr}{r^{7/4}}\right] \propto \frac{1}{N^2 r_0^{3/4}} \propto N^{-7/2} \qquad (D24)$$

Thus to leading order

$$M_1 = M_{11} + M_{12} \propto \frac{1}{N^3} \qquad (D25)$$

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TABLE I : Comparison of $\mathcal{E}_N$ (in Ry) With Various Thresholds

	MODEL ($V=\frac{2}{r_1+r_2}$)				S-Wave ($V=\frac{2}{r_{12}}$)			
N	$\mathcal{E}_N-E_N$	$\mathcal{E}_N-E_{N-1}$	$\mathcal{E}_N-E_{N-2}$	$\mathcal{E}_N-E_{N-3}$	$\mathcal{E}_N-E_N$	$\mathcal{E}_N-E_{N-1}$	$\mathcal{E}_N-E_{N-2}$	$\mathcal{E}_N-E_{N-3}$
2	-.0643				-.0041			
3	-.0296				-.0127			
4	-.0168				-.0096			
5	-.0103	>0			-.0074			
6	-.00754				-.0056			
7	-.00555				-.0043	>0		
8	-.004255				-.0034			
9	-.00336	-.00008			-.0028			
10	-.00273	-.00038	>0		-.0023			
11	-.00225	-.00052			-.0019	-.00022		
12	-.00189	-.00057			-.0016	-.00034		
13	-.00161	-.00059			-.0014	-.00040	>0	
14	-.00139	-.00058			-.0012	-.00042		
15	-.00121	-.00056			-.0011	-.00043		
16	-.00107	-.00053			-.00097	-.00045		
17	-.00094	-.00050			-.00085	-.00041		
18	-.00084	-.00047	-.00003	>0	-.00078	-.00041		
19	-.00076	-.00044	-.00007		-.00070	-.00038	-.00001	>0
20	-.00068	-.00042	-.00010		-.00063	-.00037	-.00005	
21	-.00062	-.00039	-.00012		-.00057	-.00034	-.00007	
22	-.00056	-.00036	-.00013		-.00052	-.00032	-.00009	
23	-.00052	-.00034	-.00014		-.00048	-.00031	-.00010	
24	-.00047	-.00032	-.00014		-.00046	-.00030	-.00013	
25	-.00044	-.00030	-.00015		-.00042	-.00028	-.00013	
26	-.00040	-.00028	-.00015		-.00038	-.00026	-.00013	
27	-.00037	-.00027	-.00015	-.00001	-.00035	-.00025	-.00013	
28	-.00035	-.00025	-.00015	-.00002	-.00033	-.00023	-.00013	
29	-.00032	-.00024	-.00014	-.00003	-.00030	-.00022	-.00013	-.00001
30	-.00030	-.00022	-.00014	-.00004	-.00029	-.00021	-.00013	-.00003

Figure Captions

Figure 1: $N^2 V_{N,N+1}(r)$ vs. r/r_o. The lower curves are from numerical evaluations for N=2,5,11 as indicated. The analytical approximation is the top curve.

Figure 2: $\mathcal{L}_3$ vs. E from Eq. (5.26), curve 2, (C=1/2). Note that the curve is monotonically increasing but it oscillates (infinitely rapidly as E→o) about $\mathcal{L}_3$=E (curve 1).

Figure 3: The radial function $R_N(r)$ for N=15 (denoted by *) vs. the approximation (A.1). The abscissa is $\rho=[\frac{2}{3}r]^{1/2}$ so that the average value of $r_{NN}=\frac{3}{2}N^2$ occurs at ρ=N. Beyond $r=2r_o$ the approximation in (A.1) is denoted by ★ and is barely distinguishable from the exact curve.

Fig. 1

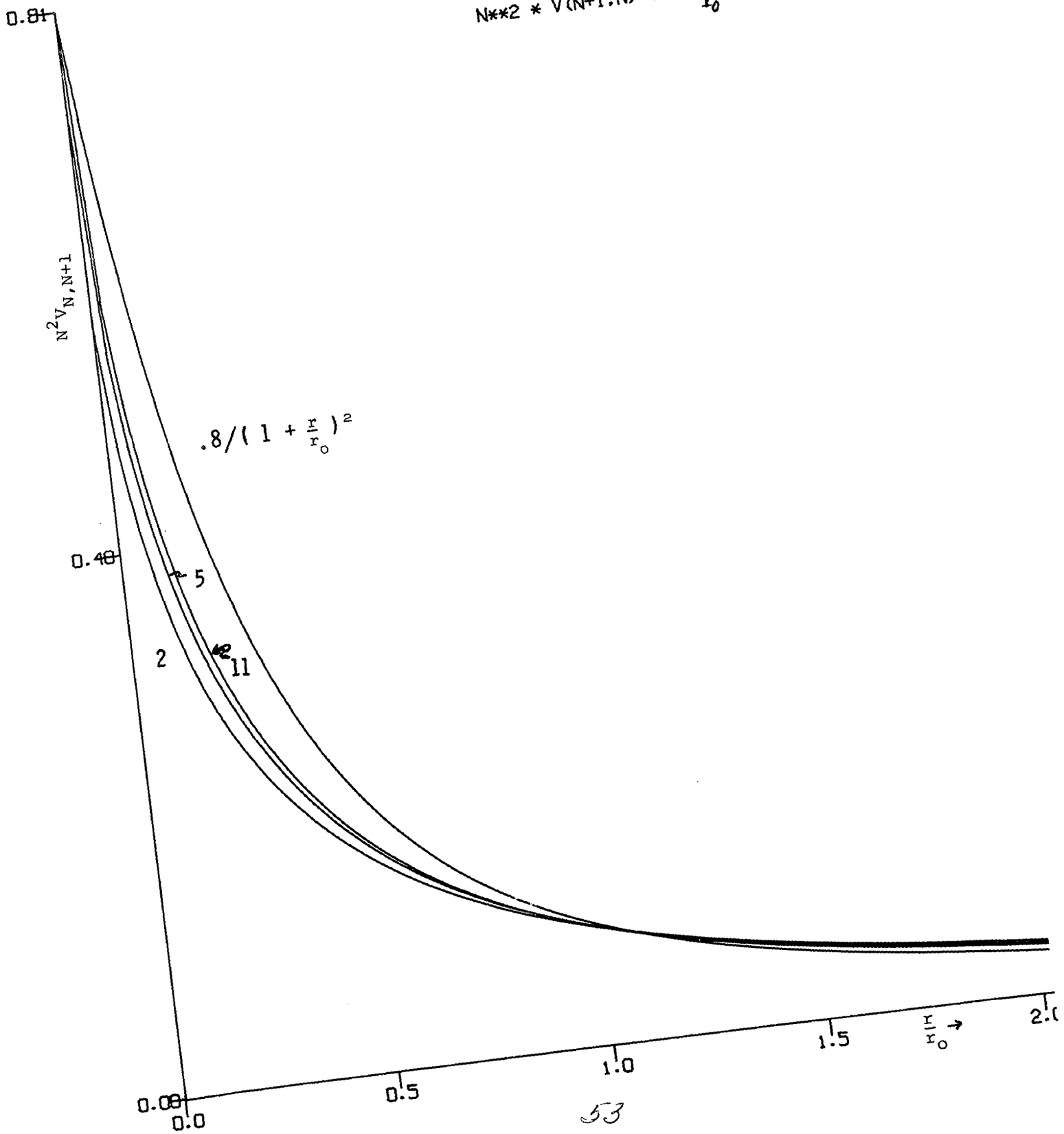
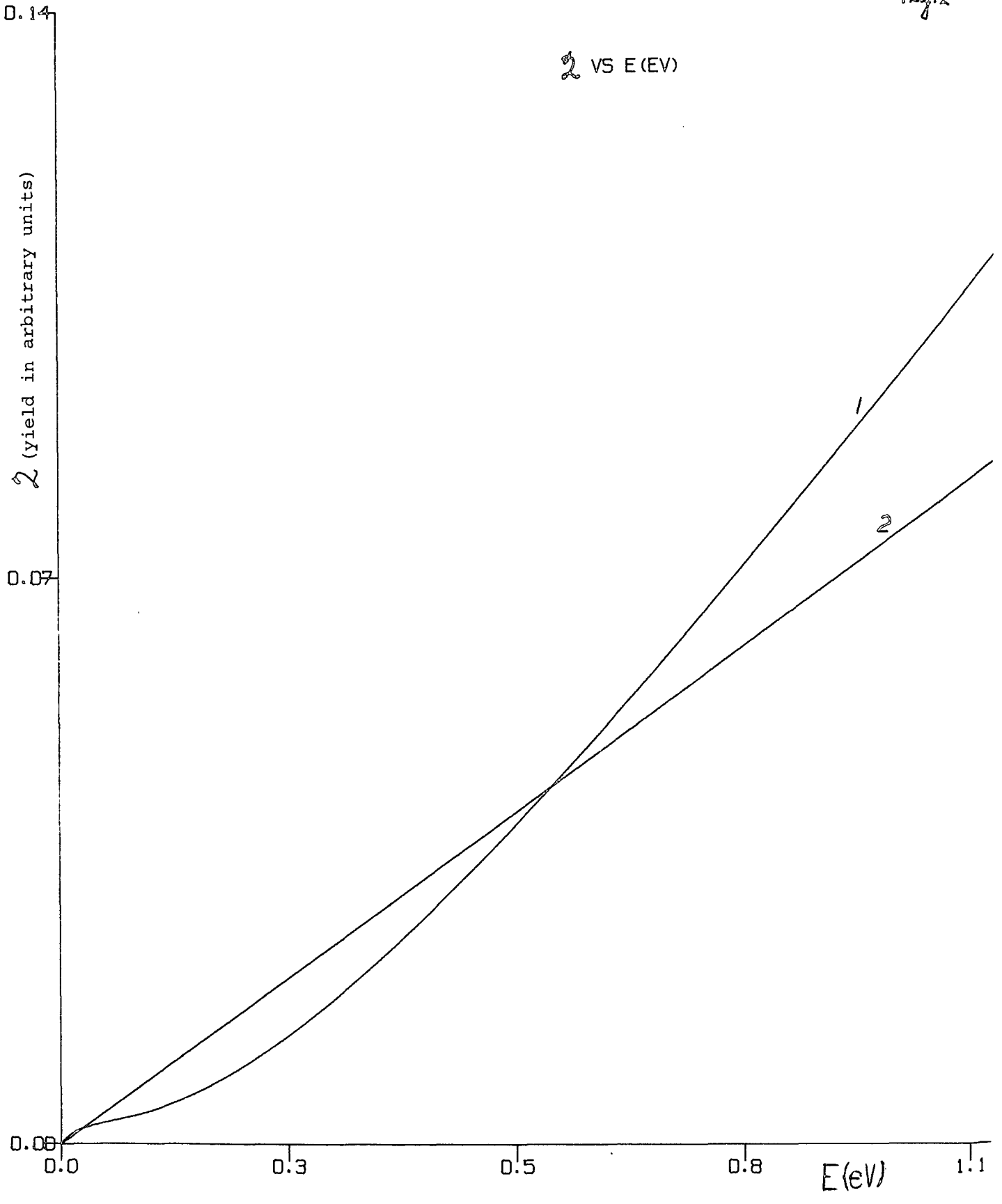

N**2 * V(N+1,N) VS $\frac{r}{r_0}$
$N^2 V_{N,N+1}$
$.8/(1+\frac{r}{r_0})^2$
0.8
0.4
0.0
5
2
11
0.0
0.5
1.0
1.5
$\frac{r}{r_0}$ →

Fig.2


η VS E (EV)
η (yield in arbitrary units)
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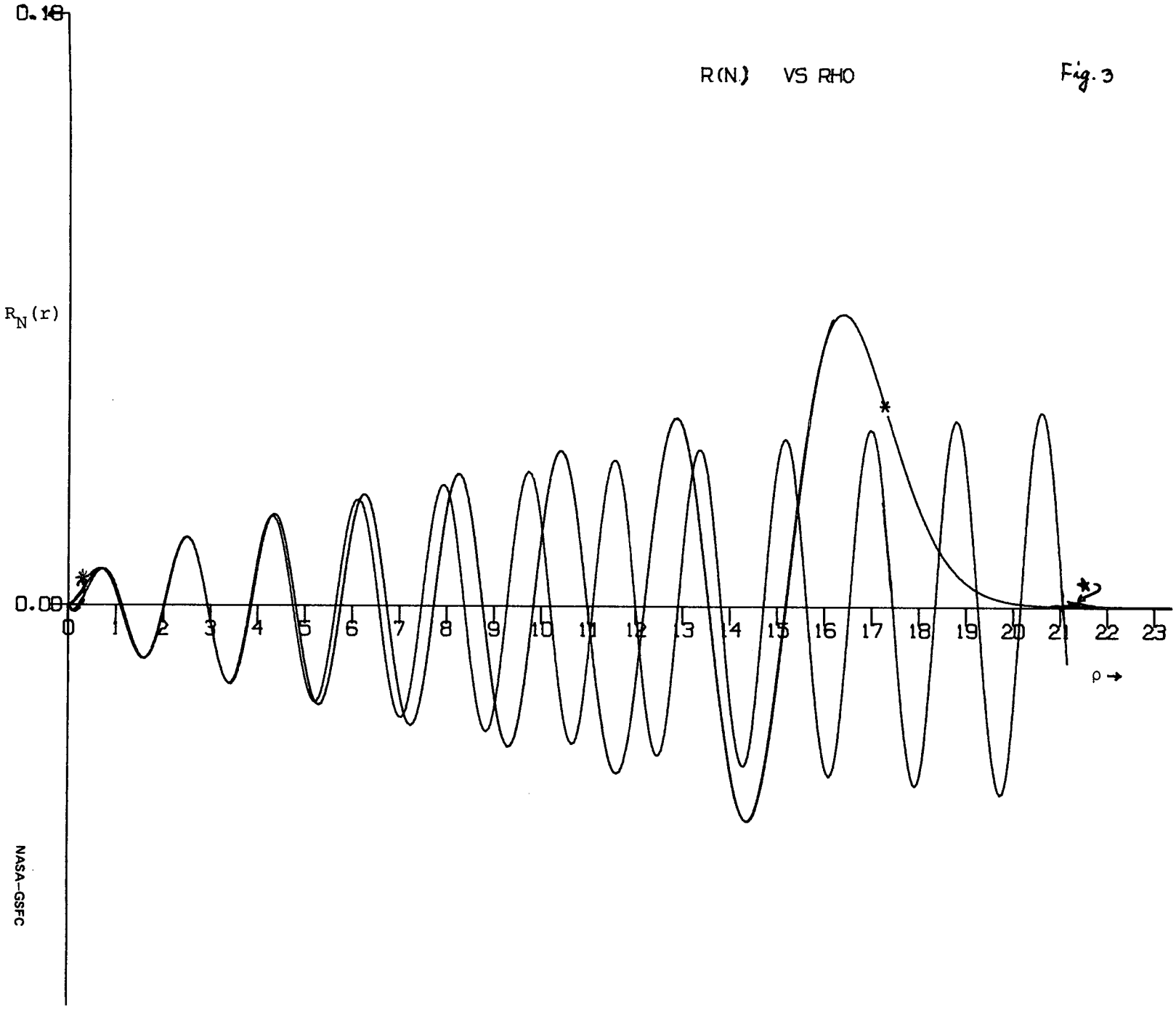
0.07
0.00
0.0
0.3
0.5
0.8
1.1
E(eV)
1
2


0.10
R(N.) VS RHO
Fig. 3
$R_N(r)$
0.00
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
ρ →
NASA-GSFC