Optical-potential approach to the electron-atom impact-ionization-threshold problem

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The problem of the threshold law for electron-atom impact ionization is reconsidered as an analytic continuation of inelastic-scattering 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 Nth excited state of the target atom. The actual calculation is carried out 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 dimensionality of the Schrödinger equation. Nevertheless, the scattering equation is still very complex. It is dominated by the optical potential which is expanded in terms of the eigenspectrum of QHQ. It is shown by actual calculation that the lower eigenvalues of this spectrum descend below the relevant inelastic-scattering 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: (i) omission of the optical potential, (ii) inclusion of the lowest term and dominant pole term, and (iii) 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, the above phenomenon of eigenvalues descending below threshold suggests that $E_N - \bar{\mathcal{E}}_N$ is 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 given.

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., autodetaching) 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 same 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 low-lying doubly excited state.

Thus we here consider the (S-wave) scattering problem itself. First we define a model which we believe contains the essentials of the electron-hydrogen ionization problem and yet greatly reduces the mathematical complexity: We replace the electron-electron repulsion $2/r_{12}$ (in rydberg units which we use throughout) by $2/(r_1 + r_2)$:

$$2/r_{12} \to 2/(r_1 + r_2) \tag{1.1}$$

and thereby reduce the S-wave Schrödinger 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 Sec. II we consider the scattering problem starting from a general close-coupling expansion. We show that because of the nature of the spectrum of QHQ 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 (Sec. II) that for purposes of evaluating inelastic-scat-

tering 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 (H_{PP}) problem is considered in Sec. 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 Sec. IV. We consider three approximations: a lowest-term approximation; an effective intermediate state (dominant-pole) approximation; and an effective energy or closure approximation. In Sec. V the threshold law for these various approximations is worked out, and some discussion of the results is given including a remark on other recent approaches to the problem based on Wannier.[4]

II. MODEL OF ELECTRON-HYDROGEN INTERACTION AND SCATTERING PROBLEM

We consider the Schrödinger equation (rydberg units throughout)

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

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

$$H = -\frac{1}{r_1}\frac{\partial^2}{\partial r_1^2} r_1 - \frac{1}{r_2}\frac{\partial^2}{\partial r_2^2} r_2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_1 + r_2}, \tag{2.2}$$

and we expand the solution in two parts:

$$\Psi_N = P\Psi_N + Q\Psi_N \tag{2.3}$$

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

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

for a total energy E, where

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

with E_N being the energy of Nth excited state of hydrogen,

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

[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 $\varphi_n(r)$ are s eigenstates of the hydrogen atom:

$$\varphi_n(r) = (1/r)R_n(r) . \tag{2.8}$$

As is by now well known, an equation equivalent to the Schrödinger equation can be derived[5] for the open-channel wave function $P\Psi_N$,

$$(PHP + \mathfrak{V}_{\text{opt}}^{Q} - E)P\Psi_N = 0 , \tag{2.9}$$

where the Q part of the optical potential is given by

$$\mathfrak{V}_{\text{opt}}^{Q} = PHQ[1/(E - QHQ)]QHP . \tag{2.10a}$$

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

$$G^{Q} = Q/(E - QHQ) . \tag{2.10b}$$

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 QHQ:

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

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) optical potential

$$\mathfrak{V}_{\text{opt}}^{Q} = \sum_{\nu} \frac{\langle PHQ_{N\nu}\Phi\rangle\langle\Phi_{N\nu}QHP\rangle}{E - \mathcal{E}_{N\nu}} . \tag{2.15}$$

The expansion (2.15) is not only useful, but is 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 ($\Rightarrow E - \mathcal{E}_{N\nu} < 0$ 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]

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

computed

$$\mathcal{E}_N = \langle \Phi_N H \Phi_N \rangle = \frac{-2}{N^2} + \langle \Phi_N | 2/(r_1 + r_2) | \Phi_N \rangle \qquad (2.16)$$

for

$$\Phi_N = \varphi_N(r_1)\varphi_N(r_2), \qquad (2.17)$$

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 eigenvalue associated with higher N' states can descend below the Nth 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.

The assertion that terms for which $E - \mathcal{E}_{N\nu} > 0$ are repulsive deserves some additional discussion in view of the fact that Gailitis[6] has shown that even after one passes a Feshbach resonance the phase shift continues to increase. This would appear to imply that a particular optical-potential term retains its attractive character even after one has passed the resonance energy. But the fact of the matter is that the scattering wave function loses a mode as it passes through a Feshbach resonance. Thus if one calculates the absolute phase shift[7] (i.e., the phase shift based on the number of nodes that are actually present in the scattered orbital), then one will find that the phase shift with such terms absent is larger than that with such terms present. This then is the meaning of the positive definiteness of terms for which $E - \mathcal{E}_{N\nu} > 0$, and it convinces us that the physical effect of such terms is repulsive.

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]

$$\Phi_N^{(j)} = \sum_{l=0}^{N-1} C_{Nl}^{(j)} \phi_{Nl}(r_1)\phi_{Nl}(r_2) P_l(\cos\theta_{12}), \qquad (2.18)$$

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.

TABLE I. Comparison of $\mathcal{E}_N$ (in Ry) with various thresholds.

	Model $[V = 2(r_1 + r_2)^{-1}]$				S wave $(V = 2r_{12}^{-1})$			
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	−0.0643				−0.0041			
3	−0.0296				−0.0127			
4	−0.0168				−0.0096			
5	−0.0103	>0			−0.0074			
6	−0.007 54				−0.0056			
7	−0.005 55				−0.0043	>0		
8	−0.004 255				−0.0034			
9	−0.003 36	−0.000 08			−0.0028			
10	−0.002 73	−0.000 38	>0		−0.0023			
11	−0.002 25	−0.000 52			−0.0019	−0.000 22		
12	−0.001 89	−0.000 57			−0.0016	−0.000 34		
13	−0.001 61	−0.000 59			−0.0014	−0.000 40	>0	
14	−0.001 39	−0.000 58			−0.0012	−0.000 42		
15	−0.001 21	−0.000 56			−0.0011	−0.000 43		
16	−0.001 07	−0.000 53			−0.000 97	−0.000 45		
17	−0.000 94	−0.000 50			−0.000 85	−0.000 41		
18	−0.000 84	−0.000 47	−0.000 03	>0	−0.000 78	−0.000 41		
19	−0.000 76	−0.000 44	−0.000 07		−0.000 70	−0.000 38	−0.000 01	>0
20	−0.000 68	−0.000 42	−0.000 10		−0.000 63	−0.000 37	−0.000 05	
21	−0.000 62	−0.000 39	−0.000 12		−0.000 57	−0.000 34	−0.000 07	
22	−0.000 56	−0.000 36	−0.000 13		−0.000 52	−0.000 32	−0.000 09	
23	−0.000 52	−0.000 34	−0.000 14		−0.000 48	−0.000 31	−0.000 10	
24	−0.000 47	−0.000 32	−0.000 14		−0.000 46	−0.000 30	−0.000 13	
25	−0.000 44	−0.000 30	−0.000 15		−0.000 42	−0.000 28	−0.000 13	
26	−0.000 40	−0.000 28	−0.000 15		−0.000 38	−0.000 26	−0.000 13	
27	−0.000 37	−0.000 27	−0.000 15	−0.000 01	−0.000 35	−0.000 25	−0.000 13	
28	−0.000 35	−0.000 25	−0.000 15	−0.000 02	−0.000 33	−0.000 23	−0.000 13	
29	−0.000 32	−0.000 24	−0.000 14	−0.000 03	−0.000 30	−0.000 22	−0.000 13	−0.000 01
30	−0.000 30	−0.000 22	−0.000 14	−0.000 04	−0.000 29	−0.000 21	−0.000 13	−0.000 03

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,

$$\Phi_{N,N+1} = (2^{-1/2}/r_1 r_2)[R_N(r_1)R_{N+1}(r_2) + (1 \rightleftharpoons 2)], \tag{2.19}$$

which have similar types of spectral properties going over finally to the purely dipole-type states (labeled $\psi_D^{(N)}$ 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. DIRECT-POTENTIAL PROBLEM

The H_{PP} problem, i.e.,

$$[PHP - E_N]P\Psi_N = 0, \tag{3.1}$$

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 $V_{nm}(r_1)$ and assuming n and m are of the order of N, then $V_{nm} \lesssim N^{-3}$ for all values of r. In perturbation theory these potentials are to be divided by the energy differences which are also of the order $\sim(n-m)/N^3$. 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 H_{PP} equation becomes in this approximation

$$\left(\frac{d^2}{dr^2} - V_{N,N}(r) + k_N^2\right)u_N(r) = 0, \tag{3.2}$$

where

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

and

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

$$= -2/r + v_{N,N}(r). \tag{3.5}$$

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

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

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

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

where r_0 is the mean radius of the Nth state,

$$r_0 = \langle N|r|N\rangle = \tfrac{3}{2}N^2, \tag{3.8}$$

and b_N the dipole moment,

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

with the value

$$b_N = 2r_0 = 3N^2. \tag{3.10}$$

This approximation of $V_{N,N}$ enables a solution of (3.7) to be analytically determined (for $k_N = 0$)

$$u_N^{(0)}(r) = (\tfrac{1}{2}r)^{1/2}J_1((8r)^{1/2}), \quad r < r_0$$

$$= r^{1/2}[A \sin(\alpha_N \ln r) + B \cos(\alpha_N \ln r)], \quad r > r_0 \tag{3.11a}$$

where

$$\alpha_N = (b_N - \tfrac{1}{4})^{1/2}. \tag{3.12}$$

The k_N dependence is handled by 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 and Ref. 10).

On matching function and derivative at $r = r_0$ and using the well-known asymptotic form[8] of J_1, one obtains to leading order (for $r \gg 1$),

$$u_N^{(0)}(r) \cong \frac{r^{1/4}}{(2\pi\sqrt{2})^{1/2}} \cos[(8r)^{1/2} - \tfrac{3}{4}\pi], \quad r < r_0$$

$$u_N^{(0)}(r) \cong \frac{r^{1/2}}{[2\pi(2r_0)^{1/2}]^{1/2}} \cos[\alpha_N \ln(r/r_0) + (8r_0)^{1/2} - \tfrac{3}{4}\pi], \quad r > r_0 \tag{3.11b}$$

IV. APPROXIMATIONS OF OPTICAL POTENTIAL

We consider here three approximations of the optical potential.

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

$$\Phi_{N+1} = Q\Phi_{N+1} = \varphi_{N+1}(r_1)\varphi_{N+1}(r_2) . \tag{4.1}$$

Substitution of this into (2.15) gives rise to an integrodifferential equation:

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

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 $u_N^{(0)}(r)$ is the homogeneous solution Eq. (3.11), $u_N^{(1)}$ is a solution of the inhomogeneous equation,

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

and C can be solved for to be

$$C = -K^{(0)}/(E - \mathcal{E}_{N+1} + K^{(1)}) , \tag{4.5}$$

with

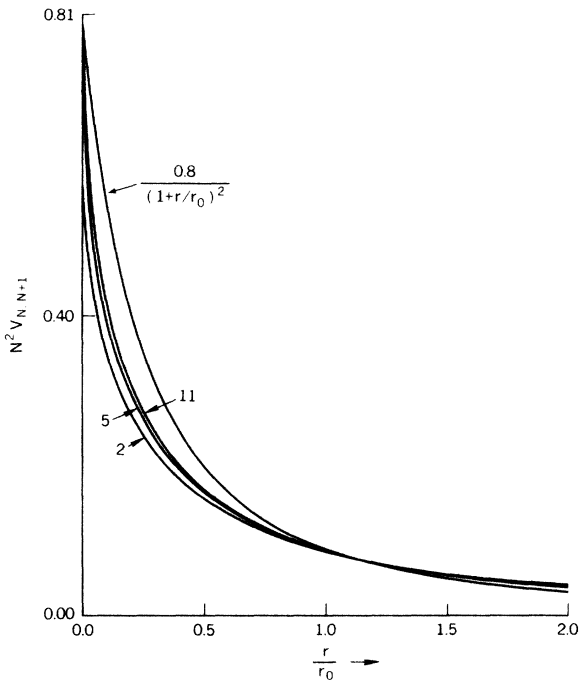

FIG. 1. $N^2 V_{N,N+1}^{(r)}$ vs r/r_0. The lower curves are from numerical evaluations for $N = 2$, 5, 11 as indicated. The analytical approximation is the top curve.

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

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:

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

In Fig. 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 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 $r/r_0 \simeq 0.5$; however, our results below are not affected. A better fit can be obtained with ($r \leq r_0$)

$$V_{N,N+1} \cong \sqrt{2} N^{-2}\{2[0.633 + (r/r_0)]^{1/2} - [1.266 + (r/r_0)]^{1/2} + (r/r_0)^{1/2}\} .$$

The solution of the $u_N^{(1)}$ equation (4.14) is effected with a Green's-function technique,

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

where the Green's function is

$$G(r, r') = (-2\pi) u_N^{(0)}(r_<) v_N^{(0)}(r_>) , \tag{4.10}$$

and $v_N^{(0)}$ is (any) irregular solution of the homogeneous equation. We choose the complementary form of (3.11) whose asymptotic form is

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

The details of the quadrature involved in (4.8) are given in Appendix A. The result is ($r<r_0$)

$$u_N^{(1)} = u_N^{(0)}(r)II(r) + v_N^{(0)}(r)I(r)\,, \tag{4.12}$$

where $I(r)$ and $II(r)$ are given in (A7) and (A10).

The evaluation of the N dependence of $K^{(0)}$ is exceedingly simple. One finds

$$K^{(0)} \propto 1/N^{1/2}\,. \tag{4.13}$$

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

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

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 Nth level,

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

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

$$\mathcal{E}_{N+1} \cong -1.27/(N+1)^2\,. \tag{4.16}$$

(This is at least semiquantitatively understandable from the classical picture of two electrons equally distant from the nucleus in which each sees the nuclear charge fractionally diminished simulating the repulsion of the electron on the other side.) To lowest order, therefore,

$$E_{N+1} - \mathcal{E}_{N+1} \cong 0.27/N^2 + O(1/N^3)\,. \tag{4.17}$$

The function $u_N(r)$ in the region $r \sim r_0$ is dominated by the term $v_N^{(0)}(r)I(r)$ by noting that for $r \sim r_0$,

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

as opposed to $II(r) \propto N^{-3/2}$ [using (A11) and (A12)]. Thus putting these behaviors together, we find

$$\lim_{N\to\infty} u_N(r)\big|_{r\cong r_0} \approx p_1(N)v_N^{(0)}(r)\,, \tag{4.19}$$

where

$$p_1(N) \equiv CN/[1 - B\sin(2\sqrt{12}N\pi)]\,. \tag{4.20}$$

The above is the essence of the $P\Psi_N$ contribution to the wave function; however, the total wave function includes a contribution $Q\Psi_N$. This may be derived from $P\Psi_N$ using the relation

$$Q\Psi = [1/(E - QHQ)]QHP\Psi\,. \tag{4.21a}$$

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

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

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

$$\left\langle \Phi_{N+1}\left|\frac{2}{r_1+r_2}\right|\frac{u_N(r_1)}{r_1}\varphi_N(r_2)\right\rangle = \int_0^\infty R_{N+1}(r)V_{N,N+1}(r)u_N(r)\,dr\,, \tag{4.22}$$

and using (4.3) for $u_N(r)$ reduces this to a form involving $K^{(0)}$ and $K^{(1)}$. One finds in fact

$$Q\Psi = q_1(N)\Phi_{N+1}\,, \tag{4.23a}$$

where

$$q_1(N) = N^2[K^{(0)} + N^{1/2}p_1(N)K^{(1)}]\,, \tag{4.23b}$$

which upon substitution reduces to

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

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

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

(ii) The second approximation we shall consider is motivated by the observation that 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

$$\mu = 0.12N \tag{4.26}$$

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

$$\Phi_{N+\mu} = (1/r_1r_2)R_{N+\mu}(r_1)R_{N+\mu}(r_2)\,. \tag{4.27}$$

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

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

On the other hand, $q_2(N)$ must be evaluated more carefully, because expression (4.21) is indeterminate. One finds nevertheless that Eq. (4.24) continues to hold. 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 re-

placed by a mean energy so that

$$\begin{aligned} v_{op}^{Q} &\to \frac{1}{E-\bar{\mathcal{E}}_N}\sum_{\nu}|PHQ\Phi_{N\nu}\rangle\langle\Phi_{N\nu}QHP| \\ &= \frac{1}{E-\bar{\mathcal{E}}_N}PHQ^2HP \\ &= \frac{1}{E-\bar{\mathcal{E}}_N}PH(Q)HP \\ &= \frac{1}{E-\bar{\mathcal{E}}_N}PV(1-P)VP, \end{aligned} \tag{4.29}$$

since $[P,H_0]=0=PQ$. In the uncoupled approximation, P reduces to

$$P\to|\varphi_N\rangle\langle\varphi_N|.$$

The optical potential v_{op}^{Q} of (2.10) becomes

$$v_{op}^{Q}=[1/(E-\bar{\mathcal{E}}_N)]\,[PV^2P-(PVP)^2], \tag{4.30}$$

where

$$V=-2/r_1+2/(r_1+r_2). \tag{4.31}$$

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

$$\begin{aligned} \langle R_N(r_2)|V^2|R_N(r_2)\rangle &\cong 4/r_1^2, \quad r_1<r_0 \\ &\cong 10N^4/r_1^4, \quad r_1>r_0. \end{aligned} \tag{4.32}$$

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

$$\begin{aligned} v_{op}^{Q} &\cong 0, \quad r_1<r_0 \\ &\cong \frac{N^4}{E-\bar{\mathcal{E}}_N}\frac{1}{r_1^4}, \quad r_1>r_0. \end{aligned} \tag{4.33}$$

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

$$\bar{\mathcal{E}}_N \propto 1/N^2. \tag{4.34}$$

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

$$|E_N-\bar{\mathcal{E}}_N|\le O(1/N^2). \tag{4.35}$$

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

$$\left(\frac{d^2}{dr^2}+V_c(r)\right)u_N(r)=0, \tag{4.36}$$

where

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

In (4.37) we have made the assumption that the optical potential in fact exceeds the dipole potential in some finite region (i.e., $r_\beta>r_0$), where r_β may be determined by the condition

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

which leads to

$$r_\beta=N(3|E_N-\bar{\mathcal{E}}_N|)^{-1/2}. \tag{4.39}$$

If (4.39) does not lead to $r_\beta>r_0$, then the equation and solution revert back to $u_N^{(0)}$ of Eq. (3.11b).

The solutions of (4.36) must again be determined by matching and one finds to lowest order, $r<r_0$,

$$u_N^{(\beta)}(r)=u_N^{(0)}(r), \tag{4.40a}$$

and for $r_0<r<r_\beta$,

$$u_N^{(\beta)}(r)\cong\begin{cases}\dfrac{r}{[2\pi(2)^{1/2}]^{1/2}}\dfrac{\cos[(8r_0)^{1/2}+\beta(1/r-1/r_0)-\frac{3}{4}\pi]}{r_0^{3/4}}, & E_N-\bar{\mathcal{E}}_N<0 \\ \dfrac{r}{[2\pi(2)^{1/2}]^{1/2}}\dfrac{\cos[(8r_0)^{1/2}-\frac{3}{4}\pi]\cosh[\beta(1/r-1/r_0)]}{r_0^{3/4}}, & E_N-\bar{\mathcal{E}}_N>0\end{cases} \tag{4.40b}$$

where

$$\beta^2=N^4/|E_N-\bar{\mathcal{E}}_N|. \tag{4.41}$$

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]

$$\mathcal{Q}=\int_0^E k_N|\eta|^2|M|^2N^3\,dw_N. \tag{5.1}$$

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

$$M=\langle\psi_N|V|\Phi_{in}\rangle, \tag{5.2}$$

which causes the transition from the unperturbed initial state

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

to a final state Ψ_N, the calculation of which we

have discussed in Secs. I–IV. 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:

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

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 is 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 absorbed in η and the calculation for u_N is done at $k_N = 0$.[10] It is important to realize that we are relying heavily on (presumed) accuracy of the distorted-wave method here. With the inclusion of coupling the rigorous validity of the k_N extrapolation would be limited by (2.6) to below the $(N+1)$ threshold, and this would not allow us to get into the ionization region. However, the falling away of the upper limit is consistent, with the dropping of coupling terms, and thus it is in the spirit of the present heuristic derivation.

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

$$E_N \to w_N = 1/N^2 . \tag{5.7}$$

This continuation is motivated by the well-known fact that a Coulomb wave for negative energy becomes a positive-energy solution by changing $N \to -i/w_N^{1/2}$ 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 w_N via (5.7), so that integration gives the E dependence of $\mathcal{Q}$ which is what we are seeking.

To gain confidence in the analytic continuation, let us consider as an example, the homogeneous solution of the H_{PP} problem, i.e., $u_N^{(0)}$ given in Eq. (3.11b). Here the matching radius is naturally taken as r_0:

$$r_m = r_0 \tag{5.8}$$

so that to leading order,

$$\frac{du_N^{(0)}}{dr} = \frac{\sqrt{2}}{r_0^{1/4}} \frac{\sin[(8r_0)^{1/2} - \frac{3}{4}\pi]}{[2\pi(2)^{1/2}]^{1/2}} ,$$

and

$$\mathcal{R}_0(r_0) = (\sqrt{2}/r_0^{1/2}) \tan[(8r_0)^{1/2} - \tfrac{3}{4}\pi] .$$

Thus using (5.5) and (5.8) for the N dependence of r_0 and α_N, we find

$$\eta \propto \frac{(r_0 \alpha_N / k_N)^{1/2}}{r_0^{1/4} \cos[(8r_0)^{1/2} - \frac{3}{4}\pi] \alpha_N \{1 + \tan^2[(8r_0)^{1/2} - \frac{3}{4}\pi]\}^{1/2}} ,$$

or finally,

$$\eta \propto \frac{r_0^{1/4}}{k_N^{1/2} \alpha_N^{1/2}} \propto \frac{1}{k_N^{1/2}} .$$

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

$$M_0 \equiv \langle [u_N^{(0)}(r_1)/r_1] \varphi_N(r_2) | V | \Phi_{\text{in}} \rangle . \tag{5.9a}$$

In Appendix D we show

$$M_0 \propto N^{-3/2} . \tag{5.9b}$$

With M being M_0 in this case and substituting for η, we find

$$\mathcal{Q}_0 \propto \int_0^E k_N \left(\frac{1}{k_N^{1/2}} \frac{1}{N^{3/2}} \right)^2 N^3 dw_N \propto \int_0^E dw_N ,$$

or

$$\mathcal{Q}_0 \propto E . \tag{5.10}$$

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-scattering cross section at threshold,[10] and this is guaranteed in our formulation by the normalization constant η. (The subscript on $\mathcal{Q}$ 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:

$$M = [1 + N^{-3/2} q_i(N)] M_0 + p_i(N) M_1 . \tag{5.11}$$

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:

$$M_1 = \langle (u_N^{(1)}/r_1) \phi_N(r_2) | V | \Phi_{\text{in}} \rangle . \tag{5.12a}$$

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

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

From (4.20) and (4.28) we see that $p_1(N)$ and $p_2(N)$ are essentially proportional to N; thus $p_i(N) \times M_1$ is smaller than the M_0 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 is one power N larger than in the $u_N^{(0)}$ case. On the other hand, the logarithmic derivative is the same,

$$\mathcal{R}_1(r_0) \cong \sqrt{2} r_0^{-1/2} \cot[(8r_0)^{1/2} - \tfrac{3}{4}\pi], \tag{5.13}$$

aside from the interchange of sine and cosine factors. The same interchange is true for $u_N^{(1)}$ vs $u_N^{(0)}$; therefore the oscillating factors continue to cancel out and we are left with

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

In comparison with η, this normalization constant is dominated by the N in the denominator which causes the threshold to contain an extra power of E

$$\mathcal{Q}_1 \propto \int_0^E w\{1 - B\sin[2(12/w)^{1/2}]\}^2 \, dw ,$$

which to leading order is

$$\mathcal{Q}_1 \propto E^2 . \tag{5.15}$$

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 a not unreasonable consequence of the repulsive optical-potential term retained. In the dominant-pole approximation, in which the term selected is at the borderline 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 obtained, together with Dr. Bhatia, numerical solutions of the exact lowest-term equations up to $N \simeq 9$ which indicates that this is the case.) This indicates that our physical understanding of the optical potential in this case is still primitive; nevertheless, the latter can be expected to have a profound effect on the threshold law. The physical effect may be an outgrowth of the two electrons having a non-negligible probability of being in regions that are excluded classically and when that happens they have a much more repulsive effect than would be expected classically.

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 b_N/r^2 in the region $r_0 < r < r_\beta$ [i.e., $r_\beta > r_0$ from (4.31)].

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

$$\eta_{2a} \propto N/(k_N r_\beta)^{1/2} . \tag{5.16}$$

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 $r_0 < r < r_\beta$ *providing* $E_N - \bar{\mathcal{E}}_N \propto -N^{-2}$:

$$M \propto M_0 \propto N^{-3/2} . \tag{5.17}$$

Thus substituting gives

$$\mathcal{Q}_{2a} \propto \int_0^E (N^2/r_\beta)\, dw_N . \tag{5.18}$$

And now considering, as implied above,

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

which implies from (4.39),

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

gives using (5.7) in (5.18)

$$\mathcal{Q}_{2a} \propto E . \tag{5.21}$$

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 $u_{ir}^{(\beta)}$ of (4.40b). Here the normalization constant turns out to be

$$\eta_{2b} \propto \frac{N}{(k_N r_\beta)^{1/2} |\cos[(8r_0)^{1/2} - \tfrac{3}{4}\pi]| \cosh[\beta(1/r_\beta - 1/r_0)]} . \tag{5.22}$$

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),

$$M \propto \{\cos[(8r_0)^{1/2} - \tfrac{3}{4}\pi]/N^3\} \times \ln r_\beta \cosh[\beta(1/r_\beta - 1/r_0)] . \tag{5.23}$$

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

$$\mathcal{Q}_{2b} \propto \int_0^E \frac{(\ln r_\beta)^2}{r_\beta} w^{1/2}\, dw . \tag{5.24}$$

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

$$\mathcal{Q}_{2b} \propto E^{5/2}(\ln E)^2 . \tag{5.25}$$

There is absolutely nothing at this time which prevents the effective optical potential, as contained in the energy difference $E_N - \overline{\mathcal{E}}_N$ from being an oscillating function of N in sign. In fact, the above-noted phenomenon wherein eigenvalues of QHQ descend below the relevant (Nth) threshold suggests just such an oscillation. Because when the state first crosses the threshold its effect is large and repulsive, but as it descends further away the attractive effect of the states above takes over until a new state descends below the new threshold.

From (4.39) we see that when $E_N - \overline{\mathcal{E}}_N$ changes sign, $r_\beta \to \infty$. If the amplitude of these oscillations is N^{-2}, then (5.18) shows that the attractive portion gives a linear rise, whereas from (5.24) the repulsive portions are essentially flat. We cannot say anything about the periodicity at this time. The apparent periodicity of the lowest state which is proportional to $N \to E^{-1/2}$ is overlaid by those of many other linearly independent states such as (2.19). One is here guided by the fact that the slope of $\mathcal{Q}$ with respect to E cannot be negative. This gives a threshold law of the form

$$\mathcal{Q}_3 \propto E[1 - C \sin(A \ln E + B)] , \tag{5.26}$$

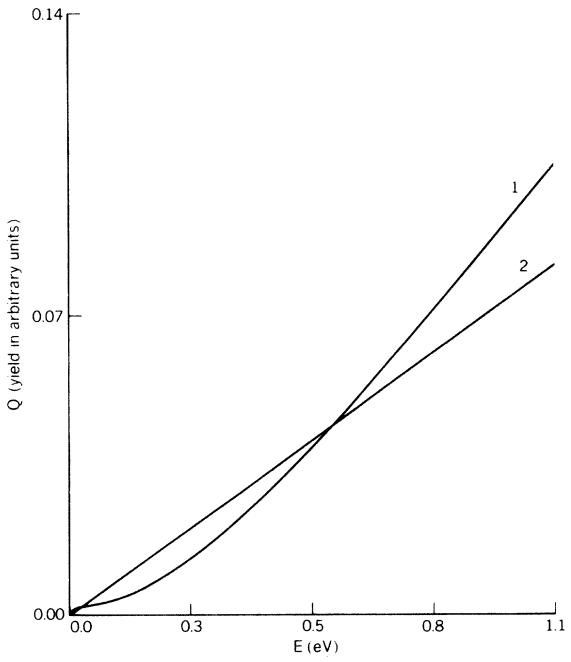

FIG. 2. $\mathcal{Q}_3$ vs E from Eq. (5.26), curve 2 ($C = \frac{1}{2}$). Note that the curve is monotonically increasing but it oscillates (infinitely rapdily as $E \to 0$) about $\mathcal{Q} = E$ (curve 1).

where A, B, and C are constants, and in order for the slope to be non-negative we must have $|C| \leq 2^{-1/2}$. That the slope of $\mathcal{Q}$ cannot be negative follows from (5.1), because the integrand is positive definite, and from (5.4) which implies that the k_N factors cancel. Thus the integrand is a non-negative function of w_N only, so that

$$\frac{\partial \mathcal{Q}}{\partial E} = \frac{\partial}{\partial E} \int_0^E g(w_N)\, dw_N = g(E) \geq 0 . \tag{5.27}$$

This is equivalent to saying that the yield $\mathcal{Q}$ itself must be a monotonically increasing function of E.

In Fig. 2 we have plotted $\mathcal{Q}$ for $A = 1$, $B = 0$, $C = \frac{1}{2}$. It can be seen that such a threshold law can be distinctly nonlinear even in the experimentally accessible region. In addition the oscillations about $\mathcal{Q} = E$ continue with ever-increasing frequency right down to the origin. Finally, the non-negative oscillations in $\partial \mathcal{Q}/\partial E$ imply ever-increasing oscillations in the energy-distribution cross section between the two outgoing electrons, which is in sharp contrast to what is expected from the semiclassical theory.[11]

VI. DISCUSSION

We have not attempted to derive a unique threshold law. Our purpose in this paper has been to present what we believe is a 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 attraction dominates in the potential as a whole. The repulsive approximations can lead to a considerable diminution even beyond a simple phase-space (PS) dependence on E:

$$\mathcal{Q}_{\rm PS} \propto \int d^3k_1\, d^3k_2\, \delta(E - k_1^2 - k_2^2) \propto E^2 . \tag{6.1}$$

Conventional wisdom on the subject might have dictated that we delete those approximations which lead to a higher power than 2; 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. For example, with that approach one would derive the same Wannier power law when the r_{12}^{-1} interaction

is replaced by our model interaction $(r_1+r_2)^{-1}$.[11] But from our treatment it would be very difficult to obtain such a result. This derives, we believe, from the fact that the Wannier approach is essentially a perturbation expansion around $r_2/r_1 \simeq 1$, whereas we have tried very hard to make no assumption of the magnitude of r_1 relative to r_2. This appears to have the effect of uncovering possible quantum-mechanical effects which would otherwise lay hidden in a series expansion in powers of $\hbar$. Of these possibilities an oscillating-derivative threshold law is clearly the most provocative. This makes a reliable calculation of $\overline{\mathcal{E}}_N$ a desirable initial endeavor as part of the general problem of synthesizing the optical potential in a definitive manner.

ACKNOWLEDGMENT

We would like to thank Dr. A. K. Bhatia not only for his contributions mentioned in the text, but for many further calculations along the lines of Ref. 1, which include the $2/r_{12}$ results in Table I. We would also like to thank Edward Sullivan for programming the model calculations and the graphs.

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:

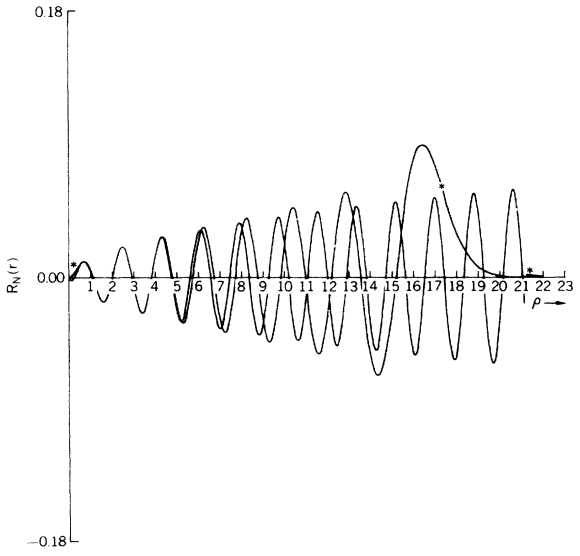

FIG. 3. Radial function $\mathfrak{R}_N(r)$ for $N=15$ (denoted by *) vs the approximation (A1). The abscissa is $\rho = (\frac{2}{5}r)^{1/2}$ so that the average value of $r_{NN}=\frac{3}{2}N^2$ occurs at $\rho = N$. Beyond $r=2r_0$ the approximation in (A1) is denoted by * and is barely distinguishable from the exact curve.

$$R_N(r) \cong \frac{(2r)^{1/4}}{(\pi N^3)^{1/2}} \cos[(8r)^{1/2} - \tfrac{3}{4}\pi], \quad r<2r_0$$
$$\cong C_N e^{-r/N} r^N, \quad r>2r_0. \tag{A1}$$

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

$$C_N = (-1)^{N-1} 2^N / N^{3/2} N\,!\, N^{N-1}. \tag{A2}$$

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 asymptotic 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 right-hand side of (A1) is divided into two regions at $r=2r_0$. The fit of R_N by the right-hand side of (A1) 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 and $\frac{4}{3}r_0 = 2N^2$, particularly around $r \lesssim r_0$, and they are much more accurate than (A1). However, reference to Fig. 3 shows that the exact function is somewhat larger than (A1) 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 right-hand side of (A1) at $r=2r_0$. For this reason we believe, for integration purposes, these compensating effects are adequately accounted by simply continuing the right-hand side to $r=2r_0$. From (4.9),

$$u_N^{(1)} = v_N^{(0)}(r) I(r) + u_N^{(0)} II(r), \tag{A3}$$

with

$$I(r) = 2\pi \int_0^r u_N^{(0)}(x) R_{N+1}(x) V_{N,N+1}(x)\, dx \tag{A4}$$

and

$$II(r) = 2\pi \int_r^\infty v_N^{(0)}(x) R_{N+1}(x) V_{N,N+1}(x) dx. \tag{A5}$$

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

$$I(r) \propto \sqrt{N} \int_0^r [x^{1/2}/(r_1+2x)^2] \times \cos^2[(8x)^{1/2} - \tfrac{3}{4}\pi]\, dx. \tag{A6}$$

Replacing the cosine-square factor by its average value ($\frac{1}{2}$) gives

$$I(r) \propto N^{1/2} \left[-\frac{r^{1/2}}{r_0+r} + \frac{1}{(2r_0)^{1/2}} \tan^{-1}\left(\frac{2r}{r_0}\right)^{1/2} \right]. \tag{A7}$$

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

$$II_<(r) \cong \int_r^{r_0} v_N^{(0)}(x) R_{N+1}(x) V_{N,N+1}(x)\, dx \qquad \text{(A8)}$$

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

$$II_<(r) \propto \frac{N^{1/2}}{\xi r_0^2} \int_{r^{1/2}}^{r_0^{1/2}} y^2 \sin[2(\sqrt{8}y - \tfrac{3}{4}\pi)]\, dy\,. \qquad \text{(A9)}$$

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

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

has also been used in deriving (A9). Here the sinusoidal factor cannot be dropped because its mean value is zero, but (A9) can be integrated to give

$$\begin{aligned} II_<(r) \propto (N^{1/2}/r_0^2)(4\sqrt{8}\{&r_0^{1/2}\cos[2(8r_0)^{1/2}] \\ &- r^{1/2}\cos[2(8r)^{1/2}]\} \\ &+ [4(8r_0) - 2]\sin[2(8r_0)^{1/2}] \\ &- [4(8r) - 2]\sin[2(8r)^{1/2}])\,. \end{aligned} \qquad \text{(A10)}$$

The expressions (A10) and (A7) into (A3) are to be used in Eq. (4.12). Note that the N dependence of $II(r)$ is dominated by the second term and that (for $r \neq r_0$) it is

$$II_<(r) \propto 1/N^{3/2}\,. \qquad \text{(A11)}$$

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 $II_>(r)$,

$$\begin{aligned} II_>(r) &\propto \left| \int_{r_0}^{2r_0} v_N^{(0)} R_{N+1} V_{N,N+1}\, dr \right| \\ &\propto \left| \int_{r_0}^{2r_0} \frac{r^{1/2}}{r_0^{1/4}} \sin[\alpha_N \ln(r/r_0) \right. \\ &\qquad \left. + (8r_0)^{1/2} - \tfrac{3}{4}\pi] \frac{r_0 R(r)\, dr}{(r_0 + 2r)^2} \right|. \end{aligned}$$

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

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

gives, aside from numerical factors,

$$\begin{aligned} &\left| \int_{r_0}^{2r_0} v_N^{(0)} R_{N+1} V_{N,N+1}\, dr \right| \\ &\qquad \leq \frac{1}{N^{1/2}} \left| \int_0^{\ln 2} e^{-y/4} \sin[\sqrt{3}Ny + (\text{const.})\, dy] \right|, \end{aligned}$$

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

$$\begin{aligned} &\left| \int_{r_0}^{2r_0} v_N^{(0)} R_{N+1} V_{N,N+1}\, dr \right| \\ &\qquad \leq \frac{1}{N^{1/2}} \left| \int_0^{\infty} e^{-y/4} \sin[\sqrt{3}Ny + (\text{const.})]\, dy \right| \\ &\qquad \leq \frac{1}{N^{1/2}} \frac{\sqrt{3}N}{\frac{1}{16} + (\sqrt{3}N)^2} = O(1/N^{3/2})\,. \end{aligned}$$

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

$$\lim_{N\to\infty} II(r) \propto II_< + II_> = O(1/N^{3/2})\,. \qquad \text{(A12)}$$

We next show that the contribution to $II(r)$ [and also for the similar contribution to $I(r)$] from $2r_0 < x < \infty$ is truly negligible. Using (A1), (4.8), (3.11), or (4.11), we find

$$\int_{2r_0}^{\infty} \begin{Bmatrix} u_N^{(0)} \\ v_N^{(0)} \end{Bmatrix} V_{N,N+1} R_{N+1}\, dr \propto \frac{C_{N+1}}{r_0^{1/4}} N^2 \int_{2r_0}^{\infty} r^{1/2} \begin{Bmatrix} \sin \\ \cos \end{Bmatrix} [\alpha_N \ln(r/r_0) + (8r_0)^{1/2} - \tfrac{3}{4}\pi] \frac{e^{-r/N+1}}{r^2} r^{N+1}\, dr\,.$$

Use of $r_0 \propto N^2$ shows the right-hand side is bounded by

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

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

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

which using Stirling's formula, is

$$\propto e^{N(\ln 6 - 2)} \simeq e^{-0.21N}\,,$$

or finally,

$$\int_{2r_0}^{\infty} \begin{Bmatrix} u_N^{(0)} \\ v_N^{(0)} \end{Bmatrix} V_{N,N+1} R_{N+1}\, dr \leq e^{-0.21N}\,.$$

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

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

Consider the first term in curly brackets; using (A12),

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

which is to leading order is proportional to

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

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

$$N^{1/2} \int_0^{r_0} \frac{r^{1/4}\cos[(8r)^{1/2} - \frac{3}{4}\pi]\, v_N^{(0)}(r) I(r)\, dr}{(r_0+2r)^2} \propto N^{1/2} \int_0^{r_0} \frac{r^{1/2}\sin\{2[(8r)^{1/2} - \frac{3}{4}\pi)]\}}{(r_0+2r)^2} N^{1/2}\left[\frac{-r^{1/2}}{r_0+r} + \frac{1}{(2r_0)^{1/2}} \tan^{-1}\left(\frac{2r}{r_0}\right)^{1/2}\right]$$

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

Now use Dwight's[13] equation (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 proportional to

$$\frac{N}{r_0} r_0^{1/2} \frac{\sin[2(8r_0)^{1/2}\pi]}{2[2(8r_0)^{1/2}]^2} \int_0^1 g(\rho)\, d\rho \propto \frac{\sin(2\sqrt{12}N\pi)}{N^2}\,.$$

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 AVERAGE ENERGY $\bar{\mathcal{E}}_N$

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

(i) Since V assumes the form

$$V = \frac{-2}{r_1} + \frac{2}{r_1 + r_2} = -\frac{2r_2}{r_1(r_1+r_2)} \to \begin{cases} -2r_2/r_1^2, & r_1 \gg r_2 \\ -2/r_1, & r_1 \ll r_2 \end{cases} \tag{C1}$$

we simply set

$$\langle \varphi_N V^2 \varphi_N \rangle \cong \frac{4}{r_1^2} \int_0^\infty \varphi_N^2\, dr_2 = \frac{4}{r_1^2}\,, \quad r_1 < r_0$$

$$\cong \frac{4}{r_1^4} \int_0^\infty r_2^2 \varphi_N^2\, dr \cong \frac{10N^4}{r_1^4} \quad r_1 > r_0 \tag{C2}$$

and, from (3.7),

$$\langle \varphi_N V \varphi_N \rangle^2 \equiv (V_{N,N})^2 \cong \begin{cases} 4/r_1^2, & r_1 < r_0 \\ b_N^2/r_1^4 = 9N^4/r_1^4, & r_1 > r_0 \end{cases} \tag{C3}$$

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

$$\mathfrak{V}_{op}^Q \cong \begin{cases} 0 \text{ [to order } O(1/r_1)] & r_1 < r_0 \\ \dfrac{N^4}{E - \bar{\mathcal{E}}} \dfrac{1}{r_1^4}, & r_1 > r_0 \end{cases}$$

or

$$\mathfrak{V}_{op}^Q = \frac{N^4}{E - \bar{\mathcal{E}}} \frac{\Theta(r_1 - r_0)}{r_1^4}\,, \tag{C4}$$

where Θ is the unit step function.

The approximation involved in (C2) is essentially the same as that employed in the evaluation of V_{NN} and (C3), so that $\mathfrak{V}_{op}^Q$ is the form (C4) 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_{Cl}^Q:

$$G^Q \equiv \frac{Q}{Q(E-H)Q} \to \frac{Q}{E - \bar{\mathcal{E}}} \equiv G_{Cl}^Q\,. \tag{C5}$$

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

$$G^Q \cong \frac{|Q\phi\rangle\langle\tilde{\phi}Q|}{\langle\tilde{\phi}Q(E-H)Q\phi\rangle} \equiv G_S^Q\,. \tag{C6}$$

It is to be emphasized here that the final-state wave function we are trying to calculate corresponds to the elastic scattering from the Nth 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

$$\mathcal{T}_{fi}^{Q} = \langle \chi_f G^{Q} \chi_i \rangle , \tag{C7}$$

with

$$\chi_i = QVP\Psi_i^{P} , \quad \chi_f = QVP\Psi_f^{P} . \tag{C8}$$

We *require* that both (C5) and (C6) give the *same* $\mathcal{T}_{fi}^{Q}$. That is,

$$\langle \chi_f G_S^{Q} \chi_i \rangle \equiv \langle \chi_f \, Q/(E - \bar{\mathcal{E}})\chi_i \rangle , \tag{C9}$$

which gives then the connection between $\bar{\mathcal{E}}$ and $\langle Q\phi, Q\tilde{\phi} \rangle$. Substituting for G^{Q} as given by (C6) allows (C9) to be solved for $\mathcal{E}$ in the form

$$\bar{\mathcal{E}} = E\left(1 - \frac{\langle \chi_f \chi_i \rangle \langle \tilde{\phi} Q\phi \rangle}{\langle \chi_f Q\phi \rangle \langle \tilde{\phi} Q\chi_i \rangle}\right) + \left(\frac{\langle \chi_f \chi_i \rangle}{\langle \chi_f Q\phi \rangle \langle \tilde{\phi} Q\chi_i \rangle} \langle \tilde{\phi} QHQ\phi \rangle\right) . \tag{C10}$$

Thus far, the trial functions $Q\phi$ and $Q\tilde{\phi}$ are left arbitrary, except the normalization (linear) parameter which was eliminated by writing G_S^{Q} in the normalization-independent form (C6). Now, we choose these trial functions such that (C10) assumes a simple form, i.e., let

$$Q\phi = \chi_i , \quad Q\tilde{\phi} = \chi_f . \tag{C11}$$

Substitution of (C11) into (C10) immediately reduces to a form

$$\bar{\mathcal{E}} = \frac{\langle \chi_f QHQ\chi_i \rangle}{\langle \chi_f \chi_i \rangle} \equiv \frac{B}{D} , \tag{C12}$$

where, using (C8), we can write

$$\begin{aligned} B &= \langle \chi_f QHQ\chi_i \rangle = \langle P\Psi_f^{P} PVQHQVP\Psi_i^{P} \rangle , \\ D &= \langle \chi_f \chi_i \rangle = \langle P\Psi_f^{P} PVQVP\Psi_i^{P} \rangle . \end{aligned} \tag{C13}$$

We can explicity estimate the N dependence of B and D for $\bar{\mathcal{E}}_N$ using the result of Sec. III for the case

$$P\Psi_i^{P} = P\Psi_f^{P} = \frac{u_N^{(0)}(r)}{r_1} \phi_N(r_2) .$$

First, consider the constant D, which becomes (using $Q = 1 - P$), as in (C4),

$$\begin{aligned} D &= \int_0^{\infty} dr_1 \, [u_N^{(0)}(r_1)]^2 \langle \varphi_{N1} [V^2 - (V_{N,N})^2] \varphi_N \rangle \\ &\cong \int_0^{\infty} dr_1 \, [u_N^{(0)}(r_1)]^2 (N^4/r_1^4)\Theta(r_1 - r_0) \\ &\cong N^4 \int_{r_0}^{\infty} dr_1 \, [u_N^{(0)}(r_1)]^2 r_1^{-4} . \end{aligned}$$

Using (3.11b) for $u_N^{(0)}$ (the part for $r > r_0$) and replacing

$$\cos^2[\alpha_N \ln(r/r_0) - (8r_0)^{1/2} - \tfrac{3}{4}\pi]$$

by $\frac{1}{2}$, we get for the integral,

$$\int_0^{\infty} dr \, [u_N^{(0)}(r)]^2 r^{-4} \propto \frac{1}{r_0^{1/2}} \int_{r_0}^{\infty} r^{-3} \, dr \propto \frac{1}{N^5} .$$

Thus

$$D \propto N^4/N^5 \propto 1/N . \tag{C14}$$

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

$$B = \langle P\Psi^{P} PVQHQVP\Psi^{P} \rangle , \tag{C15}$$

where

$$\begin{aligned} &P\Psi^{P} = U_N^{(0)}(1)\varphi_N(2) , \\ &U_N^{(0)}(1) = u_N^{(0)}(r_1)/r_1 , \\ &H = h_1 + h_2 + v , \\ &P = |\varphi_N(2)\rangle\langle\varphi_N(2)| ; \quad Q = 1 - P . \end{aligned}$$

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

$$QHQ = Q(h_1 + h_2 + v)Q = Qh_1 + Qh_2 - E_N Q + QvQ , \tag{C16}$$

so that

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

where the four terms come directly from the substitution of (C16) into (C15). Consider first

$$\begin{aligned} B_1 &= \langle U_N^{(0)} \phi_N(2) VQh_1 VU_N^{(0)}(1)\phi_N(2) \rangle \\ &= \langle U_N^{(0)}(1) V_{NN}(1) h_1 U_N^{(0)}(1) \rangle \\ &\quad - \langle U_N^{(0)}(1) V_{NN}(1) h_1 U_N^{(0)}(1) \rangle \\ &= 0 . \end{aligned} \tag{C17}$$

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

$$\begin{aligned} B_2 + B_3 = \langle U_N^{(0)}(1)\varphi_N(2) \,|\, Vh_2 V \,|\, U_N^{(0)}(1)\varphi_N(2) \rangle \\ - E_N \langle U_N^{(0)}(1)(V^2)_{NN} U_N^{(0)}(1) \rangle \end{aligned} \tag{C18}$$

and

$$B_4 = \langle U_N^{(0)}(1)[(VvV)_{NN} - 2(Vv)_{NN} + (V_{NN})^2 v_{NN}]U_N^{(0)}(1)\rangle \tag{C19}$$

where in our approximation

$$v \equiv \frac{2}{r_1 + r_2} \cong \begin{cases} 0, & r < r_0 \\ 2/r_1 - 2r_2/r_1^2, & r_1 > r_0 . \end{cases} \tag{C20}$$

Each of these terms may be evaluated in a straightforward manner except for the first term of (C18). In that case we use our approximation for V (but we neglect the cusp) before differentiating to find

$$\langle U_N^{(0)}(1)\varphi_N(2) Vh_2 V U_N^{(0)}(1)\varphi_N(2)\rangle = E_N\langle U_N^{(0)}(1)(V^2)_{NN}U_N^{(0)}(1)\rangle + \frac{(\text{const.})}{N^3} + O\left(\frac{\cos(2\sqrt{12}N)}{N^7}\right). \tag{C21}$$

The first term of (C21) cancels with the second term of (C18). All the remaining terms are of order N^{-3}. Thus

$$B \propto 1/N^3 , \tag{C22}$$

so that combining that with (C14), we get finally

$$\bar{\mathcal{E}}_N = \frac{B}{D} \propto \frac{1/N^3}{1/N} \propto N^{-2} . \tag{C23}$$

APPENDIX D: EVALUATION OF TRANSITION MATRIX ELEMENTS

We want to find the N dependence of M in the various approximations we have used. The $P\Psi$ part of M is

$$M_{P\Psi} \equiv \langle [u_N(r_1)/r_1]\varphi_N(r_2) \,|\, V \,|\, \Phi_{\text{in}}\rangle \propto \int_0^\infty \int_0^\infty dr_1\, dr_2\, u_N(r_1) R_N(r_2) \times [-2/r_1 + 2/(r_1 + r_2)] \sin kr_1\, R_1(r_2) . \tag{D1}$$

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

$$\frac{2}{r_1 + r_2} = \frac{2}{r_1} - \frac{2r_2}{r_1^2} . \tag{D2}$$

Thus

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

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 $\sin kr$ (which are independent of N). And because $(0 < \gamma \leq 1)$

$$u_N(r) \leq (r/r_0^{3/4})^\gamma \times (\text{sinusoidal function of } r) ,$$

the second integral always converges and is proportional to $N^{-3\gamma/2}$. Thus, the second term in (D4) is negligible compared to the first term. This is true whether $u_N(r)|_{r>r_0}$ is either the attractive $u_N^{(\beta)}$ of (4.40b) or simply $u_N^{(0)}(r > r_0)$ of (3.11b). Thus the N dependence of $(ME)_{p\Psi}$ is controlled by the first term of (D4) and this in turn is determined by $\langle N \,|\, r_2 \,|\, 1\rangle$ which is, trivially,

$$\langle N \,|\, r_2 \,|\, 1\rangle \propto 1/N^{3/2} . \tag{D5}$$

M_0 is a special case of $M_{p\Psi}$, so that we have finally

$$M_0 \propto M_{p\Psi}|_{\text{attractive } r^{-4}} \propto N^{-3/2} \tag{D6}$$

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

$$Q\Psi = [1/(E_N - \bar{\mathcal{E}}_N)]QVP\Psi . \tag{D7}$$

Assuming

$$Q\Psi = \vartheta_N(1)\varphi_{N+1}(z) , \tag{D8}$$

and using $P\Psi = U_N(1)\varphi_N(2)$, $Q = 1 - |\varphi_N\rangle\langle\varphi_N|$, one can reduce (D7) to

$$\vartheta(1) = V_{N,N+1}(r_1)U_N(1)/(E_N - \bar{\mathcal{E}}_N) . \tag{D9}$$

To calculate the Q part of matrix element

$$M_{Q\Psi} = \int Q\Psi V\Phi_{\text{in}} , \tag{D10}$$

we bound the $r < r_0$ contribution by

$$V_{N,N+1} \propto \frac{N^2}{(r + r_0)^2} \leq \frac{N^2}{r_0^2} \propto \frac{1}{N^2} . \tag{D11}$$

Thus

$$M_{Q\Psi} = \frac{1}{E_N - \bar{\mathcal{E}}_N}\int U_N(1)\varphi_N(2) V_{N,N+1} V\Phi_{\text{in}} \leq \frac{1}{N^2(E_N - \bar{\mathcal{E}}_N)}\int P\Psi V\Phi ,$$

or finally

$$M_{Q\Psi} \propto [N^2(E_N - \bar{\mathcal{E}}_N)]^{-1} M_{p\Psi} . \tag{D12}$$

Note that as long as $|E_N - \bar{\mathcal{E}}_N| \propto N^{-2}$, both the

$P\Psi$ and $Q\Psi$ contributions to M have the same N dependence. However, if $|E_N - \bar{\mathcal{E}}_N| < O(1/N^2)$, then the $Q\Psi$ contribution dominates.

We next consider the repulsive β^2/r^4 case which is now dominated by the contribution from r_0 to r_β. Using (4.40c) in the second term of (D4),

$$\int_{r_0}^{r_\beta} \frac{u_N(r)\sin kr\,dr}{r^2} \propto \frac{\cos[(8r_0)^{1/2} - \frac{3}{4}\pi]}{N^3} \times \int_{r_0}^{r_\beta} dr \frac{\cosh[\beta(1/r - 1/r_0)]}{r}. \tag{D13}$$

Integration by parts gives

$$\int_{r_0}^{r_\beta} (dr/r)\cosh[\beta(r^{-1} - r_0^{-1})] = \ln r \cosh[\beta(r^{-1} - r_0^{-1})]\Big|_{r_0}^{r_\beta} + \int_{r_0}^{r_\beta} dr(\ln r/r^2)\sinh[\beta(r^{-1} - r_0^{-1})]. \tag{D14}$$

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

$$M_{p\Psi}\big|_{\text{repulsive } r^{-4}} \propto \frac{\cos[(8r_0)^{1/2} - \frac{3}{4}\pi)]}{N^3} \ln r_\beta \cosh\left[\beta\left(\frac{1}{r_\beta} - \frac{1}{r_0}\right)\right]. \tag{D15}$$

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

$$M_1 = \int_0^\infty \int_0^\infty u_N^{(1)}(r_1) R_N(r_2)[2/(r_1 + r_2)] \times \sin kr_1\, R_1(r_2)\, dr_1\, dr_2, \tag{D16}$$

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

$$I(r) \to \begin{cases} r^3/N^{7/2}, & r \to 0 \\ N^{-1/2}, & r \to r_0 \end{cases} \tag{D17}$$

$$II(r) \propto N^{-3/2}, \quad 0 < r < r_0 \tag{D18}$$

Thus the two contributions to M_1 are

$$M_{11} \propto \langle N|r_2|1\rangle \int v_N^{(0)}(r) I(r) \times (2/r^2)\sin kr\, dr \propto \frac{1}{N^{3/2}} \int v_N^{(0)}(r) I(r)(2/r^2)\sin kr\, dr \tag{D19}$$

and

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

Considering the latter first and using (D18),

$$M_{12} \propto N^{-3} \int_0^\infty \frac{u_N^{(0)}(r)\sin kr}{r^2}\, dr. \tag{D20}$$

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

$$M_{12} \propto N^{-3}. \tag{D21}$$

For M_{11}, we have

$$M_{11} \propto \frac{1}{N^{3/2}} \int \frac{v_N^{(0)}(r) I(r)}{r^2} \sin kr\, dr. \tag{D22}$$

If we use $N^{-1/2}[1 - e^{-(r/N)^3}]$ to interpolate on $I(r)$ from (D17) and put all sinusoidal factors equal to 1, we can bound M_{11} by

$$M_{11} \leq \frac{1}{N^2} \int_0^{r_0} \frac{r^{1/4}}{r^2}[1 - e^{-(r/N)^3}]\, dr. \tag{D23}$$

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

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

Thus, to leading order

$$M_1 = M_{11} + M_{12} \propto 1/N^3. \tag{D25}$$

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