Lowest inelastic He^- autodetachment state ($^2P^\circ$) in a Feshbach resonance

A. K. Bhatia and A. Temkin
Atomic Physics Office, Laboratory for Astronomy and Solar Physics, Goddard Space Flight Center, Greenbelt, Maryland 20771
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The lowest inelastic ($^2P^\circ$) resonance in the scattering of electrons from helium is recalculated using the quasiprojection formalism. An eigenvalue has been found at 20.52 eV using a closed-shell target ground-state quasiprojector, and is confirmed by using an open-shell target projector (yielding $\mathcal{E} = 20.56$ eV). The width is also calculated and is very large: $\Gamma = 0.44$ eV, thus unambiguously showing that the well-known experimental structure at $\sim$20.3 eV is a Feshbach and not a shape resonance. The associated *nonresonant* continuum phase shift reveals a pronounced enhancement beyond the 2^1S threshold. This finding supports the observational inference of a second $^2P^\circ$ (shape) resonance at 20.8 eV by Phillips and Wong.

The enhancement of the threshold excitation cross section of the $2\,^3S$ state in e-He scattering provides perhaps the earliest experimental evidence of a resonance in atomic (as opposed to nuclear) physics.[1] Modern observations of this resonance using narrower-resolution beams commence with the experiment of Schulz and Fox,[2] which was immediately followed by an initial application in atomic physics of the Breit-Wigner theory by Baranger and Gerjuoy.[3] Although many experiments have since been done,[4] we show in Fig. 1, both for the historical record and because it is still quite adequate for the calculation problem, the $2\,^3S$ excitation cross section as observed by Schulz and Fox.[2]

Theoretical calculations have also been carried out. A close-coupling calculation by Burke, Cooper, and Ormonde[5] identified the resonance as $^2P^\circ$, and more recent calculations[6,7] have considerably refined and improved the quantitative agreement. Because the resonance is wide, and the decay occurs mainly in the close lying but open $2\,^3S$ channel, it was assumed that this was a shape resonance.[6,7] This designation was further supported by a recent inelastic quasiprojection of our own[8] which when originally carried out did *not* locate a $^2P^\circ$ state below the $2\,^1S$ threshold and thus seemed consistent with the above $^2P^\circ$ as a shape resonance.[9]

Very recently, however, Chung[10] has calculated a $^2P^0$ eigenvalue at $\sim$20.5 eV using a newly developed hole-projection technique.[11] In the light of the considerations of the above paragraph, this result was unexpected and yet significant if it were true. In order to test it we have redone our $^2P^\circ$ calculations, using, however, our original quasiprojector program.[12] That program only projects out the ground state, but fortunately most configurations that one needs to describe this inelastic $^2P^\circ$ resonance are automatically orthogonal to the ^3S symmetry (including exchange); thus one can simply include them with no further projection required.

The main reason for reverting to our original program[12] was that it allows a correlated (specifically an open-shell) ground-state function $\phi_0^{(\text{open})}$ to be used in our quasiprojectors. Secondly, use of the original program provided the basis for the calculations of the width, which is a second crucial factor to be compared with experiment. (Both points will be further dis-

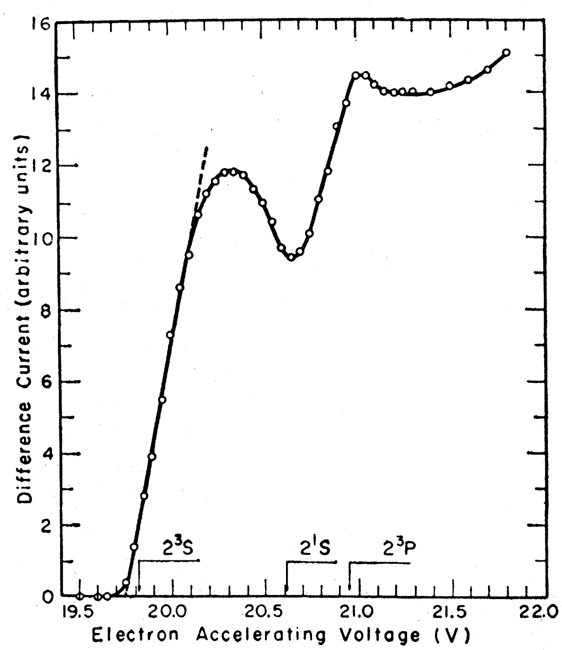

FIG. 1. Metastable helium excitation from Schulz and Fox (Ref. 2, reproduced with the kind permission of Rose Schulz).

cussed after we present our results.)

We will say little about the details of the calculation (cf. Ref. 12); it consists of minimizing the functional I,

$$I=\langle\Phi\hat{Q}H\hat{Q}\Phi\rangle/\langle\hat{Q}\Phi,\hat{Q}\Phi\rangle \quad . \tag{1}$$

$\hat{Q}$ is a quasiprojector operator which eliminates the target states; in this case $\hat{Q}$ is confined to ground-state projectors, which are outer products of $\phi_0(1\,^1S)$; ϕ_0 can in principle be represented in any desired approximation. Φ is a configuration-interaction total wave function. Above the $2\,^3S$ threshold, it is in general necessary that $\hat{Q}$ include projectors to eliminate $\phi_1(2\,^3S)$ as well[13]; that is unnecessary here because Φ is confined to configurations which are orthogonal to ^3S symmetry. With angular configurations labeled $(l_1,l_2)\,^1L_{12}l_3\,^2P\rangle$, the following configurations satisfy $\langle\phi_1(^3S),(l_1,l_2)\,^1L_{12}l_3\,^2P\rangle=0$: $(0,0)\,^1S\,1\,^2P\rangle$, $(0,1)\,^1P\,2\,^2P\rangle$, $(0,2)\,^1D\,1\,^2P\rangle$, $(0,2)\,^1D\,3\,^2P\rangle$, $(0,3)\,^1F\,2\,^2P\rangle$. Note that these orthogonalities are true for the exact $\phi_1(^3S)$ or any approximations to it.

Table I presents a compilation of results. The position results are subdivided according to which ϕ_0 was used in the quasiprojectors.[12] Referring to the $\phi_0^{(\text{closed})}$ column, we see that the position descends distinctly below He$(2\,^1S)$ threshold by the time we have used a total wave function consisting of 19 terms. (We emphasize that energy differences are calculated from the exact and not the approximate ground-state energy.[12]) Our closed-shell results are to be compared with those of Chung.[8]

The results of the respective calculations are gratifyingly close to each other, but we would emphasize that neither of these closed-shell calculations is completely convincing. This is so because the binding energy of the autodetaching state relative to the next open threshold (2^1S) is about 0.12 eV, which is much smaller than the proximity of the closed-shell energy (used in the quasiprojector) from the exact ground state (that difference being $\Delta E_0^{(\text{closed})}=1.53$ eV). The main correlation needed in improving the target state is the radial correlation of which the major part is described by the open-shell approximation $\phi_0^{(\text{open})}$ (which yields $E_0^{(\text{open})}-E_0^{(\text{closed})}=0.76$ eV). We emphasize that in addition to its improved energy, $\phi_0^{(\text{open})}$ is nonseparable; the ability of the quasiprojection formalism to encompass a correlated target state we consider to be its greatest strength.[12] The open-shell results are given in the third column of Table I, and one sees that they confirm a resonance below the $2\,^1S$ threshold. (Note, however, that in accord with Chung's theorem[11] the energy is raised in relation to the $\phi_0^{(\text{closed})}$ result.)

We have also computed the partial widths

$$\Gamma_n=2k_n|\langle\hat{P}\Psi_n'H\hat{Q}\Phi\rangle|^2 \tag{2}$$

for autodetachment to the ground state, $n=0$, and to the first excited $(2\,^3S)$ state, $n=1$. For the nonresonant scattering function we have used the exchange approximation

$$\hat{P}\Psi_n'=\mathcal{A}[u_{k_n}(\vec{r}_i)\phi_n(x_j,x_k)] \tag{3}$$

in which the radial functions $u_{k_n}(\vec{r})=(1/r)u_n(r)\times Y_{10}(\Omega)$ are determined by

$$\int Y_{10}(\Omega)\phi_n(x_2,x_3)(H-E_n^{(\text{tot})})\hat{P}\Psi_n'\,dr^{(1)}=0 \quad . \tag{4}$$

{The ground-state approximations are well known.[12]

TABLE I. Results for e-He $(^2P^o)$ resonance (in eV). (The $2\,^3S$ and $2\,^1S$ thresholds are at 19.8236 and 20.6162 eV, respectively.)

Physical quantity	$\mathcal{E}$		Γ_{2^3S}	Γ_{1^1S}
Target ground state			$\phi_0^{(\text{closed})}$	
Target $2\,^3S$ state	$\phi_0^{(\text{closed})}$	$\phi_0^{(\text{open})}$	$\phi_1^{(\text{open})}$	$\phi_0^{(\text{closed})}$
No. of radial configurations				
15	20.703 39	20.739 36		
19	20.557 26	20.580 55	0.326	0.0018
23	20.556 74	20.578 59	0.364	0.0021
31	20.526 05	20.561 43	0.424	0.0024
40	20.524 89	20.560 29	0.437	0.0024
Chung[a]	(20.536, 20.495)[a]			
Experiment[b]	20.3 ± 0.3		(Total width) 0.5	

[a] Reference 10. The two results correspond to two somewhat different calculations.
[b] The experimental results represent a rough average of the results of those in Refs. 4 and 2.

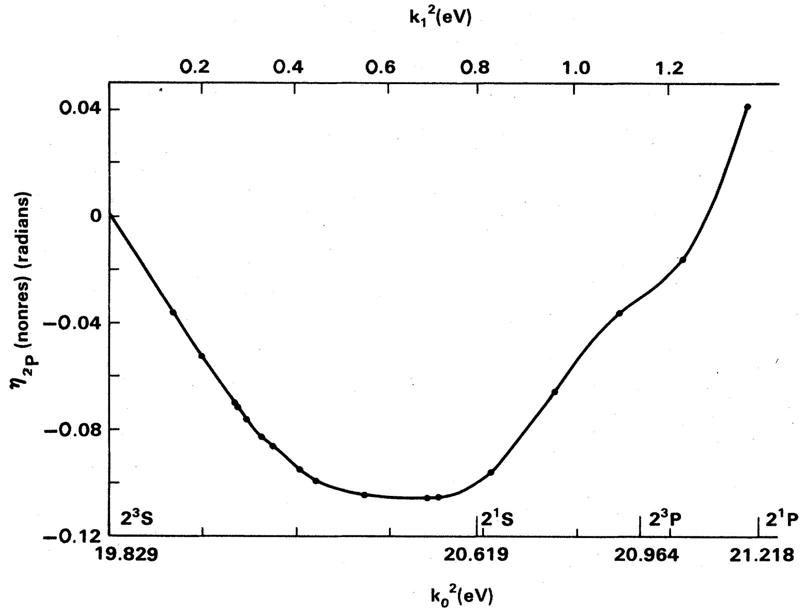

FIG. 2. Nonresonant phase shift for ^2P wave scattering from He ($2\,^3S$).

For $\phi_1(2\,^3S)$ we use $\phi_1^{(\mathrm{open})}=\exp[-(2r_1+0.32r_2)]-(1\rightarrow 2).\}$

Results are given in the fourth and fifth columns of the table. The main finding is that the total width, $\Gamma_t=0.44$ eV, is large and in general accord with the experiment[4] (cf. for example Fig. 1). In fact, to our knowledge, this is the largest width of any neutral target Feshbach resonance that has ever been calculated. One also sees the total width, $\Gamma_t=\Gamma_{2\,^3S}+\Gamma_{1\,^1S}$, is dominated by the partial width to $2\,^3S$ state. This same behavior was found by us in an e-O VII calculation,[14] and the reason for it, which is in fact quite general, is that the oscillations of the inelastic continuum orbital (in this case k_1p) match those of one of the excited electrons (in this case $2p$). Specifically both $2p$ and k_1p ($k_1 << k_0$) have essentially no nodes, whereas k_0p oscillates rapidly, which causes much greater cancellation in the matrix element. Note also that this type of Feshbach resonance, wherein the symmetry but not the orbitals of the core state ($1s2s\,^1S\rightarrow 1s2s\,^3S$) is altered in the autoionization process, has no counterpart for the one-electron target.

That autodetachment to $2\,^3S$ dominates should not be confused with the idea that $\hat{Q}\Phi$ itself must contain a substantial amount of $\Phi_1(2\,^3S)$ (in fact, it contains none). However, nothing precludes the possibility than an additional enhancement in the nonresonant phase shift might be contributing significantly to this resonance. To examine that we plot in Fig. 2 the phase shift associated with our nonresonant $2\,^3S$ continuum in the resonant region. But we see no increase in the phase shift in the region of the lowest $^2P^\circ$ resonance (20.3 ± 3 eV). What we find instead is that the nonresonant phase does start to rise but only at and beyond the $2\,^1S$ threshold. This suggests that there should be a second $^2P^\circ$ resonance, this one a shape resonance (although it may not be completely developed). It is provocative and lends credence to their result that a second $^2P^\circ$ resonance (at 20.8 eV) has been experimentally inferred by Phillips and Wong.[15]

In summarizing that situation we would say (keeping in mind that $n=2$ threshold of H gets heavily split in He) that a second $^2P^\circ$ shape resonance in e-He is the analog of the famous $^1P^\circ$ shape resonance in e-H scattering just above the $n=2$ threshold,[16] whereas the lower $^2P^\circ$ resonance bears some similarity to (but is not the exact counterpart of) the dominant $^3P^\circ$ e-H Feshbach resonance below the $n=2$ threshold.[17]

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